3D Numerical Forward Modeling of Complex Resistivity

Field Data

by

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ABSTRACT

The detection and tracking of organic contamination is one of the most difficult problems in environmental investigations. The geophysical techniques of complex resistivity (CR) and ground penetrating radar (GPR) both have the ability to detect organic contamination in the subsurface. While GPR works well for contaminant detection in clay-free environments, the presence of small amounts of clay can inhibit its contaminant-detecting ability. CR, on the other hand, works well for detecting clay-organic reactions. A difficult problem to solve before conducting CR field surveys is the determination of the proper type, orientation, and size of electrode array to use for a given target and background medium. The goal of this thesis is to develop a forward modeling computer program to model the CR response for a given electrode array geometry and field setting. The modeling program (CR3D) is a finite-volume forward modeling code based on a direct current (DC) resistivity code developed at the University of British Columbia and the University of California at Berkeley.

With the CR technique, chemical reactions in the earth’s subsurface are detected and distinguished from one another by their frequency dependency and non-linear characteristics. Frequency dependence is introduced into the CR3D modeling through a Cole-Cole type model.
In this thesis, field data are presented for organic chemically contaminated sites at the Denver Federal Center (Lakewood, Colorado), and Hill Air Force Base, Operable Unit 2 (Layton, Utah). A case history for the Hill Air Force Base site where laboratory data, field data, and computer-modeled data are compared is also presented.

This study also investigated the phase and resistivity responses for profiles of various electrode arrays over a buried, conductive, polarizable block. Results are shown for Wenner profiles for various heights, widths, lengths, and depths of burial of the block. Also, results are presented for a comparison of a Wenner, collinear dipole-dipole, parallel dipole-dipole, and expanding potential array profile over a buried cube.

With the computer code developed in this thesis, the CR response for any arbitrary non-focussed electrode configuration can be modeled for a given target and site geometry.
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LIST OF ACRONYMS

AC Alternating Current
A/D Analog to Digital
AFB Air Force Base
BiCG Biconjugate Gradient
CERCLA Comprehensive Environmental Response, Compensation, and Liabilities Act
CG Conjugate Gradient
CPA Constant Phase Angle
CR Complex Resistivity
CSM Colorado School of Mines
DC Direct Current (signal at 0 Hz)
DCE Dichloroethene
DFC Denver Federal Center
DNAPL Dense Non-Aqueous Phase Liquid
EDM Electronic Distance Measuring device
EM Electromagnetic
EPA Environmental Protection Agency
FE Frequency Effect
GIF Geophysical Inversion Facility
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<tr>
<td>GPR</td>
<td>Ground Penetrating Radar</td>
</tr>
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<td>IP</td>
<td>Induced Polarization</td>
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<tr>
<td>IRP</td>
<td>Installation Restoration Program</td>
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<tr>
<td>MIP</td>
<td>Magnetic Induced Polarization</td>
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<td>MOA</td>
<td>Multiple Orientation Array</td>
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<tr>
<td>NLCR</td>
<td>Non Linear Complex Resistivity</td>
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<tr>
<td>PCE</td>
<td>Tetrachloroethylene (also called perchloroethylene)</td>
</tr>
<tr>
<td>PHD</td>
<td>Phase Hilbert Distortion</td>
</tr>
<tr>
<td>RF</td>
<td>Radio Frequency</td>
</tr>
<tr>
<td>RHD</td>
<td>Resistivity Hilbert Distortion</td>
</tr>
<tr>
<td>RMS</td>
<td>Root-Mean-Squared</td>
</tr>
<tr>
<td>S/N</td>
<td>Signal to Noise Ratio</td>
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<tr>
<td>SP</td>
<td>Self Potential or Spontaneous Polarization</td>
</tr>
<tr>
<td>SRS</td>
<td>Source Recovery System</td>
</tr>
<tr>
<td>TCA</td>
<td>Trichloroethane</td>
</tr>
<tr>
<td>TCE</td>
<td>Trichloroethylene</td>
</tr>
<tr>
<td>THD</td>
<td>Total Harmonic Distortion</td>
</tr>
<tr>
<td>UBC</td>
<td>University of British Columbia</td>
</tr>
<tr>
<td>UCB</td>
<td>University of California, Berkeley</td>
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<tr>
<td>USGS</td>
<td>United States Geological Survey</td>
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LIST OF SYMBOLS

\[ \alpha \] Cole-Cole Distribution Parameter

\[ \Delta V_{i,j,k} \] Elemental Volume used in 3D Discretization

\[ \Delta V \] Electrical Potential Difference (voltage)

\[ \phi \] Phase Shift (lead or lag) (mrad)

\[ \rho \] Resistivity (\(\Omega\)m)

\[ \sigma \] Electrical Conductivity (mho/m)

\[ \sigma' \] Real Part of the Complex Conductivity

\[ \sigma'' \] Imaginary Part of the Complex Conductivity

\[ \sigma_{DC} \] Conductivity at Zero Frequency (DC)

\[ \tau \] Time Constant (sec)

\[ \omega \] Angular Frequency

A Positive Current Electrode

B Negative or Sink Current Electrode

AB Spacing between Current Electrodes

MN Spacing between Potential Electrodes

m Chargeability
LIST OF UNITS

Ωm  Ohm-meter

cm  Centimeters =10⁻² m

Hz  Hertz

Km  Kilometers =10⁻³ m

m  Meters

MHz  MegaHertz =10⁻⁶ Hz

mrad  Milliradians =10⁻³ Radians
ACKNOWLEDGMENTS

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DEDICATION

I would like to dedicate this manuscript to my parents, Vito and Vicki, for the unending patience, their selfless sacrifices, and their whole-hearted support of my educational journey.
1.1 Introduction

The detection and tracking of organic contamination is one of the most difficult problems in environmental investigations. The geophysical techniques of complex resistivity (CR) and ground penetrating radar (GPR) both have the ability to detect organic contamination in the subsurface. Whereas GPR works well for contaminant detection in clay-free environments, the presence of small amounts of clay can inhibit its contaminant-detecting ability. CR, on the other hand, works well for detecting clay-organic reactions. GPR detects organic contaminants on a volume basis and is an effective technique for repeated surveys where contaminants are moving in the ground. CR detects organic contaminants by the frequency spectrum of surface active chemical reactions and is a more unique and sensitive measurement technique. In this thesis, results are presented for CR surveys conducted at two organic chemically contaminated field sites using CR equipment built at the Colorado School of Mines (CSM).

Selecting a proper electrode array for a particular field situation in electrical prospecting is not a trivial problem. Parameters such as the size, orientation, and type of electrode array, the size, shape, and orientation of the target, and the electrical properties of the target and the host rock or soil all factor into the survey design. To assist in the
planning of CR surveys, I produced a 3D finite-volume forward modeling code for CR field data.

Ideally, laboratory samples from a field area can be analyzed prior to field work to determine the electrical properties of the subsurface. Cole-Cole parameters extracted from the laboratory measurements can then be input into a program to determine the complex conductivity at various CR frequencies, which in turn can be entered into the forward modeling program to calculate the phase and resistivity response for a particular setting and electrode configuration.

1.2 History of Induced Polarization and Complex Resistivity

The origins of induced polarization and complex resistivity can be traced back to the initial observation of electrical polarization effects in soils and rocks by Conrad Schlumberger around 1911 (Collett, 1990). The discovery was first described in Schlumberger’s 1912 German patent, followed by a 1920 monograph “Étude sur la prospection électrique du sous-sol” which was the first publication to conclusively describe an induced polarization response (Sumner, 1976). Although attempts to use IP for petroleum exploration were made in the 1930’s, and subsequently as a well-logging tool in the former Soviet Union in 1941, significant published research did not appear until after World War II.

Research conducted by the United States Naval Ordnance Lab on an electrical polarization method for detecting explosive mines in water during WWII eventually led
to D.F. Bleil’s post-war efforts with the United States Geological Survey in field testing the induced polarization technique over a mineralized area (Collett, 1990). Harry Seigal of Newmont noted Bleil’s work and demonstrated that the IP method was reliable in 1948 (Wait, 1959). Following the establishment of Newmont Exploration Ltd. in 1949, extensive field and theoretical work was conducted involving the IP method. Prior to 1950, IP measurements were made in the time domain. In 1950, the first frequency domain systems were field tested by Newmont. From 1951-1960, several universities, government agencies, and mining companies in the United States, the former Soviet Union, and Europe became interested in the induced polarization method for metallic mineral exploration (Angoran et al., 1974; Sumner, 1976; Collett, 1990).

Whereas the traditional two-frequency IP method had gained worldwide acceptance by the 1960’s, spectral induced polarization and complex resistivity (CR) were only in a developmental stage. By the late 1960’s, researchers in Russia, the United States, and Canada were investigating the use of nonlinear electrical impedance techniques for sulfide discrimination (Collett, 1990). Early CR work included phase and amplitude measurements by W.J. Scott in 1967 (Scott, 1971), and by Kennecott Exploration, Inc. in 1968 (Van Voorhis et al., 1973). Complex resistivity equipment and service companies became available by 1973 (Hallock, 1974; Zonge and Wynn, 1975; Collett, 1990).

From the late 1970’s to the present, work has been conducted involving the use of the complex resistivity method for the detection of chemical reactions in rocks and soils. Olhoeft (1985) provides an excellent description of the nonlinear complex resistivity
method for detection of oxidation-reduction, ion exchange, and clay-organic reactions. Measurements in the laboratory (Olhoeft, 1985; Sadowski, 1988; Olhoeft and Jones, 1997; Jones, 1997) and in the field (Olhoeft, 1986; Olhoeft and King, 1991; and Olhoeft and Wardwell, 1998) have shown the CR method to be useful for noninvasive detection of clay-organic reactions.

1.3 Electrical Properties

The CR method is used to measure the earth’s electrical properties; CR is an electrical, ground-contact geophysical technique that measures the in-phase and out-of-phase components of the earth’s total resistivity as a function of frequency (Sumner, 1976). Electrical properties exhibit one of the broadest variations in magnitude of any of the physical properties (electrical resistivity spans 29 orders of magnitude) (Olhoeft, 1979). Water is the greatest factor in the large range of magnitude for electrical properties in earth materials (Olhoeft, 1981). The electrical resistivity of rocks and soils is primarily governed by the amount and connectivity of porosity available to be filled with water, the amount of water filling the pore space, the electrical conductivity of the pore-filling solution, and by the reactive mineral content (Olhoeft, 1986). In general, the resistivity of earth material decreases with increased porosity, reactive material content, water content, and water salinity (Olhoeft, 1986). In addition, the resistivity is usually lowered with the addition of inorganic contamination and increased with the addition of organics (Olhoeft, 1986).
Electrical properties are determined by a host of physical and chemical processes which can be divided into two general classes: charge transport processes (conduction) and charge separation processes (polarization) (Olhoeft, 1981).

### 1.3.1 Charge Transport

A complete description of charge transport mechanisms is given in Olhoeft (1981), a brief summary of which is included below. The two most important charge transport or conduction processes in the determination of electrical properties are charge migration and tunnelling. Migration is defined as the diffusion (the random motion) or percolation (regular motion) of matter in response to an electric field. Tunnelling is defined as the quantum statistical movement of charge through an energy barrier. Migration basically corresponds to the DC electrical conduction of charge along surfaces or through bulk matter, while tunnelling governs the movement of charge across interfaces of electrically dissimilar materials.

Earth materials that display frequency independent electrical resistivity undergo simple charge transport with the most complex particle interactions on the level of simple scattering (Olhoeft and Scott, 1980). Simple charge transport is generally conducted through pore fluid in unblocked pore spaces. However, when an interface or other energy barrier is present, the transfer of electric charge across the barrier appears as an impedance in CR measurements (Jones, 1997). The two most important mechanisms for charge transfer across energy barriers are ion exchange processes and oxidation-reduction
reactions (Olhoeft and Scott, 1980). Chemical charge transfer processes will be discussed further in Section 1.4.2.

In field surveys, methods such as CR, IP, and DC resistivity make bulk measurements of conduction processes. However, in some geological environments, surface conduction (transport) can have a significant effect on the measured CR signal. Surface conduction can be considered as a special case of (or 2D counterpart to) the bulk conduction in 3D media (Henzler, 1975). Surface conductance is defined as a function of mobilities and surface excess concentrations of electrons and “holes” (Bockris and Khan, 1993). For a more complete description of surface conductance, see Bockris and Khan (1993). In relation to CR, surface conductance becomes important in mineralogical clay systems where interfacial regions can approach or exceed the particle size. Under an applied field, the mobile cations in the diffuse double layer of a clay can increase the ion concentration, resulting in increased surface conductivity and polarization (Jones, 1997). Increases in excess surface charge can be linked directly to large dispersions in IP measurements (Wong, 1979). For extensive descriptions of the double-layer and behavior of clays in regards to geophysical electrical measurements, see Canan (1999) and Jones (1997).

1.3.2 Electrical Polarization

Along with charge transport, polarization mechanisms determine the electrical properties of a medium. Polarization is defined as “the physical separation of charge in
distance from its normal equilibrium by some applied force”, including electrical fields, chemical reactions, and mechanical deformation (Olhoeft, 1981). Although several polarization mechanisms determine electrical properties at high frequencies (>10^7 Hz), the two most important polarization mechanisms in the complex resistivity frequency range (0.001-1000 Hz) are orientational and interfacial polarization. Orientational polarization is the re-alignment or reorientation of polar molecules without distortion of shape due to an external field; water molecules (liquid or ice) are the primary agents of orientational polarization in rocks and soils (Olhoeft, 1981). Interfacial polarization describes the separation and build-up of charge at local variations in electrical properties during the migration of charge due to an external electric field (Olhoeft, 1981). The impedance caused by the accumulation of charges (whether caused by local electrical or chemical potentials) can be seen in the complex resistivity response.

Interfacial polarization can be further classified as either membrane or electrode polarization. Membrane polarization occurs at solid-liquid boundaries (such as negatively-charged clay particles in an electrolyte-filled pore space) where diffuse clouds of ions can form and impede the movement of charges in the presence of an applied electric field (see Figure 1.1). Electrode polarization occurs in the presence of an external electric field when a metallic mineral blocks an electrolyte-filled pore passage, thus resulting in an accumulation of ions on either side of the particle (Telford et al., 1990). Figure 1.2 shows one example of electrode polarization.
Figure 1.1 Depiction of ions in a pore space forming an ion concentration barrier which creates membrane polarization. (a) Pore path before application of an electric potential. (b) Pore path after application of a driving force (after Sumner, 1976).
Figure 1.2 Electrode polarization. The upper pore depicts electrolytic flow and the bottom pore shows an electrode polarization effect (after Telford et al., 1990).
For systems containing strictly simple charge transport, the electrical properties of the rocks will be independent of frequency. However, in the presence of polarization mechanisms, electrical properties such as resistivity become frequency dependent (Olhoeft and Scott, 1981).

1.3.3 Frequency Dependence

The frequency dependence of a system is governed by either diffusion or kinetics-limited processes. The slowest step in a process determines whether a system is diffusion or kinetics-limited. For example, if a process is limited by the speed of a reaction, it is said to be kinetics-limited. Alternately, if the movement of particles to and from an interface is the limiting step, the process is termed diffusion-limited (Olhoeft, 1985). The interfacial impedance of diffusion-limited processes follows a square-root of the frequency trend known as the Warburg impedance (Olhoeft, 1985; Sumner, 1976). The behavior of the Warburg impedance is different from that of a classical capacitor in that the impedance of a capacitor varies with the inverse of the frequency while the Warburg impedance varies with the inverse of the square root of the frequency. In diffusion-limited systems, the frequency dependence is mostly controlled by the distribution of particle sizes and pore sizes (Wong, 1979; Olhoeft, 1985). In contrast, the frequency dependence of kinetics-limited reactions is dependent on chemical reaction rates and independent of particle and pore size distributions (Olhoeft, 1985).
The frequency dependence of earth materials can be represented by equivalent circuits using the standard resistor, capacitor, and inductor electronic components, along with the Warburg element that gives rise to the Warburg impedance described above. Resistors are frequency independent, behave in a linear fashion over frequency, and obey Ohm’s current voltage law. Capacitors and inductors are both frequency dependent and behave in a linear fashion over frequency and stimulus amplitude. The Warburg element is frequency dependent and behaves in a nonlinear fashion over amplitude. Figure 1.3 shows the frequency dependence (or lack thereof) of a resistor and a capacitor. The resistor displays no frequency dependence, while the capacitor shows a $90^\circ$ out-of-phase behavior. The frequency dependence of the Warburg element and an inductor are shown in Figure 1.4. The Warburg element displays a $45^\circ$ out-of-phase response with a $\sqrt{\omega}$ frequency dependence. The inductor has a $-90^\circ$ out-of-phase frequency dependence. As shown in Pelton et al. (1978), earth systems can be simulated with equivalent circuits. Figure 1.5 shows a diagram of a rock with two water-filled pores, one of which is blocked by graphite mineralization. The unblocked upper pore can be represented by a resistor that simulates the resistance of the pore water; the blocked lower pore is represented by a resistor, which simulates the pore water, and a Warburg element, which simulates the impedance at the graphite-water interface. The effect of the two branches in parallel simulates the rock as a whole.
Figure 1.3 Frequency dependence of a resistor and capacitor plotted in the complex plane. 1.) Note that the resistor is independent of frequency and plots only on the real axis. \( V \) is voltage, \( I \) is current, \( R \) is resistance. 2.) The capacitor is frequency dependent and its response plots on the imaginary axis 90° out-of-phase. \( c \) is capacitance, and \( t \) is time.
Figure 1.4 Frequency dependence of an inductor and the Warburg element plotted in the complex plane. 1.) Note the -90° out-of-phase behavior of the inductor. V is voltage (volts), L is inductance (henrys), I is current (amperes), and t is time (seconds). 2.) Also note the 45° out-of-phase dependence of the Warburg element response with the square root of the angular frequency.
Figure 1.5 Example of a rock and its equivalent circuit representation. 1.) Rock with water-filled pores. The lower pore is blocked by graphite mineralization. The rock can be represented by the circuit shown in 2.). $R_0$ represents the resistance of the water in the upper pore. $R_1$ represents the resistance of the water in the lower pore, and $W$ is the Warburg element which represents the impedance at the graphite-water interface.
1.3.4 Amplitude and Phase

In CR measurements, an alternating current (AC) is injected into the ground through current electrodes and potentials are measured at receiver electrodes. If an AC sine wave is established as a reference, the amplitude and phase shift between the injected current and the received voltage can be determined. Figure 1.6 shows a plot of an injected current signal and measured voltage response. The time shift between the two signals is termed the phase shift. The phase shift or phase angle can also be quantified by decomposing the measured voltage into in-phase and out-of-phase components with respect to the current signal (see Figure 1.7). The phase angle can be defined:

\[ \phi = \tan^{-1} \frac{V_{out}}{V_{in}} \]  

(1.1)

where \( \phi \) is the phase angle, \( V_{out} \) is out-of-phase component of the voltage, and \( V_{in} \) is the in-phase voltage component. CR phase angles are measured in milliradians (mrad) and are either plotted versus frequency on a log-log scale, or in the complex plane. The phase data collected in this thesis are all plotted versus frequency on a log-log scale.

Changes in phase angles over frequency are a measurement of the frequency dependence of a system. Zonge et al. (1972) and Weller et al. (1996) show that phase-angle measurements can be translated into traditional IP frequency effect (FE) and vice versa.

The amplitude and phase of the complex resistivity can be defined as follows:
Figure 1.6 CR phase determinations. $\phi$ is the phase lag between the input current (solid line) and measured voltage (dashed line) (modified after Sumner, 1976). Resistivity is calculated from the ratio of the amplitudes.
Figure 1.7 Components of the CR phase-lag angle (modified after Sumner, 1976). $V_{\text{out}}$ is the out-of-phase component of the voltage with respect to the current, and $V_{\text{in}}$ is the in-phase component of the voltage with respect to the current.
\[ |\rho| = \frac{V_o}{I_o} \]  
\[ \phi = \phi_V - \phi_I \]

where \(|\rho|\) is the magnitude of the resistivity, and \(V_o\) and \(I_o\) are the voltage and current as shown in Figure 1.6. \(\phi\) is the phase angle in general terms. When the current signal is used as the reference, \(\phi_I\) is zero and the phase angle is equal to \(\phi_V\).

### 1.4 Effect of Physical and Chemical Factors on CR Responses

Electrical properties measured with the complex resistivity technique are dependent on both the physical and chemical nature of the subsurface. Above \(10^8\) Hz, physical processes determine measured electrical properties; however, in the CR frequency band, chemical reactions dominate the electrical properties of water-rock interactions (Olhoeft, 1985). The presence or absence of water also plays an important role in the electrical properties of rocks and soils. In absolutely dry rocks, physical factors completely govern all electrical properties. However, if a polar solvent such as water is introduced into the system, a whole suite of solvent-rock interactions becomes a factor in the determination of the measured electrical properties (Olhoeft, 1987). The effect of specific physical factors and chemical processes on CR responses are discussed below.
1.4.1 Physical Factors

In a rock or soil system, the particle and pore size distribution and connectivity, the habit and texture of mineralization, the bulk density, and the efficiency of grain-to-grain contacts can all be factors in the measured electrical properties. Wong (1979) developed a mathematical model that strongly correlated with experimental data and described the effect of particle size on electrical conductivity and phase spectra versus frequency. Along with particle size distribution, the electrical conductivity of a pore-filling solution, the pore size and shape, and the connectivity between pores will affect the overall electrical conductivity of a wet-rock system (Olhoeft, 1985).

In geological systems where two materials of dissimilar electrical properties are mixed together, one of the most common physical phenomena seen while measuring electrical properties is the Maxwell-Wagner effect. When a force such as an external electric field is applied to a heterogeneous material, charges become trapped in the energy differences at the interfaces between two electrically different materials (Olhoeft, 1985). The charges that accumulate at particle edges and grain boundaries during the application of the external field will relax back to their original distribution when the external field is removed. It is the diffusion of charges back to their original distribution that creates the measured frequency dependence in electrical properties (Olhoeft, 1985).
1.4.2 Chemical Reactions

Although physical factors are important in the determination of electrical properties at high frequencies (>10⁸ Hz) and in the absence of water and chemical reactions, low frequency electrical properties are dominated by the effects of chemical reactions. Some chemical processes such as oxidation-reduction, cation-exchange, and clay-organic processes can appear as electrical relaxations from approximately 100 Hz to below 0.001 Hz (Olhoeft, 1987).

The rusting of a metallic mineral in the presence of water is a common example of an oxidation-reduction reaction. For example, an iron wall may experience the oxidation of iron into hematite and the reduction of water; the transfer of electrons through energy barriers between the iron and water appears as an impedance that can be observed using the complex resistivity method (Olhoeft, 1985).

A second type of chemical reaction observable with complex resistivity is ion-exchange. Since cations are smaller and move more quickly than anions, ion-exchange processes usually involve the exchange of cations. A common ion-exchange reaction is the substitution of one salt cation for another in water softeners (Olhoeft, 1985). Clay and zeolite minerals are particularly prone to ion-exchange reactions, although other hydrated minerals can also undergo ion exchange at higher temperatures (due to geothermal activity, for instance). Distinguishing ion-exchange reactions from oxidation-reduction reactions in complex resistivity data will be discussed in terms of measurements of nonlinearity in Section 1.5.
Clay-organic reactions make up a third type of chemical process that can be observed with the complex resistivity technique. Although clay-organic electrochemistry is not well understood, organic molecules have been known to preferentially attach to clay surfaces, thus inhibiting cation exchange processes (Olhoeft, 1985). As with oxidation-reduction and ion-exchange reactions, clay-organic reactions display marked changes in measurements of nonlinearity (see Section 1.5). Jones (1997) also notes that some organic compounds can interact with the cations in clays, resulting in larger chemical complexes with different mobilities. Ultimately, conducting pathways within the clay can become blocked and the overall conductivity can be decreased. The noninvasive nature of complex resistivity and its ability to detect clay-organic reactions make complex resistivity an important tool for monitoring clay barriers around waste sites (Olhoeft, 1986). A recent study concerning the attack of a clay barrier wall by tetrachloroethylene (PCE) contamination is discussed in Chapter 3.

1.5 Nonlinearity Measurements with the CR Technique

In complex resistivity measurements, the level of nonlinearity helps distinguish chemical reactions from one another and from physical processes. The following discussion of nonlinearity comes primarily from papers by Olhoeft (1979, 1985, 1987) which address low frequency electrical properties and complex resistivity. In complex resistivity measurements, nonlinearity in the relationship between current density and electric field strength arises when energy barriers are large relative to the applied energy.
However, increasing the voltage above certain levels can also result in abnormal increases in the rate of current; this is also a nonlinear electrical phenomenon (Katsube et al., 1973). Diffusion-limited systems such as oxidation-reduction reactions are described by absolute rate equations which are inherently nonlinear (Olhoeft, 1979). Two measures of nonlinearity in complex resistivity measurements are the total harmonic distortion (THD) (which is a measure of the distortion of the waveform) and the Hilbert Distortion (HD) (which is a measure of the distortion of the transfer function’s frequency dependence).

The total harmonic distortion of a measurement can be determined by measuring the harmonic content of the input and output of a system, and taking the root-mean-squared (RMS) difference between the harmonics of the input and output. In a linear system, the output should contain no new harmonic content. Any differences between the harmonic content of the input and output indicate that the system is nonlinear. Hence, the THD is a measure of nonlinearity. The THD plots for laboratory data from Hill Air Force Base and the Denver Federal Center can be found in Chapter 3 and Appendix C.

A second measure of nonlinearity is Hilbert Distortion (HD). In complex resistivity measurements, the real and imaginary parts of the transfer function between stimulus and response are related by the Hilbert Transform or Kramers-Kronig relations (Olhoeft, 1979; Macdonald, 1998). In order to calculate the Hilbert Distortion of a system, one must measure the frequency dependence of the transfer function, and then use the Hilbert Transform to calculate new real and imaginary parts of the measured
transfer function. The difference between the synthetic and measured transfer functions is the Hilbert Distortion. For the laboratory and field data displayed in Chapter 3 and Appendices B and C, the Hilbert Distortion is calculated for both the amplitude of the resistivity (RHD) and the phase spectra (PHD).

A system can exhibit any combination of the above types of nonlinearity; the type of nonlinearity displayed by a system assists in distinguishing between various types of chemical reactions. In complex resistivity measurements, high degrees of nonlinearity indicate chemical as opposed to physical activity. In general, higher phase and nonlinearity measurements indicate greater chemical activity. Nonlinear behavior in the earth’s subsurface is usually caused by charge transfer processes—namely oxidation-reduction reactions and ion-exchange processes. Ion-exchange processes normally have higher Hilbert Distortion than oxidation-reduction reactions; whereas oxidation-reduction reactions usually have higher THD than ion-exchange processes. In laboratory studies, Jones (1997) notes that the addition of organic contaminants to clays has an effect on the nonlinearity measurements of clay-organic systems. As further studies are made on the effects of a wide spectrum of contaminant-clay systems, nonlinear complex resistivity measurements will become more useful in detecting specific sources of contamination in the earth’s subsurface.
CHAPTER 2

COMPLEX RESISTIVITY FIELD METHODOLOGY

2.1 Survey Design

In order to successfully conduct a complex resistivity survey, several factors must be considered concerning the target, an appropriate electrode array, the geologic/geoelectric environment, and sources of noise, interference, and error. The first step in any electrical survey is to determine the problem to be solved. Complex resistivity has proven to be successful in detecting a wide variety of field targets. For instance, CR has been used to detect the presence or absence of clay-organic reactions in the ground (Olhoeft, 1986), to locate disseminated sulfides (Zonge, 1981), to indirectly detect hydrocarbon reservoirs (Snyder et al., 1981), and to map nonreacting ground versus ground where oxidation-reduction or ion exchange reactions are transpiring (Olhoeft and Scott, 1980). Once the intended target is identified, a suitable survey can be designed.

2.1.1 Geoelectric Environment

An understanding of the geologic and geoelectric environment is extremely beneficial to the planning of a CR survey. Knowledge of the conductivities and thicknesses of subsurface layers assists in estimating the probable signal to noise ratio, possible levels of electromagnetic coupling, and the effective polarizability of polarizable
targets (Bertin and Loeb, 1976). Electromagnetic and direct current methods can help establish the electrical environment. Although it is not regularly performed, reconnaissance work using electromagnetic methods or ground penetrating radar can also locate pipes and buried structures such as walls or dikes that may have a bearing on the positioning of the array on the surface of the ground. Coarse preliminary surveys can be used to identify major anomalies to be investigated with finer measurements (Bertin and Loeb, 1976).

Important geoelectric parameters for designing a survey include the resistivity and polarizability contrasts between the host medium and the target, and the depth, size, shape, and orientation of the target. Before attempting a survey, the geophysicist must determine whether or not a target will be detectable with the given equipment. Van Nostrand’s (1953) classic text discusses the necessary parameters to detect an infinitely conducting sphere using the DC resistivity method. He concluded that in order to detect a sphere of radius ‘r’ buried at a depth ‘d’, the maximum ratio of r:d was 0.5. He described his conclusion as a guideline, and not a rule. Van Nostrand’s conclusion is the limiting case for a perfectly conductive sphere. In actual field environments, the maximum ratio will need to be greater due to noise and non-perfectly conducting targets. In field situations where the resistivity contrast between the target and host is insignificant, the target can still be detected with CR if there is an appreciable contrast in polarizability between the target and the host medium (as is often the case with clay-organic reactions).
The depth at which a target can be detected is dependent not only on the size, shape, and orientation of the target in the subsurface, but also on the type and orientation of the electrode array on the surface (Apparao et al., 1992). Various electrode arrays and their effectiveness in detecting targets will be discussed in Section 2.2. Excellent reviews on the responses given for targets with varied orientations, depths, sizes, and shapes for the DC resistivity problem are given in Van Nostrand and Cook (1966) and Kunetz (1966). Some CR examples of various target scenarios will be shown in Chapter 4 using the CR3D computer modeling code developed for this thesis.

The feasibility of detecting certain targets is dependent on the capabilities of available equipment. For instance, an older CR system that measures from 0.01 to 110 Hz as described by Zonge and Wynn (1975) or from 0.01 to 5.0 Hz (Pelton et al., 1978) may not be suitable for detecting a low frequency (0.001-0.01 Hz) clay-organic reaction. Also, a CR system designed for mining applications in wilderness areas may not have the proper shielding to make measurements in a culturally noisy urban setting.

2.1.2 Sources of Noise, Interference, and Error

Despite careful planning and survey design, the field environment can add several unforeseen sources of error, interference, and noise. Some sources of noise are ubiquitous and hence, unavoidable; however recognizing the source of such noise can help the geophysicist interpret the data. Some common sources of noise in CR measurements include fences, pipes, and power lines. Leakage currents, capacitive
coupling, EM coupling, radio and television signals, and telluric currents are sources of interference often encountered in the field. Topography and inaccuracy in electrode positioning can introduce error into CR measurements.

Grounded fences, pipelines, telephone lines, and power lines can result in contamination of measurements due to their channeling of current along preferential paths in the earth (Zonge and Hughes, 1981). A detailed description of the effects of fences and pipelines on induced polarization and CR data is given in Wynn and Zonge (1975), the highlights of which are presented below. Fences appear to each have their own individual signature as opposed to the more uniform effects of a metallic pipeline. A single grounded fence can conceal an ore body during a mining survey. The effect of a fence or pipeline on phase measurements is often similar to that of a polarizing, dike-like feature. Although the exact character of fence effects is not known for certain, contributing factors may include: 1). The focusing of currents due to a very good conductor giving rise to nonlinearities in the current behavior 2). The fence acting as a grounded antenna and collecting and retransmitting survey signals, resulting in a phase lag 3.) The fence effect is a true polarization effect from the corrosion of the metal in the fence or posts. Extremely high resistivity contrasts (>100:1) in rocks can give anomalous spectra similar to those due to fence effects. Power lines can also contribute fence-like noise. The grounding system for telephone lines and power transmission lines can simulate an enormous grounded fence. 60 Hertz (50 Hz in most European and Asian countries) transmission lines also produce a ground wave through inductive coupling
with the earth that can be received hundreds of meters from the source. Thus, 60 Hz noise is difficult to escape while conducting CR surveys. Underground pipelines and cathodic protection for pipelines can also contaminate CR field data.

Running survey lines perpendicular to a fence or pipeline can minimize the anomalous effect on CR data. Sumner (1976) also recommends insulating the fence, using lower frequencies or currents, or ideally, removing the fence altogether. However, complex resistivity surveys conducted in or near urban areas will most likely be affected by 60 Hz noise and shifts in ground potential due to power load changes. Even after efforts have been put forth to minimize cultural noise, CR data are still prone to cultural contamination. Hence, successfully identifying and removing such effects can be very useful. Zonge and Hughes (1981) present a field example where the effect of a pipeline was successfully identified and removed, thus rendering the remaining data useful.

Leakage currents resulting in capacitive coupling can cause spurious effects in CR data, especially at high frequencies. Leakage currents are usually the result of breaks in cables or defective wire insulation (Zohdy, 1968; Telford et al., 1990; Olhoeft, 1998) or wet cables due to rain or condensation. Once leakage currents exist, capacitive coupling may occur between current and potential wires, or between current electrodes and potential wires (Telford et al., 1990). The probability for spurious effects due to leakage currents increases greatly under wet field conditions (Zohdy, 1968). Before attempting to deal with EM coupling and IP dispersions, the effect of leakage currents must be noted and removed (Washburne, 1982).
Telluric currents and EM coupling are also sources of interference in CR surveys. The nature of electromagnetic coupling, its effects on CR data, and its minimization will be discussed in some detail in Section 2.3. Telluric currents are induced in the earth primarily by solar-wind-influenced variations in the earth’s magnetic field (Sumner, 1976). For deep target work, such as locating sulphide systems in conductive environments, the necessary use of low frequencies can cause telluric noise to render CR data unusable (Halverson, 1990). As frequencies are lowered in a survey, the telluric noise introduced by the natural field spectrum will increase (Jepson, 1969). Figure 2.1 shows the low-frequency electromagnetic field spectrum. Large self-potential-type effects can also be present near (within 10 Km of) mining or industrial operations due to power line surges and grounded DC mining machinery. The noise can appear in the CR record anywhere from DC to 120 Hz (or higher due to harmonics) (Wynn and Zonge, 1975). Sometimes telluric currents have a predominant direction which, if known for the survey area, allows the geophysicist to orient the survey lines perpendicular to the direction of maximum telluric voltage amplitude, thus minimizing the telluric noise level (Bertin and Loeb, 1976; Sumner, 1976). However, the best orientation of survey lines to detect a target with a particular orientation and strike or to avoid EM inductive coupling from a wall or fence could be antithetical to the best orientation of survey lines to minimize telluric effects. Additionally, conducting surveys in the early morning or in the evening avoids the peak telluric activity that usually occurs at mid-day. Halverson
Figure 2.1 The low-frequency electromagnetic field spectrum (modified after Sumner, 1976).
(1990) recommends using very low frequencies and cancelling-out telluric effects as opposed to using high frequencies and attempting to remove EM coupling effects.

In addition to logistical problems caused by topographic features such as hills and valleys, the apparent resistivities of a CR survey can be affected by topography. For example, a steep-sided, flat-topped hill will effectively concentrate current at the foot of the slopes, and reduce current at the tops of the slope (Coggon, 1971). The concentration of current will increase the apparent resistivity at the bottom of a valley and decrease the apparent resistivities at the top of a hill. Hence, when extreme topography is encountered in the field, the surveyor should note the location and extent of the topographic feature, and examine the data to see if changes in apparent resistivity correlate to changes in topography.

Human error is probably the most common source of inaccuracy in complex resistivity surveys. Although the possibilities for human error are limitless, some frequently encountered mistakes in CR surveying include: inaccurate placement of current and potential electrodes, connecting potential or current electrode cables backwards (thus reversing the polarity of the signal), wetting the connection between the potential electrodes and their cables while wetting the electrodes (causing nonlinearities due to the possible polarization of charges at the metal-water interface), forgetting to turn on all the components in the system (differential amplifier boxes, power amplifier), allowing the current signal to clip prior to data collection, and forgetting to null the SP before beginning data collection. Many of these errors can be recognized in the field
before a full data collection sweep is completed. Thus, a careful field crew and a knowledgeable party chief can help reduce much of the human error in the field.

2.1.3 Survey Logistics

Once the equipment and type of array have been selected, then the electrode spacing, direction of survey lines, type of electrodes, and density of measurement stations must be determined within the logistical constraints of the survey area. The required spacing between the current electrodes (AB spacing), the potential electrodes (MN spacing), and the current and potential dipoles or poles (in the case of dipole-dipole, pole-pole, and pole-dipole arrays) is determined with consideration for the depth of the target, the anticipated level of EM coupling, and logistical constraints. For a symmetrical quadripole array (Wenner, Schlumberger) with a given MN spacing, increasing the AB spacing increases the depth of investigation. For environmental applications, AB spacings are sometimes less than 100 m, whereas mineral exploration often requires spacings of hundreds to thousands of meters. Increasing the AB spacing increases the level of EM coupling. An increase in the MN spacing increases susceptibility to telluric currents at low frequencies (Zohdy, 1998). Logistical constraints such as fences, highways, bodies of water, rough terrain, and private property can also limit the size and location of the electrode spread. In remote areas, survey design is sometimes limited to the arbitrary location of roads or trails (i.e. when the trails or roads are surrounded by swamps, trees, lava flows). For instance, a collinear dipole-dipole array or a
Schlumberger array would be much easier to use on narrow trail than an AB rectangle array.

The direction of the survey lines can be important if the intended target is a linear feature. For an elongated vein-like mineralization zone, it is preferable to run survey lines perpendicular to the strike of the target zone (Bertin and Loeb, 1976). Survey lines are often oriented perpendicular (as opposed to parallel) to fences to minimize coupling. Obviously, topographic features such as steep hills and ravines are also practical factors that must be considered when deciding on the orientation of the survey lines.

The density of measuring stations depends on the necessity of detailed information and the budget of the survey. However, it is preferable to collect excess information at a higher survey cost than to obtain too little information from which it is impossible to draw conclusions.

2.2 Electrode Arrays

Selecting a proper electrode array is dependent on the target, the orientation of the geologic and geoelectric environment, logistical constraints, and the required resolution and probing depth needed to detect the target. Although many geophysical practitioners use the same electrode array for every situation, the array selection should be guided by the purpose of the survey, the geologic situation, and the amount of information desired (Coggon, 1973). The section below describes some of the advantages and disadvantages
of several electrode arrangements. A comparison of the EM coupling for various arrays is presented in Section 2.2.5.

2.2.1 Symmetric Quadripole Arrays

Historically, a great deal of work in DC resistivity and IP investigations was carried out using symmetric quadripole arrays. The Schlumberger and Wenner arrays fall into this category. The potential electrodes are located between the current electrodes, or vice versa in a reciprocal Schlumberger array. Carpenter (1955) describes $\alpha$, $\beta$, and $\gamma$ Wenner arrays, with the $\alpha$ configuration being the standard Wenner. See Figure 2.2 for diagrams of the symmetrical quadripoles. For the Schlumberger array, the potential electrode pair is kept within about the middle 1/5 of the current electrode spacing. In most settings a 15:1 or 20:1 AB:MN ratio will still produce an acceptable signal to noise (S/N) ratio depending on the ability of the equipment to inject current into the ground, the sensitivity of the measuring equipment, and the ambient noise (Zohdy, 1998).

The Wenner array is similar to the Schlumberger array, except that the potential electrode pair is always 1/3 of the AB spacing and centered in between the current electrodes. In regard to rapidity of execution, the Wenner array requires all four electrodes to be moved for each station of a profile or sounding. The Schlumberger arrays requires the movement of all four electrodes during a profile, but only periodic movement of all four electrodes during a sounding. For the Wenner and Schlumberger arrays, the AB and MN cables can be quite long and heavy; thus, the survey rate is
Figure 2.2  Symmetric quadripole arrays. 1.) Schlumberger array 2.) Reciprocal Schlumberger array  3.) Wenner array
generally slower than for a pole-pole array (Bertin and Loeb, 1976). The decrease in primary potential difference ($\Delta V$) due to increased spacings is not as rapid as with the dipole-dipole array. For equivalent spacings, the $\Delta V$ for a symmetrical quadripole array is twice that of a pole-dipole array (all else being equal). The symmetric quadripoles arrays are better for conducting soundings, while the pole-dipole array is a better configuration for profiling.

2.2.2 Dipole-Dipole and Bipole-Dipole Arrays

A second grouping of arrays is the dipole-dipole and bipole-dipole arrays. For the dipole-dipole array, the current and potential dipoles are the same size, whereas in the bipole-dipole, the current bipole is much larger than the potential dipole. Depending on the relative positions of the current and potential electrodes, the dipole-dipole array can be termed a collinear, azimuthal, radial, perpendicular or parallel (equatorial when $\theta = 90^\circ$) array (Frohlich, 1967) (see Figure 2.3). According to Roy and Apparao (1971), the equatorial and azimuthal arrays have the deepest depth of investigation, followed by the perpendicular, radial, and parallel arrays (in order of decreasing depth of investigation). The collinear polar dipole-dipole array has the best vertical resolution, and the equatorial and azimuthal arrays have the poorest vertical resolution.
The collinear dipole-dipole array has been one of the most popular arrays for measurements in mining exploration (Jepson, 1969). The advantages of the dipole-dipole array include relatively short cables (compared to quadripole or pole-pole arrays),
Figure 2.3 Six of the possible dipole-dipole arrangements. 1.) Parallel array--when \( \theta = 0^\circ \) or \( 180^\circ \), it is a collinear dipole-dipole array. When \( \theta = 90^\circ \), it is an equatorial array. 2.) Azimuthal array--when \( \theta = 90^\circ \), it is an equatorial array. 3.) Radial--when \( \theta = 0^\circ \) or \( 180^\circ \), it is a collinear dipole-dipole array. 4.) Perpendicular array. 5.) Equatorial array (\( \theta \) always = \( 90^\circ \)). 6.) Collinear dipole-dipole array (modified after Frohlich, 1967).
minimum EM coupling, and good resolution for complex situations and detecting vertical, dike-like conductors (Jepson, 1969; Coggon, 1973). Weaknesses include: poor S/N and inability to provide dip information above 30° (Sumner, 1976; Hohmann, 1975). The poor signal to noise ratio is related to the rapid decrease in the primary voltage with increasing the spacing between the dipoles (Bertin and Loeb, 1976).

2.2.3 Gradient Arrays

The gradient arrays make up a third class of arrays. According to Bertin and Loeb (1976) and Ward (1990) the “AB rectangle” or “rectangle of resistivity” arrays are types of gradient arrays. However, the gradient array has traditionally been considered a collinear array. Two types of gradient arrays are shown in Figure 2.4. The primary electric field is uniform within a rectangle measuring AB/3 (parallel to the current electrodes) by AB/2 (perpendicular to the current electrodes). Hence, the potential electrodes should remain within the above rectangle and should be centered between the current electrodes. For a standard, mining exploration gradient array, the ratio between the current and potential electrode spacings is usually between 20:1 and 50:1.

One of the advantages of the gradient array is its ease of survey execution once the array is set up. The current electrodes and the transmitting unit remain in one place during data collection resulting in more rapid survey execution. Additional cables and current electrodes can be set up for the next survey station to avoid loss of time while switching to the next rectangle (Bertin and Loeb, 1976). Also, gradient arrays are easy to
Figure 2.4 Gradient arrays with potential electrodes within the middle 1/3 of the current electrode spacing. 1.) Standard gradient array. 2.) Modified gradient array, AB rectangle, or rectangle of resistivity array.
use with multi-channel data acquisition systems. According to Coggon (1973), the gradient array has good horizontal resolution and produces superior dip information in comparison with the dipole-dipole and pole-dipole arrays.

Unfortunately, the gradient array has several shortcomings. In mining applications, where the AB:MN ratio is always high, the primary $\Delta V$ signal is relatively weak. Hence, part of the survey design with the gradient array should include calculations to determine if the primary voltage will be large enough to detect the target in the geoelectric environment for a given sized array (Bertin and Loeb, 1976). Data collected with a gradient array also contain very little information about target depth (Coggon, 1973; Sumner, 1976). Coggon (1973) also maintains that gradient array responses to thin, vertical structures are weak (compared to the dipole-dipole array), and that gradient anomalies are strongly affected by overburden irregularities. Gradient array surveys are also limited by the necessity of a clear, open space to lay out a rectilinear grid. In heavy brush or forest situations, the rectangle of resistivity (Zohdy et al., 1974) array may not be a logistical possibility, whereas the collinear dipole-dipole or pole-dipole might be practical (Bertin and Loeb, 1976).

2.2.4 Arrays With Electrodes at “Infinity”

A fourth group of electrode arrangements includes arrays with one or more electrodes at “infinity”. This group can be further divided into the focussed and
unfocussed arrays. The focussed unipole array and the unfocussed pole-pole and pole-dipole arrays will be described below (see Figure 2.5).

All of the configurations described thus far have been unfocussed arrays. Focussed borehole probes such as the Laterolog (Doll, 1951) have been in common use for nearly fifty years. The application of current focussing in surface arrays is not as traditional. The goal of a focussed array is to channel a constant amount of current flowing in a beam of fixed geometry and current density into the ground (Jackson, 1981). An example of a focussed surface array is the unipole array.

For the unipole array, the current sink is located at “infinity” and the potential electrodes are centered in between the two positive current electrodes. Dey et al. (1975) give an account on the nature and performance of the unipole array. The unipole array acts as a pure anomaly detector since the primary electric field at the potential electrodes is zero over a half-space or over a laterally homogeneous, horizontally layered half-space. Therefore, any signal received at the potential electrodes indicates a lateral resistivity contrast. The strength of the unipole array is its ability to detect and resolve lateral inhomogeneities. The simplicity of anomalies detected with the unipole array allows targets such as conductive dikes at depth to be located. One of the weaknesses of the unipole array is the logistical problem of locating an electrode at “infinity” for large arrays. Also, keeping the current equally split between the two positive current electrodes is not a trivial task.
Figure 2.5 Arrays with electrodes at infinity. 1). Pole-dipole array. 2). Pole-pole or two-electrode array. 3). Unipole array--one half of the positive current is injected at each of the A electrodes. P₁ and P₂ are the potential electrodes.
A second type of array with electrodes at infinity is the pole-pole or two-electrode array. For the pole-pole array, both a current and a potential electrode are removed to infinity. In the realm of electrical methods applied towards environmental, groundwater, and engineering problems, the pole-pole array has undergone recent renewed popularity (Beard and Tripp, 1995).

The primary advantage of the pole-pole array is its large depth of investigation with respect to comparable Schlumberger, dipole-dipole, and unipole arrays (Roy and Apparao, 1971). In DC resistivity field results, the pole-pole array produced higher amplitude anomalies over conducting, vein-shaped targets than symmetrical quadripole and focussed arrays (Apparao and Roy, 1973). The pole-pole array also produced the largest anomalies for time-domain induced polarization profiles over sulphide and graphite mineralizations (compared to pole-dipole, Wenner, and Schlumberger arrays) (Roy and Jain, 1973). The relatively quick rate of surveying and the need for only a small survey crew are both strengths of the pole-pole configuration (Sumner, 1976). The primary drawback of the pole-pole array is its lack of resolution compared to the dipole-dipole, pole-dipole, or symmetrical quadripole arrays (Roy and Apparao, 1971; Beard and Tripp, 1995). In contradiction to Roy and Jain (1973), Beard and Tripp (1995) maintain that the insensitivity of the pole-pole array to polarizable structures should keep it from being used in IP surveys. Another drawback is the logistical difficulty of placing two electrodes at infinity for large electrode spreads.
The pole-dipole array (also called a half-Schlumberger array) consists of one current electrode at infinity and the other current electrode at a given spacing from the potential dipole. Data collection can be conducted as a traditional profile by moving three electrodes, or by keeping one current electrode stationary and surveying the area around it with the potential electrodes (Jepson, 1969). Soundings can also be performed with the pole-dipole array. The depth of investigation for the pole-dipole (or half-Schlumberger) array is less than that of the pole-pole array, but greater than the collinear dipole-dipole array. The primary $\Delta V$ signal decreases less rapidly for the pole-dipole array than for the dipole-dipole array (Bertin and Loeb, 1976). Keeping the transmitter, power unit, and B current electrode stationary results in only having to move the light receiver and long A cable during a survey. The principal drawback to using the pole-dipole array is the difficulty of data interpretation due to the asymmetry of anomalies for symmetric bodies (Coggon, 1973; Beard and Tripp, 1995). The logistics of placing a current electrode at infinity can also become a drawback for large surveys.

Since no electrode can actually be placed at infinity, a short discussion on the placement of the infinity electrode is in order. For the pole-dipole array, a general field guide is to place the infinity electrode at 10 times the distance between the current pole and the closest potential electrode. The pole-pole array requires the infinity electrodes to be placed at a distance 100 times the length between the current and potential poles (Zohdy, 1998). The rationale for the two infinity distances is based on the fact that the signal drops off at a rate of $1/r^2$ for the pole-dipole array, and $1/r$ for the pole-pole array.
(hence the greater distance for the pole-pole infinity electrodes) (Zohdy, 1998). For the modified unipole array, Apparao and Gangadhara Rao (1974) calculated the errors involved with the placement of infinity electrodes. They discovered that the infinity electrodes should be located at over 12 times the distance between the positive current electrodes. Placing the infinity electrodes at only 2.5 times the distance between the positive current electrodes resulted in a maximum error of more than 40% (with respect to the expected voltage value over homogeneous ground) in the measured voltage for a resistivity profile.

Ideally, the infinity electrode(s) should be placed far enough from the other electrodes so that its contribution is negligible. Alternatively, the infinity electrode can be placed in a position where its contribution to each of the potential electrodes (assuming the infinity electrode is a current electrode) is equal. For a homogeneous earth (or a horizontally stratified, laterally homogeneous medium), an infinity electrode placed along the perpendicular bisector of the line between the potential electrodes will create the same potential at each of the potential electrodes (Kunetz, 1966). In the field, however, a laterally inhomogeneous earth will create asymmetries in the contributions to each of the potential electrodes and the infinity electrode should be placed at an appreciable distance from the survey line along the perpendicular bisector of the MN spacing (Kunetz, 1966; Roy and Jain, 1973; Zohdy, 1998). Figure 2.6 shows the preferred placement for the infinity electrode for a pole-dipole array. Apparao and Roy (1973) calculated the effect of placing infinity electrodes perpendicular to a profile line
Figure 2.6 Preferred placement of “infinity” electrode for a pole-dipole array
for a pole-pole array. They determined that the amount of error introduced by the infinity electrodes was dependent on both the distance of the infinity electrodes from the profile line, and the relative position of the measuring poles along the profile line. The systematic error or bias introduced into the absolute apparent resistivity by placing the infinity electrodes at 10 times the distance between the two poles was about 15% at all the stations of a profile. For infinity electrodes placed at 5 times the distance between the poles, a systematic error of 28% was introduced into the absolute apparent resistivity at each station along the profile. If it is not practical to place the infinity electrodes at sufficient distances from the measuring electrodes, then a correction should be made for the resulting errors. Alternatively, the correct formulas to calculate the apparent resistivity could be used (as opposed to the pole-pole approximation) and the results could then be interpreted accordingly.

2.2.5 EM Coupling Effects for Various Electrode Arrays

The geometry of the electrode array plays a role in determining the level of EM coupling contained in CR data. In terms of EM coupling rejection, Sumner (1976) groups arrays into the following three categories: Good rejection—collinear dipole-dipole, parallel dipole-dipole; Fair rejection—Wenner, Schlumberger, pole-dipole; Poor rejection—non-collinear gradient, pole-pole. Although not discussed in this thesis, it should be noted that the magnetic induced polarization method (MIP) avoids EM inductive coupling completely (see Seigal, 1974; Seigal and Howland-Rose, 1990). Also,
the coupling in the gradient array is greatly reduced for traverses away from the line of the current electrodes (Ramachandran Nair and Sanyal, 1980). Several authors agree with Sumner’s assessment of the dipole-dipole array as a superior configuration for EM coupling reduction compared to the pole-dipole array (Coggon, 1973; Dey and Morrison, 1973; Wynn, 1979). Figure 2.7 shows the EM coupling over a homogeneous earth for a Wenner array, a collinear dipole-dipole array, a collinear bipole-dipole array, and two positions on a gradient array grid. The Wenner and gradient array both have much higher susceptibility to EM coupling than the collinear dipole-dipole and the collinear bipole-dipole (where the collinear dipole-dipole is a subset of the collinear bipole-dipole with n=1). In general, electrode configurations with the potential electrode pair within the current electrodes (Wenner, Schlumberger, gradient) are more severely affected by EM coupling than electrode arrays where the current and potential electrode pairs are completely separated (dipole-dipole, pole-dipole).

2.3 Electromagnetic Coupling

Electromagnetic coupling is one of the greatest sources of interference in complex resistivity measurements. Since the early 1960’s, when induced polarization measurements were first being made with large electrode spacings in conductive environments, the distorting effects of inductive coupling were recognized (Hallof,
Figure 2.7 A comparison of EM coupling for Wenner, gradient, collinear dipole-dipole, and collinear dipole-dipole arrays over a homogeneous earth (after Wynn and Zonge, 1977).
1974). Electromagnetic coupling and a polarizable earth effect the measured potential difference in a similar fashion. Hence, a substantial portion of the complex resistivity response over polarizable half-spaces can be due to EM coupling (Dey and Morrison, 1973; Washburne, 1982). The following sections will describe the nature of EM coupling, its behavior in various geologic settings, methods for its minimization and removal, and its effect on data collected with various electrode configurations.

2.3.1 General Description of EM Coupling

Electromagnetic coupling, inductive coupling, and mutual impedance are all terms associated with frequency dependent complex resistivity responses. In this thesis the terms inductive coupling and EM coupling will be synonymous, as prescribed by Wynn and Zonge (1977). Major and Silic (1981) define inductive coupling as the frequency dependent mutual inductive impedance between the transmitter and receiver terminals. When inductive coupling is present in induced polarization work, the total mutual impedance is defined as an interaction between the frequency dependent EM induction phenomena and the frequency dependent resistivity. In other words, the total mutual impedance in a CR survey is composed of a complex resistivity contribution from the earth-return currents, and an inductive coupling contribution caused by the induction between the cable loops above the earth’s surface or

\[ Z(\omega) = Z_{CR}(\omega) + Z_{IC}(\omega) \]  

(Brown, 1985). Where \( Z(\omega) \) is the frequency dependent mutual impedance for a
polarizable, horizontally layered, conductive earth, \( \omega \) is the angular frequency in \text{rad/sec}, 
\( Z_{CR} \) is the complex resistivity contribution, and \( Z_{IC} \) is the inductive coupling contribution. 
For mathematical treatments of mutual impedance, see Sunde (1967); Dey and Morrison (1973); and Brown (1985).

The level of EM coupling encountered during a CR survey is dependent on the electrode geometry and the polarizability, conductivity contrast, and subsurface geometry of the surveyed earth (Washburne, 1982). The frequency range used in the CR survey also determines the extent to which EM coupling will affect the measurements. For phenomena such as some clay-organic reactions, the frequencies of detection (<0.1 Hz) are low enough to assign negligible values to the EM coupling contribution. Wynn (1979) maintains that the EM coupling contribution to the CR response usually does not become significant until 1.0 Hz. For the field examples included in Chapter 3, the targeted clay-organic reactions are detected at frequencies below 1 Hz, thus EM coupling is assumed to be insignificant.

### 2.3.2 EM Coupling in Various Geologic Settings

The geologic environment of the CR survey has a direct effect on the level of EM coupling. Dey and Morrison (1973) examined the theoretical effect of geologic layering, conductivity contrasts of layers, and varying layer thicknesses on the percent frequency effect of electromagnetic coupling versus a quantity, \( L^2 (\sigma_1 f) \). \( L \) is the length of the receiving dipole, \( \sigma_1 \) is the conductivity of the top layer overlying a half-space, and \( f \) is the
higher of the frequencies used. Their results are based on modeling for the pole-dipole and dipole-dipole arrays. The EM coupling response for a two layer earth is generally less than that of a homogeneous half-space when the overburden is less resistive than the underlying half-space. When the overburden is more resistive than the underlying half-space, the layered earth gives higher EM coupling responses than a homogeneous half-space of the overburden’s resistivity. The EM coupling effect increases as the ratio of the conductivity of the underlying half-space and the overburden increases. In the case of a resistive overburden, increasing the thickness of the overburden results in less EM coupling. For a conductive overburden, the opposite is true.

In terms of phase angles, the phase lag (negative phase angle) increases rapidly with frequency for a conductive overburden in a two layer earth model (Wynn, 1979). For a resistive overburden, the phase lag initially increases with frequency, but then reaches a maximum, decreases, and crosses over the real axis to a phase lead at high frequencies (Wynn, 1979; Washburne, 1982). EM coupling over extremely conductive ore bodies can even cause negative IP responses (Hohmann, 1975). A good collection of Argand or Cole-Cole plots depicting EM coupling for various geologic situations is given in Meyer (1990).

2.3.3 EM Coupling Minimization and Removal

In dealing with EM coupling, the geophysicist can either attempt to minimize and avoid coupling in the field, or to model and remove the effect of coupling from the
collected data. The effects of EM coupling can be minimized by strictly using low
frequencies ($\leq 0.1$ Hz) and staying away from conductive ground (Wynn and Zonge,
1977). Although using frequencies $\leq 0.1$ Hz is not practical for many mining
applications, detecting some clay-organic reactions is possible. Using short or
completely separated cables for the connections between the transmitting and receiving
dipoles and minimizing the array spacings while maintaining a proper depth of
investigation for target detection are other options for limiting coupling effects (Bertin
and Loeb, 1976).

Since the above recommendations are not feasible for many applications, several
investigators have devised EM coupling modeling and removal schemes. Hallof (1974)
was one of the first researches to develop an EM “decoupling” routine. He suggested
fitting a straight line or quadratic polynomial to phase measurements made at two
discrete frequencies. The intersection of the straight lines or polynomial fits with the
ordinate at zero frequency allegedly represented the decoupled response (Wynn and
Zonge, 1975). Hallof’s scheme was criticized by Wynn (1979) for only being effective
half the time for normal field conditions, by Song (1984) for the assumption that the true
IP response is flat at low frequencies (invalid for sulphides and alluvial clays), and by
Wynn and Zonge (1975) for not taking into account the frequency dependent properties
of some rocks.

Wynn and Zonge (1975) developed their own method for coupling removal that
was heavily dependent on laboratory work and curve matching EM coupling effects for a
particular environment. Pelton et al. (1978) used the observation that the Cole-Cole frequency dependence of EM coupling was much higher than the frequency dependence for most mineralized environments to automatically “remove” coupling effects through inversion.

Despite the claims of success from the above investigators of successful coupling removal, Wait and Gruszka (1986) are somewhat skeptical. Their studies suggest that EM coupling removal is only valid below 10 Hz. They concluded that the electrochemical effects responsible for the complex and frequency dependent behavior of resistivity were “inextricably intertwined” with EM coupling effects and thus, bold assertions of automatic or complete EM coupling removal should be “viewed with concern”. The best way to avoid EM coupling is to use the MIP method, which has no EM coupling.

2.4 Conducting a CR Survey

Once the survey has been properly designed, the execution of the surveying is straightforward in theory. However, countless obstacles and unexpected developments make field work an art as well as a science. The majority of the following description will be drawn from field work I helped conduct using a complex resistivity system developed and built by members of the Colorado School of Mines (see field examples and equipment description in Chapter 3).
The first step in most surveys is to establish the location of the electrode spread on an existing map through visual inspection, measuring tapes, or preferably Electronic Distance Measuring (EDM) devices. Next, the current electrodes (stainless steel rods) and potential electrodes (porous pots or elemental lead) are planted and the cables are laid out to their respective electrodes. The ground surrounding the electrodes is then wetted with water to enhance ground contact. Once the electrodes have been wetted, and the cables are connected to the electrodes and pre-amplification boxes, the self-potential (SP) is removed using a manual SP-bucker on the pre-amp box and a voltmeter. If an electrode needs to be reset, or a cable re-connected, then the SP must be removed again. Experience has shown that the SP should be allowed to settle for several minutes after the electrodes have been wetted before it is bucked out.

Before collecting field data, the system should be checked for leakage currents and SP effects. The check can be executed by collecting data over the potential pairs while isolating one of the current leads from the ground, the other current lead, and the current electrodes. If the system has no leakage currents, and the SP has been properly nulled, then all the potential channels will show zero potential (Olhoeft and Wardwell, 1998). In the case that the potentials are not zero, field data collection should not proceed until the source of the potential has been determined and nulled. The SP should be checked at each differential amplifier box and the potential and current cables should be examined for breaks.
For data collection with the Colorado School of Mines (CSM) system, a computer program cycles through frequencies from 1000-0.001 Hz in a 1, 2, 5 sequence of each order of magnitude (including 1000 Hz) for a total of nineteen frequencies. A complete suite of frequencies takes about thirty-six minutes in a low-noise environment. The data collection time is short compared to the set-up time for one station of a gradient, Schlumberger, or Wenner configuration. During data collection, setting up additional electrodes for the next station can shorten the overall survey time.
CHAPTER 3

COMPLEX RESISTIVITY FIELD EXAMPLES

3.1 CR Field Equipment

Complex resistivity data were collected at Hill Air Force Base, Layton, Utah, and the Denver Federal Center, Lakewood, Colorado, using a sixteen-channel CR data acquisition system built at the Colorado School of Mines during the spring and summer of 1997. The system was designed by Dr. Gary Olhoeft (CSM) (Olhoeft, 1979; Olhoeft, 1985) with assistance from Dr. David McGlone (Smoke Creek Instruments, Inc.). The system was assembled by Drs. McGlone and Olhoeft, and several graduate and undergraduate students (including myself). The sixteen-channel system was part of a ninety-six channel system originally built for deployment at a controlled DNAPL spill test at Dover Air Force Base. Due to construction difficulties with the Dover test cell, the project was transferred to Hill AFB where a well-characterized DNAPL-contaminated site was available to demonstrate the CR method.

A general diagram of the sixteen-channel system is shown in Figure 3.1. The system is composed of the major components listed below. The power is supplied by a gas-powered generator. For the Hill AFB project, a 5000W Kawasaki generator was borrowed from Dr. Olhoeft. At the Denver Federal Center, a 4000W Honda generator was borrowed from Dr. Dave Campbell of the United States Geological Survey.
Figure 3.1 General diagram of a 16-channel CSM complex resistivity field system (one of six 16-channel systems).
The current is injected into the ground through two stainless steel rods measuring 1.22 m in length and 1.77 cm in diameter. The sinusoidal AC signal is generated by one of a pair of phase-locked, rackmounted Stanford Research Systems DS 345, 30 MHz Synthesized Function Generators. The second function generator, phase-locked to the first function generator, is used as the analog to digital (A/D) time-base clock. The signal is amplified by a Crown DC 300A Series II power amplifier which is located in a shock-proof rackmount case. The single Crown amplifier is capable of producing 600 W of power. At one Hill Air Force Base site, two Crown M-600 amplifiers were bridged together for 4000 W of power in order to penetrate resistive soils.

The potential is measured simultaneously between the reference channel and all of the fifteen potential electrode pairs. The potential electrodes are composed of elemental, metallic lead and measure 5.08 cm in length and 1.77 cm in diameter. From the potential electrodes, the signal travels through 30.5 m triax, driven shield cables which are connected to differential amplification boxes. The differential amplification boxes consist of a circuit board and two 12 Volt, lead-acid batteries; one box is used for each channel. The boxes also contain potentiometers that allow “SP bucking” prior to data collection. As described in Section 2.4, the SP bucker knobs on the differential amplifier boxes are used in conjunction with a voltmeter to null any SP that may exist between potential electrode pairs prior to data collection. From the differential amplification boxes, the signal travels through 15.2 meter twisted pair, shielded twinax cables to the isolation amplifier. The isolation amplifier ensures that the field signals are
at a safe level for handling by the data acquisition boards. One isolation amplifier box accommodates signals from 16 differential amplification boxes; a toggle switch allows a gain of 1 or 10 to be applied to individual channels. Each of the sixteen channels is protected by an Analog Devices AD210 isolation amplifier. The isolated signals are sent via 3.33 m long cables to the Analogic SSH-8 sample and hold boards located in a rackmount PC. The PC contains one ioTech Personal 488 IEEE board, two eight-channel Analogic SSH-8 boards, and one Analogic FAST 16-1-1 A/D board. Following digitization, the field signal is sent to the data collection software on the PC written by Dr. Olhoeft.

The fifteen field data acquisition channels are all measured against the voltage drop over a standard power resistor (or set of resistors) which is contained in a rackmount box (this is considered the zero or reference channel). An image of the field system is shown in Figure 3.2. The 12 V batteries in the differential amplification boxes are recharged overnight using a sixteen-channel recharger box powered by Tripp-Lite PR-40 power supplies. The technical schematics and specifications for the isolation amplifier, differential amplifiers, and battery chargers can be found in Appendix D.

3.2 Description of a Typical NLCR Field Data Display

Although CR data can be plotted as real and imaginary parts in the complex plane, the computer programs used in CSM surveys display measurements as functions of magnitude and phase versus frequency. In addition to the conventional magnitude and
Figure 3.2 Complex resistivity field system. 1.) Computer monitor 2.) Rackmount computer containing A/D boards 3.) Phase-locked function generators 4.) Sixteen-channel isolation amplifier 5.) Input cables from differential amplifier boxes 6.) Crown power amplifier 7.) Standard resistor box
phase measurements, the CSM system also calculates the Hilbert Disortion of the resistivity (RHD) and phase (PHD). Although the THD can be recorded with the CSM equipment, it was not calculated for the field data in this thesis due to the high level of noise at the field site. A typical NLCR field data plot is shown in Figure 3.3. The data in Figure 3.3 were collected at Hill Air Force Base. The figure consists of four primary rectangles in which the phase, resistivity, PHD, and %RHD are plotted. The heading in the top left-hand corner above the data plots is the name of the file that contains the raw NLCR data. The three numbers and symbols to the right of the file name correspond to the channels that are being plotted. In the case of Figure 3.3, Channels 4, 9, and 14 all have the same MN spacing, and thus are plotted together. The MN spacing for the arrays used at Hill AFB are shown in Table 3.1 (see Figure 3.10 for electrode array geometry).

<table>
<thead>
<tr>
<th>Channels</th>
<th>MN Spacing</th>
</tr>
</thead>
<tbody>
<tr>
<td>1, 6, 11</td>
<td>1 m</td>
</tr>
<tr>
<td>2, 7, 12</td>
<td>2 m</td>
</tr>
<tr>
<td>3, 8, 13</td>
<td>4 m</td>
</tr>
<tr>
<td>4, 9, 14</td>
<td>8 m</td>
</tr>
<tr>
<td>5, 10, 15</td>
<td>16 m</td>
</tr>
</tbody>
</table>

Table 3.1 MN spacings for expanding potential array used at Hill AFB.
Figure 3.3 An example of an NLCR spectral field data plot. Data for three channels of an array used at Hill AFB are shown.
The top rectangle contains phase data plotted as the log of the negative of the phase in milliradians (mrrads) versus the log of the frequency (Hz). The second rectangle contains the linearly-scaled magnitude of the apparent resistivity (ohm-m) plotted versus the log of the frequency (Hz). The rectangle below the resistivity contains the PHD (mrrads) plotted versus the log of the frequency (Hz). The bottom rectangle contains the plot of the %RHD calculations. The %RHD is the deviation between the calculated Hilbert resistivity magnitudes and the measured resistivity magnitudes at each frequency. The scale at the bottom of the figure corresponds to all four of the above rectangles. The scale extends from 0.001 Hz to 1000 Hz on a logarithmic scale.

3.3 CR Surveys at Hill Air Force Base

The cancellation of the Dover AFB controlled DNAPL spill left the U.S. Air Force and CSM personnel in search of an appropriate location for the clay-organic reaction-detecting capabilities of CR to be demonstrated. Hill AFB was selected due to the well-characterized nature of the contamination at Operable Unit 2 (OU2) (Olhoeft and Wardwell, 1998).

3.3.1 Location and Background of Hill AFB Contamination

Hill AFB is located near Layton, Utah, about 40 km northwest of Salt Lake City (see Figure 3.4). The CSM complex resistivity study was conducted in and near the
Figure 3.4 Hill Air Force Base location map (modified after Olhoeft and Wardwell, 1998).
northeast part of the base known as Operable Unit 2 (OU2) (see Figure 3.5). The following site descriptions are taken primarily from Olhoeft and Wardwell (1998). Historically, Hill AFB has produced hazardous waste associated with industrial processes related to missile assembly and aircraft repair such as metal plating, painting, paint-stripping, and degreasing. Unknown quantities of trichloroethylene (TCE) and sludge from vapor degreasers were dumped into Chemical Disposal Pit 3 at OU2 from 1967 to 1975. Also, an unknown volume of plating tank bottoms was disposed of at OU2 during the 1940’s. Chemical Disposal Pit 3 consists of two unlined trenches into which chemicals and waste were dumped. The nature of the waste disposal procedure at OU2 led to contamination leaking from the trenches and migrating off of Hill AFB and into the shallow water supply system to the east of the base.

In 1996, the second phase of the Installation Restoration Program (IRP) selected Chemical Disposal Pit 3 as a site for further contaminant characterization work. The first phase of the IRP had involved ranking sites according to their offsite contaminant migration potential. Site characterization and DNAPL source characterization work included GPR surveys, site modeling, well field design and installation, and alluvium characterization. Through soil and groundwater analysis, the DNAPL layer was determined to consist mainly of chlorinated and non-chlorinated solvents with a smaller fraction of co-solved oil and grease. The solvents were primarily TCE (75%) with lesser amounts of 1,1,1-trichloroethane (TCA), tetrachloroethylene (PCE), methylene chloride,
Figure 3.5 OU2 location map (modified after Olhoeft and Wardwell, 1998)
toluene, and Freon. At OU2, approximately 5,685 gallons of residual DNAPL exist in the vadose zone, and 110,000 gallons of free-phase DNAPL exist in sand and clay layers.

In 1987, the United States Environmental Protection Agency (EPA) placed Hill AFB on the National Priorities List under the Comprehensive Environmental Response, Compensation, and Liabilities Act (CERCLA). Response actions which have been taken at OU2 include: collection and treatment of contaminated water flowing from springs and seeps, provision of municipal water connections to five homes that were affected by OU2 contamination, installation of fences around contaminated springs and seeps to prevent access by livestock, installation of a clay-slurry containment wall around the contaminant source area, and the construction of a Source Recovery System (SRS). The SRS, which began operation in 1992, was designed to remove DNAPL from the Chemical Disposal Pit 3 area. Through 1997, the SRS had recovered more than 30,000 gallons of DNAPL.

3.3.2 Geologic and Hydrogeologic Setting of OU2

OU2 is located on a plateau approximately 90 meters above the Weber River Valley. The CR study area at OU2 on the east side of Perimeter Road is capped by the Provo/Alpine Formation, which consists of mixed clays, silty clays, sand, and gravel. A layer of sand and gravel underlies the Provo/Alpine Formation, which is underlain by the Alpine Formation slump zone. The hillside located between Hill AFB and the Weber River Valley is known as the Weber Delta Landslide Complex. The entire OU2 study
area is underlain by Alpine Formation clays. The area west of Perimeter Road is underlain by weathered clay with interbedded silts and sands. A generalized geologic cross-section of OU2 is shown in Figure 3.6.

The hydrologic setting at OU2 is made up mainly of three shallow aquifer systems and a deep aquifer system. The shallow, unconfined systems consist of a shallow system (less than 3 meters to groundwater off-Base and less than 7 m to groundwater on-Base) in the vicinity of Chemical Disposal Pit 3, a hillside groundwater system (11-21 meters to groundwater) on the east side of Perimeter Road, and the Weber River alluvium (1.5-4.5 meters to groundwater) to the north and east of OU2. For all three systems, the saturated thickness is generally less than 9 meters. The three shallow aquifer systems are depicted in Figure 3.6. The deep aquifer system below OU2 is a confined system that is located 91-152 meters below the surface. Although the Delta and Sunset Aquifers are separate bodies to the west of OU2, it is unclear whether they are one body below OU2. The area surveyed in the CR study is located above the shallow aquifer in the vicinity of Chemical Disposal Pit 3.

3.3.3 Data Collection at OU2

From 20 October 1997 to 24 October 1997, ten complex resistivity data sets were collected at OU2 by the CSM research team. The research team consisted of four graduate students (myself, Barry Kirkendall, Stanley Vozzella, and Terrie Rowley) led by Dr. Olhoeft. The primary objective of the surveys was to use CR to track and locate the
Figure 3.6 Geological cross-section of OU2, Hill Air Force Base (modified after Olhoeft and Wardwell, 1998).
migration of organic contamination through the electrochemical signature from clay-organic reactions. The first step in setting up the CR arrays was locating the buried clay slurry containment wall. The clay slurry wall was installed around the former Chemical Disposal Pit 3 to contain the source of contamination. The auger-mixed wall extended to a depth of approximately 30.5 meters, but was not visible from above ground; thus necessitating the use of GPR to determine its location. The orientation and location of the containment wall with respect to the CR survey area and Perimeter Road are shown in Figure 3.7.

The GPR work was performed using a Sensors & Software pulseEKKO 1000 system, 225 MHz antennas, and a calibration wheel. The first line was run from north to south, followed by an east to west line. The clay-slurry wall gave distinct anomalies which can be seen in Figure 3.8. Once the containment wall was located in the field, the next step was to set up the CR surveys. The location and orientation of the GPR and CR surveys with respect to the containment wall, the fence marking the AFB boundary, and the Utah State Plane Coordinate System are shown in Figure 3.9.

The first CR data set was collected on 20 October using Array 1. The CR equipment consisted of a 16-channel subset of the 96-channel CSM system (see Section 3.1 and Appendix D for details). Although the optimum location for the array would have been directly above the containment wall, the size and location of the array was limited due to heavy construction equipment traffic (Olhoeft and Wardwell, 1998). Array 1 was a modified gradient or rectangle of resistivity array which can be termed (and will
Figure 3.7 Orientation and location of the complex resistivity test area with respect to the containment wall and Perimeter Road.
Figure 3.8 GPR radargram of Line 2 at OU2, Hill AFB showing anomalies indicating the location of the clay-slurry containment wall.
Figure 3.9 Location and orientation of the GPR and CR surveys with respect to the containment wall, the AFB boundary, and the Utah State Plane coordinate system.
be referred to as throughout this thesis) an “expanding potential array”. The current electrodes are spaced 32 meters apart and potential electrodes are placed within the current electrodes along three parallel lines. The potential pairs were spaced at 1, 2, 4, 8, and 16 meters separation. Figure 3.10 is a schematic of the expanding potential array referred to as Array 1. The locations of the electrode positions were surveyed using a Sokhisha SET-2 total station EDM. The CR data collection was executed following the procedure described in Section 2.4. The first set of data collected with Array 1 was excessively noisy. However, the second, third, and fourth sets were much cleaner. The level of noise could be correlated to the power state of a sump pump located within 4 meters of Array 1. The second, third and fourth data sets were all collected the morning of 21 October when the sump pump was turned off for maintenance, whereas the first data set was collected when the pump was running.

Following the collection of four data sets with Array 1, data collection proceeded on the east side of Perimeter Road with Array 2. Array 2 was located outside the AFB boundary, but still within OU2. The ground below Array 2 was found to be more resistive than the ground under Array1, which called for the use of two bridged Crown M-600 amplifiers to increase the voltage. Array 2 was identical in type and dimensions to Array 1. As with Array 1, the positions of the electrodes, a well and several surrounding survey stakes were located with the EDM equipment. Several of the AFB boundary fence posts were also surveyed for reference. Two CR data sets were collected with Array 2 on 21 October and three additional data sets were collected 22 October.
Figure 3.10 Expanding potential array lay-out used for Array 1, 2, and 3 at OU2. The potential electrodes are spaced at 1 m for Channels 1, 6, and 7, 2 m for Channels 2, 7, and 12, 4 m for Channels 3, 8, and 13, 8 m for Channels 4, 9, and 14, and 16 m for Channels 5, 10, and 15. The AB spacing is 32 m. Channel 0 is a reference voltage across a standard resistor.
Array 3 was positioned on 21 October and used for data collection on 22 October. Array 3 was located parallel and to the northeast of Array 2 (see Figure 3.9 for location). GPR lines were run over the center branches of both Array 2 and Array 3. One set of CR data was collected using Array 3 with the same dimensions and type as Arrays 1 and 2. On 23 October the current electrodes for Array 3 were expanded to a spacing of 64 m, and the potential spacings were increased to 2, 4, 6, 8, 16, and 32 meters. However, a steady rain turning to snow pre-empted CR data collection when leakage currents became excessive. Additional EDM surveying was performed on 24 October, but an incoming blizzard disallowed any further CR work.

3.3.4 Sources of Noise and Interference at OU2

As would be expected at an air force base, the environment at Hill AFB for CR and GPR data collection was noisy. Sources of interference included incoming and outgoing aircraft (and their radio communications), air force communications equipment, heavy construction equipment activity, and in the case of Array 1, sump pumps. A potential source of interference for Array 2 was the chain-link AFB boundary fence and a buried metallic natural gas pipeline that was detected under the array using GPR.
3.3.5 OU2 Data Processing and Analysis

Ten Nonlinear Complex Resistivity (NLCR) data sets, six GPR lines, and several EDM data were collected by the CSM research team from 20 October-24 October 1997 at OU2. The NLCR data field data were processed using NLCR_FLD, a program written by Dr. Olhoeft. NLCR_FLD produces plots of phase, resistivity, RHD, and PHD for each of the field channels. The results of the data analysis are thoroughly explained in Olhoeft and Wardwell (1998). The primary target in the CR surveys was the suspected reaction of the organic contaminant plume with the clay-slurry containment wall. Through comparison of laboratory and field data, it was determined that the slurry wall was most likely being attacked by PCE. Laboratory data for the clay slurry wall contaminated with PCE is shown in Figure 3.11. A similar low frequency phase relaxation can be seen in Channel 9 of the field data shown in Figure 3.12.

3.4 CR Surveys at the Denver Federal Center

The CSM CR system was also deployed for a study at a contaminated site at the Denver Federal Center (DFC). This study was part of a concerted effort for a class project in GP521 by three CSM graduate students during the Spring of 1998. Borehole complex resistivity surveys were run by Kim Oshetski, CR laboratory work on soil samples was conducted by Kristen Sneddon, and I conducted the surface CR surveys.
Figure 3.11 Laboratory data for a PCE-contaminated sample of the clay-slurry containment wall at OU2, Hill AFB. Laboratory measurement made by Stanley C. Vozzella. Cole-Cole fitting program written by Jones (1997).
Figure 3.12 Complex resistivity field data collected at OU2, Hill AFB. The three plotted channels have an MN spacing of 8 m and an AB spacing of 32 m. The low frequency (<0.1 Hz) trend in the data for Channel 9 resembles the laboratory data for PCE reacting with the clay-slurry wall (see Figure 5.4).
3.4.1 Location and Background of DFC Field Area

The DFC is located in Lakewood, Colorado, approximately 19 km west of Denver, Colorado. The study area is located at the eastern boundary of the DFC, just north of McIntyre Gulch (see Figure 3.13). The contaminant plume targeted in this study is thought to have originated from leaking storage tanks located near Building 52 at the DFC (see Figure 3.13). In 1978, the Federal Highway Administration installed 560-gallon and 250-gallon tanks at the DFC to store solvents and waste solvents used in asphalt testing (Oulton, 1996). In September of 1988, the tanks were suspected of leaking and were subsequently drained. However, in 1995, contaminants were discovered in wells near a planetarium on the east side of Kipling Street directly across from the DFC. The proximity of schools and homes to the detected contamination prompted the installation of an iron-filings reaction wall to mitigate the migration of the contaminant plume. TCA was the primary contaminant found in water samples, although TCE and DCE were also present (Caruana, 1998).

The ‘permeable reactive barrier’ in Figure 3.14 is a funnel-and-gate reaction wall designed to curtail contaminant migration. The “funnels” in the wall consist of metal sheetpile that was driven vertically into the ground. As water reaches the wall, it is funneled to the reaction cells. Figure 3.14 illustrates the “funneling” action created by the wall. The “gates” are cells composed of a layer of gravel, zero-valence iron filings, and a second layer of gravel. Figure 3.15 shows a plan view cross-section of a gate. In
Figure 3.13 Site map of the Denver Federal Center showing location of the reaction wall and Cell One (modified after Caruana, 1998).
Figure 3.14 Diagram of the funnel and gate method. The reaction wall at the Denver Federal Center has four such funnels and gates. GW is ground water, and PRB stands for permeable reactive barrier (after Powell et al., 1998).
Figure 3.15 Plan view of a gate in a “funnel and gate” permeable remediation barrier (modified after Powell et al, 1998)
theory, as the contaminated water passes through the cell, it reacts with the iron and comes out clean on the far side of the wall (Powell et al., 1998). At the DFC, the hydraulic gradient is towards the east, hence the water should be pure as it leaves federal land. There are four reaction cells in the wall, the southernmost (Cell One) of which is located just north of McIntyre Gulch. The surface CR surveys in this project were all located near Cell One.

3.4.2 Geologic Setting at the DFC Study Area

A four-meter thick layer of alluvium lies approximately 60 cm below the surface at the DFC study area. The alluvium is underlain by roughly 1-3 m of weathered bedrock, which in turn is underlain by unweathered claystone/sandstone bedrock. Figure 3.16 shows a generalized south-north cross-section of the reaction wall area. Note that the sheetpile extends down to the unweathered bedrock below Cell One (the southernmost ‘gate’ in the diagram).

3.4.3 Data Collection at the DFC Site

From 11 March 1998 to 23 April 1998, field work was conducted at the DFC. As with the clay-slurry containment wall at Hill AFB, the first task to be performed in the CR surveys was to locate the buried reaction wall at the DFC. Although the reaction cells were visible from the surface, the sheetpiling was buried at a depth of approximately 60 cm. The first technique employed to map the location of the wall was GPR. GPR was
Figure 3.16 Denver Federal Center permeable barrier wall schematic cross section (modified after Caruana, 1998)
chosen because of its sensitivity to conductive targets such as the large metal sheetpile wall. A Sensors & Software pulsEKKO 1000 GPR system with a pair of 450 MHz antennas was employed. At the time of the GPR surveys, the exact properties of the soil were unknown, although clay was reportedly present. No obvious anomalies were observed in the five lines of radar data that were collected over the wall. The lack of a clear anomaly was attributed to the suspected high-loss property of the clayey soil. Although the lines were run roughly perpendicular to the strike of the 0.635 cm thick sheetpile wall, no clear anomaly was detected in the field. Modeling the radar data may have allowed detection of the wall, a real-time anomaly detector was more desirable for the purpose of mapping the exact location of the wall in the field.

A second effort to map the wall was made using a Geonics EM-31 borrowed from the United States Geological Survey (USGS). The EM-31 was essentially used as a subsurface metal detector. The location of the wall was easily detected as the needle on the EM-31 would “peg” while the equipment was over the wall. The width of the anomaly was approximately 30 cm at various locations along the wall. By placing survey flags at the beginning and ending “peg” locations during fifteen traverses to the north and south of Cell One, the location and trend of the wall were determined. The wall was mapped from 10 m north of Cell One, to the terminating point of the wall near McIntyre Gulch. The fact that the wall ended over 3 meters from McIntyre Gulch raised the question of whether contaminated water was flowing around the edge of the remediation
wall and off of DFC land. Contaminated water may have also been flowing over the top of the reaction wall as water table levels changed with the seasons.

The two objectives for performing CR surveys at the DFC were to determine whether the reaction wall was properly remediating the water leaving federal land, and to try various CR electrode arrays in the field to gain a better understanding of the effects of electrode geometry. Once the reaction wall had been mapped, three locations were selected for conducting CR surveys. The first two locations were 33 m and 15 m to the west of the wall (see Figure 3.17). The reason for choosing these two locations was to determine how clay-organic reaction response varied with distance from the wall. The CR response due to the metal wall was also expected to vary with distance from the wall. The third location was directly over the remediation wall, just south of Cell One (see Figure 3.18). Four different potential electrode arrays were set up within the shaded box in Figure 3.18. Three of the arrays contained potential electrode pairs that were located completely on one side of the wall with potential pairs of the same MN spacings on the opposite side of the wall. This area was chosen to determine if clay-organic reactions were present on the western side of the reaction wall, and not on the eastern side. The detection of a reaction on one side of the wall and the absence of that reaction on the other side would be evidence that the reaction wall was properly remediating the contaminated water. This assumes that a clay-organic reaction is present and can be detected and isolated using CR equipment in the DFC study environment.
Figure 3.17 Spatial diagram of locations for DFCD3, DFCS1, DFCW11A, and DFCW11B. The shaded areas represent the region where the potential electrodes were placed. See Figures 3.18, 3.19, and 3.20 for the configurations of the above arrays. (Note: figure not to scale)
Figure 3.18 Spatial diagram of locations for electrode configurations MOA_1, MOA_2, MOA_3, and MOA_4. The shaded area represents the region where the potential electrodes were placed. See Figures 3.21, 3.22, 3.23, and 3.24 for the configurations of the above arrays. The AB spacing is 40 m, and the shaded area is 12.5 m x 12.5 m. (Note: figure not to scale)
The CR equipment used for the DFC project was the same 16-channel CSM system that was deployed at Hill AFB (with the exception of a 4000W gas-powered generator borrowed from the USGS). The first electrode array (named DFCD3) was set up 33 m from the reaction wall. The size of the array was limited by a fence to the north and McIntyre Gulch to the south. The array was the same modified gradient array used at Hill AFB with slightly different dimensions (see Figure 3.19). The AB spacing was 34 m and the MN spacings were 1, 2, 4, 8, and 16 m. The distance between each parallel branch of the array was 7 m. Setting up the array took two people approximately four hours. The field procedure described in Section 2.4 was used for the CR surveys at the DFC. Field data collected with Array DFCD3 can be found in Appendix B. A second type of array was set up along the center branch of the DFCD3 array. This collinear experimental array (DFCS1) can be termed an “expanding electrode” array (see Figure 3.20). DFCS1 is a symmetric quadripole array with an AB spacing of 34 m and MN spacings of 0.50, 1.0, 1.5, 2.0, 3.0, 4.0, 6.0, 8.0, 12.0, 16.0, 18.0, 20.0, 22.0, 24.0, and 28.0 m. The data collected with this array can be found in Appendix B.

The same array used for DFCD3 was employed at a second location 15 m from the reaction wall (see Figure 3.17). The data from this array (DFCW11A) can be found in Appendix B. A second type of modified gradient array was set-up using the same current and potential electrode positions as array DFCW11A. The cables leading to the differential amplifiers were simply switched to create the configuration (DFCW11B) shown in Figure 3.21. The AB spacing was kept at 34 m while the inner three potential
Figure 3.19 Expanding potential electrode array DFCD3 and DFCW11A. The potential electrodes are spaced at 1 m for Channels 1, 6, and 7, 2 m for Channels 2, 7, and 12, 4 m for Channels 3, 8, and 13, 8 m for Channels 4, 9, and 14, and 16 m for Channels 5, 10, and 15. The AB spacing is 34 m. Channel 0 is a reference voltage over a standard resistor.
Figure 3.20  Collinear expanding potential array DFCS1. AB=34 m, MN for Ch 1=0.5 m, Ch 2=1.5 m, Ch 3=3.0 m, Ch 4=6.0 m, Ch 5=12 m, Ch 6=1.0 m, Ch 7=2.0 m, Ch 8=4.0 m, Ch 9=8.0 m, Ch 10=16.0 m, Ch 11=18.0 m, Ch 12=20.0 m, Ch 13=22.0 m, Ch 14=24 m, Ch 15=28 m.
Figure 3.21 Gradient-type potential electrode array DFCW11B. The current electrodes are spaced 34 m apart collinear with Channels 6-10. The MN spacing for Channels 1, 2, 4, 6, 7, 9, 11, 12, and 14 is 1 m. The MN spacing for Channels 3, 5, 8, 10, 13, and 15 is 4 m.
electrode pairs for each branch had MN spacings of 1.0 m. The two outer pairs on each branch had MN spacings of 4.0 meters. The data collected with DFCW11A can be found in Appendix B.

Four experimental electrode configurations were set up directly over the remediation wall (see Figure 3.18). All four arrays used the same current and potential electrode positions; hence the MOA (Multiple Orientation Array) prefix. The potential electrodes were placed on a 12.5x12.5 m grid with a 2.5 m space between each electrode. The current electrodes were positioned perpendicular to the wall with an AB spacing of 40 m.

The first array (MOA_1) used for data collection was a gradient-type array consisting of five branches of three potential pairs, each with an MN spacing of 2.5 m (see Figure 3.22). The center potential pair on each branch was bisected by the remediation wall; i.e. M was on one side of the wall, and N on the other. Five pairs of electrodes were located entirely on one side of the wall, and five pairs were located entirely on the opposite side of the wall. This was designed to note differences in CR responses before and after the reaction wall. The data collected with MOA_1 can be found in Appendix B.

The second array (MOA_2) was similar in design to MOA_1, but with larger MN spacings (see Figure 3.23). The outer MN pairs had spacings of 5 m, while the inner pair had an MN spacing of 7.5 m. As with MOA_1, the center MN pairs were bisected by the
Figure 3.22 Potential electrode array MOA_1 with current electrodes spaced 40 m apart collinear with Channels 7, 8, and 9. All fifteen channels have an MN spacing of 2.5 m.
Figure 3.23 Potential electrode array MOA_2. The current electrodes are spaced 40 m apart and are collinear with Channels 5, 6, and 13. The potential electrodes are have a spacing of 5 m for Channels 1-10 and 7.5 m for Channels 11-15.
wall, while the outer pairs were completely on one side of the wall. None of the electrodes were moved in the transition from MOA_1 to MOA_2. The potential electrode cable leads were simply changed at each of the differential amplifier boxes. The data from MOA_2 can be found in Appendix B.

The third electrode array (MOA_3) differed in orientation with respect to MOA_1 and MOA_2. Twelve of the potential pairs were oriented parallel to the reaction wall with MN spacings of 5 m (see Figure 3.24). Three potential pairs were oriented with the wall as a perpendicular bisector and MN spacings of 2.5, 7.5, and 12.5 m. The potential pairs oriented parallel to the wall were expected to give a different response due to maximized coupling to the wall versus the potential pairs oriented perpendicular to the wall. The data collected with MOA_3 can be found in Appendix B.

The final array (MOA_4) was set-up with twelve potential pairs oriented at various angles to the remediation wall, and three pairs set up perpendicular to the wall (see Figure 3.25). The MN spacings were 17.7, 14.6, 12.7, 13.5, 9.0, and 5.6 m for the angled potential pairs, and 12.5, 7.5, and 2.5 m for the perpendicular pairs. The data from MOA_4 can be found in Appendix B.

3.4.4 Sources of Noise and Interference at the DFC Site

The CR data collection environment at the DFC study site was not as noisy as the Hill AFB site. However, interference may have been introduced into the data from two
Figure 3.24  Potential electrode array MOA_3. The current electrodes are spaced 40 m apart along the center of the potential electrode grid perpendicular to the wall. The MN spacing for Channels 1-12 is 5 m. Channel 13 has an MN spacing of 2.5 m, Channel 14 has an MN spacing of 7.5 m, and Channel 15 has an MN spacing of 12.5 m.
Figure 3.25 Potential electrode arrangement MOA_4. The current electrodes are spaced 40 m apart on either side of the wall along the same lines as Channels 13-15. The MN spacings are as follows:Channels 1 and 6=17.7 m, Channels 2 and 5=14.6 m, Channels 3 and 4=12.7 m, Channels 7 and 12=13.5 m, Channels 8 and 11=9.0 m, Channels 9 and 10=5.6 m, Channel 13=12.5 m, Channel 14=7.5 m, and Channel 15=2.5 m.
chain-link fences running parallel and perpendicular to the reaction wall (see Figure 3.17). The buried wall itself most likely contributes to the measured CR signal. Other potential sources of interference in the area include several radio-frequency (RF) transmitting antennas in the area and 60 Hz powerline interference.

3.4.5 DFC Data Processing and Analysis

Eight CR data sets were collected at the DFC from 9 April 1998 to 21 April 1998. The CR raw field data were originally processed using Dr. Olhoeft’s NLCR_FLD program. However, five data sets were found to have channels whose signal was 180° out-of-phase with the reference channel. The reversed polarity resulted from hooking up the high and low potential leads backwards at the differential amplifier boxes. The original NLCR_FLD program was modified to correct the polarity of the reversed channels.

The data analysis consists primarily of comparing the results from geometrically identical arrays (DFCD3 and DFCW11A) versus distance from the reaction wall, and comparing channels on either side of the reaction wall within the same array (MOA_1, MOA_2, MOA_3). The DFCW11A data for all fifteen channels show a distinct increase in phase at low frequencies compared with data collected with DFCD3. Figures 3.26 and 3.26 are representative of the phase differences in all fifteen channels. Figure 3.26 shows the differences in phase between the three channels of DFCW11A and DFCD3 with MN
Figure 3.26 Data for DFCW11A (see Figure 3.19 for geometry of arrays) and DFCD3 with MN spacing=4 m. The top group of graphs is for array DFCW11A whose center is 18 m from the sheetpile wall (see Figure 3.16) and the second group of graphs is for array DFCD3 whose center is 33 m from the sheetpile wall. Note the larger phase response at lower frequencies (<1 Hz) for DFCW11A.
Figure 3.27 Data for DFCW11A (see Figure 3.19 for geometry of arrays) and DFCD3 with MN spacing=16 m. The top group of graphs is for array DFCW11A whose center is 18 m from the sheetpile wall (see Figure 3.16) and the second group of graphs if for array DFCD3 whose center is 33 m from the sheetpile wall. Note the larger phase response at lower frequencies (<1 Hz) for DFCW11A.
spacings of 4 m. Figure 3.27 shows the phase difference between the three channels of DFCW11A and DFCD3 with MN spacings of 16 m (the outermost channels). The reason for the increase in the low frequency phase response for DFCW11A data could be the proximity of the array to the corroding sheetpile of the reaction wall.
CHAPTER 4

COMPLEX RESISTIVITY FORWARD MODELING

4.1 Previous Models

The last thirty years have witnessed an explosion in geo-electrical modeling. Most geophysical problems are, in fact, three-dimensional, but in the past have been treated as 1D or 2D problems due to the lack of necessary computational power. Some early efforts in DC 2D forward modeling include Lee’s (1975) model for certain geometric inhomogeneities using a surface integral solution, the finite-difference approach by Mufti (1976), and the finite-volume Dey and Morrison (1979a). Coggon (1971) developed a 2D finite element model for the DC forward problem, and both 2D finite element (Coggon, 1971) and 2D finite difference (Coggon, 1973) models for the forward IP problem. Dodds et al. (1977) developed a 2D IP forward model using the transmission surface or network technique. The 3D DC forward problem has been solved using several methods, including solving surface integrals (Barnett, 1972; Lee, 1975; Daniels, 1977—for buried electrodes; Das and Parasnis, 1987; and Beard et al., 1996), the finite volume method (Dey and Morrison, 1979b; Spitzer, 1995; and Zhao and Yedlin, 1996), the transmission-network method (Zhang et al., 1995), and the Chebyshev domain decomposition method (Zhao and Yedlin, 1993). The finite-difference and transmission-network approaches for large, three-dimensional problems have only
become computationally feasible in the last decade. 3D IP models have been developed by using surface integral methods by Barnett (1972), Hohmann (1975) and for the case of buried electrodes, by Daniels (1977). Oldenburg and Li (1994) solve the forward IP problem by creating two forward DC models using an original and a perturbed conductivity distribution. They then calculated the apparent chargeability from the two DC resistivity forward models.

Although the numerical modeling of IP and DC forward problems has a rich history, the development of CR or spectral induced polarization forward models is relatively recent. Two 3D forward models currently available in the literature are described by Weller et al. (1996) and Shi et al. (1998). Weller et al. (1996) use the finite volume approach described by Dey and Morrison (1979b). They solve the forward problem for complex conductivities for each current electrode separately and use the superposition of pole-pole arrays to model various electrode arrays. The intrinsic complex conductivities used in the model are assigned using the model of constant phase angle (CPA). The CPA model states that if the frequency dependence of the real and imaginary parts of the conductivity can be described with the same function, the phase angle becomes independent of frequency (Weller et al., 1996). The CPA model assumes that the frequency dependence of the apparent phase angle can be ignored for small to moderate contrasts in the intrinsic phase of the model. Although the CPA model is suitable for describing low-level disseminated IP sources, it is not suitable for modeling highly frequency-dependent clay-organic or oxidation-reduction processes. The finite
volume equations are written in matrix form as: \( \mathbf{Gv} = \mathbf{s} \). The conductance matrix, \( \mathbf{G} \), depends on the complex conductivities and geometry of the gridded model; \( \mathbf{v} \) is a vector that consists of the unknown potentials, and \( \mathbf{s} \) is the current source vector. Weller et al. solve the system of equations using Jacobs’ (1981) complex bi-conjugate algorithm that extends the application of the conjugate gradient method to complex, indefinite systems. The computer code was written in C++ by Matthias Seichter as part of his PhD research at the Technische Universität Braunschweig, Germany (Seichter, 1998).

Shi et al. (1998) use the transmission network analogue as opposed to the finite volume discretization scheme. The network consists of network nodes, boundary nodes, and impedance branches. Unlike Weller et al. (1996), Shi et al. (1998) work with complex resistivities instead of complex conductivities. They solve a linear set of equations: \( \mathbf{Kv} = \mathbf{s} \), where \( \mathbf{K} \) is a matrix that depends on the resistivity and geometry of the gridded model, \( \mathbf{v} \) is a vector consisting of potential field samples at grid points, and \( \mathbf{s} \) is a source vector determined by integrating the current distribution over grid elements. The quantities \( \mathbf{K}, \mathbf{v}, \) and \( \mathbf{s} \) are all complex. The equations are solved using a complex bi-conjugate gradient method described in Jacobs (1986). The computer modeling code was written in Fortran as part of Weiquan Shi’s PhD research at the Earth Resources Laboratory at the Massachusetts Institute of Technology (Shi, 1998).
4.2 CR3D Model

The modeling program used in this thesis (CR3D) is an adaptation of a 3D DC resistivity forward modeling code developed at the University of British Columbia (UBC) Geophysical Inversion Facility (GIF). The source code was provided by Dr. Yaoguo Li with the consent of Dr. Doug Oldenburg. Their code is based on Dey and Morrison’s (1979b) 3D finite volume resistivity modeling approach. I converted the DC resistivity code into a CR modeling code by replacing all the real conductivity references in the code with complex conductivities. I then wrote a complex conjugate gradient solving routine based on the conjugate gradient template described in Barrett et al. (1994) to solve the system of complex equations. The solver incorporated a sparse matrix-vector multiplication subroutine developed at the UBC-GIF, which I modified to accommodate complex numbers. Advice and C++ code provided by Dr. Andreas Weller were also incorporated into the solver routine.

4.2.1 Fundamental Equations

The equations related to the forward CR modeling problem can be formulated following the DC resistivity developmental scheme of Dey and Morrison (1979b) and the complex conductivity approach of Weller et al. (1996). The model consists of a complex conductivity distribution in a 3D Cartesian (x,y,z) coordinate system with +z being in the downward direction. In the following discussion, the conductivities, potentials, and source current are complex quantities. Assuming an isotropic conductivity, the vector of
current density and the vector of the electric field are parallel and the current density can be expressed by Ohm’s Law (ignoring displacement currents):

$$\mathbf{J}(x, y, z) = \sigma(x, y, z)\mathbf{E}(x, y, z)$$  \hspace{1cm} (4.1)

where $\mathbf{J}$ is the current density vector, $\sigma$ is the conductivity, and $\mathbf{E}$ is the stationary electric field vector. The conservative nature of stationary electric fields produces the following relation:

$$\mathbf{E}(x, y, z) = -\nabla V(x, y, z)$$  \hspace{1cm} (4.2)

where $V$ is the electric potential. For a current source located at $(x_s, y_s, z_s)$, the injected current function is:

$$q(x, y, z) = I \delta(x-x_s)\delta(y-y_s)\delta(z-z_s)$$  \hspace{1cm} (4.3)

where $\delta$ denotes the Dirac delta function. Assuming a flow of steady current, the equation of continuity gives:

$$\nabla \cdot \mathbf{J}(x, y, z) = q(x, y, z)$$  \hspace{1cm} (4.4)

The electric potential in a non-uniform isotropic medium is given by the following equation (Weller et al., 1996):

$$-\nabla \cdot (\sigma(x, y, z) \nabla V(x, y, z)) = q(x, y, z)$$  \hspace{1cm} (4.5)

Although Eq. [4.5] is derived for steady current flow, it is also applicable to low-frequency alternating currents when EM inductive coupling effects can be ignored (Weller et al., 1996).
4.2.2 3D Discretization

CR3D follows the discretization approach of Dey and Morrison (1979b). The finite-volume method involves discretizing the subsurface into a grid of rectangular prisms on arbitrarily spaced meshes (the mesh spacings need not be the same size). The elemental volume discretization method of Dey and Morrison (1979b) is used to describe the complex conductivity, $\sigma_{i,j,k}$, enclosed by the nodes $i, j, k; i+1, j, k; i+1, j+1, k; i, j, k+1; i+1, j, k+1; i, j+1, k+1; \text{and } i+1, j+1, k+1$. The $i, j, \text{ and } k$ subscripts correspond to the x, y, and z directions, respectively. A complex potential is assigned to each of the $(i, j, k)$ nodes surrounding $\sigma_{i,j,k}$. Figure 4.1 shows $\sigma_{i,j,k}$, and the general grid spacing and indexing method used in the discretized model. The node $(i, j, k)$ represents the elemental volume, $(\Delta v_{i,j,k})$, which is described by the following relation for a point in the interior of the prismatic grid:

$$\Delta v_{i,j,k} = \frac{(\Delta x_i + \Delta x_{i-1})(\Delta y_j + \Delta y_{j-1})(\Delta z_k + \Delta z_{k-1})}{8}$$  \hspace{1cm} (4.6)

Eq. [4.6] is the result of potential node $(i, j, k)$ being at the junction of eight rectangular prisms with generally different conductivities (Weller et al., 1996). For nodes on the ground surface (in the limit of $z \rightarrow 0$) the elemental volume is given by:

$$\Delta v_{i,j,k} = \frac{(\Delta x_i + \Delta x_{i-1})(\Delta y_j + \Delta y_{j-1}) \cdot \Delta z_k}{8}$$  \hspace{1cm} (4.7)

To solve for the unknown potential at each node $(i, j, k)$, Eq. [4.5] is integrated over the corresponding elemental volume $\Delta v_{i,j,k}$ as follows:
Figure 4.1 Discretized 3D prismatic grid. The volume enclosed by nodes $i, j, k; i+1, j, k; i+1, j+1, k; i, j, k+1; i+1, j, k+1; i, j+1, k+1; i+1, j+1, k+1$ is assigned a complex conductivity, $\sigma_{i,j,k}$. 
\[ - \iiint_{\Delta v_{i,j,k}} \nabla \cdot [\sigma(x, y, z) \nabla V(x, y, z)] \, dx \, dy \, dz \quad (4.8) \]

\[ = \iiint_{\Delta v_{i,j,k}} I \cdot \delta(x_i - x_j) \delta(y_j - y_k) \delta(z_k - z_j) \, dx \, dy \, dz \]

\[ = I_{i,j,k} \]

where \( \Delta v_{i,j,k} \) is the elemental volume surrounding node \((i,j,k)\)

\( V \) is the complex electric potential

Green’s theorem yields the relation (Weller et al., 1996; Dey and Morrison, 1979b):

\[ \iiint_{\Delta v_{i,j,k}} \nabla (\sigma \nabla V) \, dV = - \oint_{S_{i,j,k}} \sigma \frac{\partial V}{\partial n} \, ds \quad (4.9) \]

The relationship of Eq. [4.9] and the form of its right hand side allow Eq. [4.8] to be written:

\[ - \oint_{S_{i,j,k}} \sigma (x, y, z) \frac{\partial V(x, y, z)}{\partial n} \, ds = I_{i,j,k} \quad (4.10) \]

where \( S_{i,j,k} \) is the surface enclosing the elemental volume \( \Delta v_{i,j,k} \)

\( n \) is the outward normal

\( I_{i,j,k} = I \) only within elemental volumes in which a current source is located; in all other elemental volumes, \( I_{i,j,k} \) is assumed to be zero (Weller et al., 1996). The surface integral along the surface \( S_{i,j,k} \) in Eq. [4.10] can be divided into six sub-surfaces whose normal directions are parallel to the grid axes. For an interior node in the discretized grid,
approximating the partial derivatives, \( \frac{\partial V}{\partial n} \), with the central difference formula allows Eq [4.10] to be written:

\[
G_{\text{top}} V_{i,j,k-1} + G_{\text{bottom}} V_{i,j,k+1} + G_{\text{left}} V_{i-1,j,k} + G_{\text{right}} V_{i+1,j,k} + G_{\text{front}} V_{i,j,k-1} + G_{\text{back}} V_{i,j,k+1} + G_{p} V_{i,j,k} = I_{i,j,k} \quad (4.11)
\]

The geometric coefficients \( G_{\text{top}}, G_{\text{bottom}}, G_{\text{left}}, G_{\text{right}}, G_{\text{front}}, G_{\text{back}}, G_{p} \) all have the physical meaning of a conductance and are built according to the rule (Weller et al., 1996):

\[
G = \bar{\sigma} \frac{A}{l} \quad (4.12)
\]

where \( \bar{\sigma} \) is an average conductivity, \( A \) is the cross sectional area, and \( l \) is the distance between two adjacent nodes. Figure 4.2 shows the orientation and spacing of the nodes along with the locations of the geometric coefficients. The geometric coefficients are defined as follows:

\[
G_{\text{top}} = -\frac{1}{4\Delta z_{k-1}} (\sigma_{i-1,j,k-1} \Delta x_{i-1} \Delta y_{j} + \sigma_{i,j,k-1} \Delta x_{i} \Delta y_{j} + \sigma_{i-1,j,k-1} \Delta x_{i-1} \Delta y_{j+1} + \sigma_{i,j,k-1} \Delta x_{i} \Delta y_{j+1}) \quad (4.13)
\]

\[
G_{\text{bottom}} = -\frac{1}{4\Delta z_{k}} (\sigma_{i-1,j,k} \Delta x_{i-1} \Delta y_{j} + \sigma_{i,j,k} \Delta x_{i} \Delta y_{j} + \sigma_{i-1,j,k-1} \Delta x_{i-1} \Delta y_{j+1} + \sigma_{i,j,k-1} \Delta x_{i} \Delta y_{j+1}) \quad (4.14)
\]

\[
G_{\text{left}} = -\frac{1}{4\Delta x_{j-1}} (\sigma_{i-1,j-1,k} \Delta y_{j-1} \Delta z_{k-1} + \sigma_{i,j,k-1} \Delta y_{j} \Delta z_{k-1} + \sigma_{i-1,j,k-1} \Delta y_{j-1} \Delta z_{k} + \sigma_{i,j,k} \Delta y_{j} \Delta z_{k}) \quad (4.15)
\]

\[
G_{\text{right}} = -\frac{1}{4\Delta x_{j}} (\sigma_{i-1,j-1,k} \Delta y_{j-1} \Delta z_{k-1} + \sigma_{i,j,k-1} \Delta y_{j} \Delta z_{k-1} + \sigma_{i-1,j,k-1} \Delta y_{j-1} \Delta z_{k} + \sigma_{i,j,k} \Delta y_{j} \Delta z_{k}) \quad (4.16)
\]

\[
G_{\text{back}} = -\frac{1}{4\Delta y_{j-1}} (\sigma_{i,j-1,k-1} \Delta z_{k-1} \Delta x_{i} + \sigma_{i,j,k-1} \Delta z_{k-1} \Delta x_{i} + \sigma_{i,j-1,k-1} \Delta z_{k} \Delta x_{i} + \sigma_{i,j,k} \Delta z_{k} \Delta x_{i}) \quad (4.17)
\]
Figure 4.2 3D discretization grid (modified after Seichter, 1998) showing orientation and spacing of nodes. Node \((i, j, k)\) is surrounded by six neighboring nodes. A geometric coefficient, \(G\), is located on each of the branches connecting the nodes.
\[ G = \frac{-1}{4\Delta y_j} (\sigma_{i-1,j,k-1} \Delta z_{k-1} \Delta x_{i-1} + \sigma_{i,j,k-1} \Delta z_{k-1} \Delta x_i + \sigma_{i,j,k} \Delta z_k \Delta x_{i-1} + \sigma_{i,j,k} \Delta x_i \Delta z_k) \]  \hspace{1cm} (4.18)

\[ G = -(G+G+G+G+G) \]  \hspace{1cm} (4.19)

At each node in the interior of the discretized grid, Kirchoff’s current law can be applied to state that the current flowing into one node must be equal to the sum of the currents flowing out of the node (Weller et al., 1996):

\[ I_{i,j,k} = I_{\text{top}} + I_{\text{bottom}} + I_{\text{left}} + I_{\text{right}} + I_{\text{front}} + I_{\text{back}} \]  \hspace{1cm} (4.20)

where the currents on the right hand side of Eq.[4.20] are each equal to the product of a coupling coefficient and the potential difference between node \((i, j, k)\) and a neighboring node:

\[ I_{\text{top}} = G(V_{i,j,k-1} - V_{i,j,k}) \]  \hspace{1cm} (4.21)

\[ I_{\text{bottom}} = G(V_{i,j,k+1} - V_{i,j,k}) \]  \hspace{1cm} (4.22)

\[ I_{\text{left}} = G(V_{i-1,j,k} - V_{i,j,k}) \]  \hspace{1cm} (4.23)

\[ I_{\text{right}} = G(V_{i+1,j,k} - V_{i,j,k}) \]  \hspace{1cm} (4.24)

\[ I_{\text{back}} = G(V_{i,j-1,k} - V_{i,j,k}) \]  \hspace{1cm} (4.25)

\[ I_{\text{front}} = G(V_{i,j+1,k} - V_{i,j,k}) \]  \hspace{1cm} (4.26)
Hence, Eq. [4.20] shows that the potential, $V$, at node $(i, j, k)$ is only dependent on the surrounding nodes $(i, j, k-1)$, $(i, j, k+1)$, $(i-1, j, k)$, $(i+1, j, k)$, $(i, j-1, k)$, and $(i, j+1, k)$.

### 4.2.3 Cole-Cole Model

The intrinsic complex conductivities used in CR3D models were calculated using a form of the Cole-Cole model. Although the Cole-Cole model was originally formulated to calculate dielectric dispersions (Cole and Cole, 1941), it has been found to be applicable to IP and CR modeling (Pelton et al., 1978; Washburne, 1982; Jones, 1997).

The Cole-Cole model proposed by Pelton et al. (1978) is of the form:

$$
Z(\omega) = R_0 \left[ 1 - m \left( 1 - \frac{1}{1 + (i\omega\tau)^c} \right) \right]
$$

(4.27)

where:

- $Z(\omega)$ = the complex impedance at angular frequency $\omega$
- $\omega = \text{the angular frequency } 2\pi f$, where $f$ is the frequency
- $R_0 = \text{the resistance at zero frequency (DC)}$
- $m = \text{the volume chargeability}$
- $i = \sqrt{-1}$
- $\tau = \text{the time constant in seconds}$
- $c = \text{the time constant distribution parameter}$

The Cole-Cole model described by [4.27] is one form of a large family of relaxation models. Comparisons of Cole-Cole models with other relaxation models (Debye, Cole-Davidson, and others) are given in Pelton et al. (1983). In order to model multiple
relaxations, an additive Cole-Cole model (as presented in Jones [1997], minus the dielectric term) of the following form is used in this thesis:

\[
s' + i s'' = \sigma_{dc} \left[ 1 + \sum_j m_j \left( \frac{(i \omega \tau_j)^{\alpha_j}}{1 + (i \omega \tau_j)^{\alpha_j}} \right) \right]
\]

(4.28)

where:

- $s'$ = the real part of the complex conductivity
- $s''$ = the imaginary part of the complex conductivity
- $\sigma_{dc}$ = the conductivity at zero frequency (DC)
- $\alpha$ = the Cole-Cole time constant distribution parameter
- $m$ = the volume chargeability
- $\tau$ = the time constant
- $i = \sqrt{-1}$
- $\omega$ = the angular frequency (2\pi f), where f is frequency
- $j$ = subscript for a particular relaxation

Equation [4.28] differs from Pelton’s Cole-Cole model (Equation [4.27]) in that it is in terms of conductivity and it takes into account multiple relaxations. The complex resistivity is simply the complex reciprocal of the complex conductivity:

\[
\rho' - i \rho'' = (s' + is'')^{-1}
\]

(4.29)

To calculate the complex conductivities of the host medium and each inhomogeneity, the user must assign a $\sigma_{dc}$, $m$, $\alpha$, and $\tau$ to each inhomogeneity and the host medium in an
input file. The complex conductivities for each inhomogeneity and the background conductivity are then calculated at each user-specified frequency using Eq. [4.28].

4.2.4 Boundary Conditions

Two boundary conditions must be applied to the discretized halfspace in order to simulate field conditions. In the field, the subsurface is bounded by what is assumed to be a perfectly insulating layer of air. In the computer model, the Neumann boundary condition (Dey and Morrison, 1979; Weller et al., 1996) is applied to the surface defined by \( z = 0 \):

\[
\frac{\partial V}{\partial n} = 0
\]  \hspace{1cm} (4.30)

where \( n \) = outward normal and \( V \) = electric potential.

Eq. [4.30] states that no current flows through the \( z = 0 \) boundary. In the field, the earth is considered to be infinite in lateral extent and depth. In the computer model, the boundaries in the lateral directions and at depth are defined using the mixed boundary condition proposed by Dey and Morrison (1979b). The form of the mixed boundary condition is:

\[
\frac{\partial V}{\partial n} + V \frac{\cos \theta}{r} = 0
\]  \hspace{1cm} (4.31)

where \( r \) = the length of the vector \( \mathbf{r} \) that connects the current source and a node on the boundary

\( \theta \) = the angle between \( \mathbf{r} \) and the outward normal \( n \) at the boundary plane
The above boundary condition takes advantage of the asymptotic behavior of the electric potential at distant bounding planes (Dey and Morrison, 1979b).

4.2.5 Solution of the System of Equations

The use of a finite-volume 3D discretization allows the solution for the complex potentials at each node of the discretized grid using the equation:

$$K V = s$$  \hspace{1cm} (4.32)

where $K$ is a matrix dependent on the geometry and physical property distribution in the grid; $V$ is a vector containing the unknown potentials at each node in the grid; and $s$ is a vector containing the source terms for the injection current. $K$, $V$, and $s$ all contain complex quantities. The system of equations is solved using a form of the bi-conjugate gradient (BiCG) method. The BiCG method has proven useful in solving problems in electromagnetics (Smith et al., 1990; Smith, 1996) and complex resistivity (Weller et al., 1996; Seichter, 1998; Shi et al., 1998; Shi, 1998). For symmetric matrices, Jacobs (1981; 1986) developed a form of the BiCG method that reduces to the conjugate gradient (CG) method extended to complex numbers. I wrote a Fortran CG solver code for complex numbers based on the CG template described by Barrett et al. (1994) and C++ code written by Mattias Seichter and provided by Dr. Andreas Weller. The solver code incorporates a UBC-GIF routine for vector-matrix multiplication for sparse matrices stored in Yale or row-major format.
4.2.6 Assumptions and Limitations of CR3D

The modeling code, CR3D, is not intended to be used to solve all CR forward problems; it contains assumptions and limitations. One of the most significant assumptions in the formulation of the forward problem is the exclusion of EM inductive coupling effects. As opposed to treating the total current density (and subsequently the complex conductivity) as the sum of conduction and displacement currents (Olhoeft 1985; Jones, 1997), the contribution of the displacement current is assumed to be zero. In extremely resistive environments, propagation cannot be neglected and the above assumption is violated. Equations for steady current flow are assumed to be valid at low frequencies (Weller et al., 1996). The frequencies used in CR surveys (0.001-1000 Hz) are assumed to be low enough so that scattering effects are not a factor. At low frequencies (<1.0 Hz), EM inductive coupling effects can be considered negligible (Wynn, 1979). It should be noted that data collected in environments with highly conductive surface layers or with large electrode spreads can still be affected by EM inductive coupling even at low frequencies (Dey and Morrison, 1973). It is not recommended to use CR3D to model problems in which the targeted reactions occur at high (>10 Hz) frequencies. For the modeling of most low-frequency clay-organic reactions, the above assumption is valid.

CR3D allows the user to add blocks of inhomogeneities into a homogeneous half-space. The level of anisotropy for a particular model is defined by the user (i.e. adding vertical dikes or layering). The formulation of the forward CR problem used in this
thesis assumes that the system is linear. Hence, nonlinear calculations such as THD, PHD, and RHD are not included in the forward modeling.

CR3D is currently limited by the size of the discretized 3D space. The memory limitations of current computer resources limit the total number of nodes (and equations) that can be stored and solved. As advances in technology produce computer resources with larger memory capacities, the size and fineness of the 3D model will be allowed to increase. The format for discretizing inhomogeneities as blocks also makes the modeling of dipping or rounded inhomogeneities difficult. In order to simulate a dipping dike, for example, the user would need to define several rectangular blocks with small offsets.

4.3 CR3D Modeling Examples

The following modeling examples were generated on a PC (Pentium II, 400 MHz, 384 MB RAM) running on a Linux Redhat 5.2 platform using a NAGWare f90 Release 2.2 compiler. The first example is a comparison with the results given in Figure 6 of Weller et al. (1996). A Schlumberger sounding was performed over a three layer model (using a 3D modeling algorithm) with the following parameters shown in Table 4.1. A comparison between Weller et al.’s (1996) results and CR3D results is shown in Figure 4.3; the results are in good agreement with one another. Note that the results computed with CR3D only range from an AB/2 of 10 to 80.
Figure 4.3 Schlumberger sounding over a three layer model (see Table 4.1 for model parameters). Comparison of CR3D results vs. Weller et al. (1996) Figure 6. The “1-D filter method” (as described in Anderson [1979]), “Dirichlet BC” (potentials at boundaries equal zero), and “asymptotic BC” (mixed boundary conditions described in Section 4.24) are the original data from Weller et al. (1996). The CR3D data were produced by the code developed for this thesis using the boundary conditions described in Section 4.2.4.
Table 4.1 Parameters used in a Schlumberger sounding over a three layer polarizable earth.

A second example using the CR3D program was based on an earth model that consisted of a buried block (inhomogeneity) in a homogeneous country rock (half-space). A depiction of the 3D model is shown in Figure 4.4. The Cole-Cole parameters for the model are given in Table 4.2.

| Layer | $|\rho|$ in $\Omega$m | $\phi$ in mrad | $\sigma'$ | $\sigma''$ | Thickness in m |
|-------|----------------------|----------------|----------|-----------|---------------|
| 1     | 100                  | 5              | 0.01     | 0.00005   | 10            |
| 2     | 10                   | 25             | 0.1      | 0.0025    | 40            |
| 3     | 100                  | 5              | 0.01     | 0.00005   | $\infty$     |

Table 4.2 Cole-Cole parameters for a buried block model.

Resistivity and phase plots versus frequency for the inhomogeneity and the background are shown in Figures 4.5 and 4.6, respectively. The peak of the phase anomaly for the inhomogeneity ($\approx 100$ mRad) occurs roughly at 1.0 Hz, while the phase anomaly for the background is nearly zero ($<0.001$ mRad) below 10 Hz. Hence, the following profiles were run at 1.0 Hz to produce the largest possible phase anomaly. Wenner profiles over
Figure 4.4 3D model of a block buried in a homogeneous half-space. The x-width, y-width, depth extent, and depth of burial of the block were varied for this study, while the Cole-Cole parameters were kept constant. The buried gray cube is centered within the larger model-space cube. Note: $\rho_{bc} = 1/\sigma_{bc}$. 

\[ m = 0.2 \]
\[ \tau = 0.2 \]
\[ \alpha = 1.0 \]
\[ \rho_{\infty} = 30 \text{ ohm-m} \]

\[ m = 1e-5 \]
\[ \tau = 1e-4 \]
\[ \alpha = 1.0 \]
\[ \rho_{\infty} = 150 \text{ ohm-m} \]
Figure 4.5 Resistivity and phase plots versus frequency for an inhomogeneity with one Cole-Cole dispersion ($m = 0.2$, $\tau = 0.2$, $\alpha = 1.0$, and $\rho_{dc} = 30 \text{ ohm-m}$).
Figure 4.6 Resistivity and phase plots versus frequency for a background medium with one Cole-Cole dispersion (m= 1e-5, \( \tau = 1e-4, \alpha = 1.0, \) and \( \rho_{bc} = 150 \text{ ohm-m} \)). Note that the phase values are very low (1e-8 mRad - 1e-2 mRad).
block models with varying x-width, y-width, depth extent, and depth of burial were simulated (see Figure 4.7 for an illustration of parameters). X-width refers to the width of the block in the x direction (parallel to the line of survey). Y-width describes the width of the block in the y direction (perpendicular to the line of survey). Depth extent refers to the length of the block in the z direction, and depth of burial is the distance from the “earth’s surface” to the top of the block.

To run a model, the real and imaginary parts of the complex conductivities for the inhomogeneity (or inhomogeneities) and the background are calculated using [4.28]. The complex conductivities are then assigned to a 3D mesh. The mesh for the models described in this chapter is shown in Figures 4.8 and 4.9. Figure 4.8 shows the mesh in the x-y plane. The x-y mesh measures 54x54 mesh cells which correspond to a “distance” of 16800; the units of “distance” are arbitrary (i.e. it could be 16800 m, cm, yards, etc.) and the number is the summation of the cell widths in a particular direction. For example, in the x-direction, the cell widths are: 3200, 1600, 800, 400, 200, 44*100, 200, 400, 800, 1600, and 3200 (44*100 symbolizes 44 cells of width 100) which totals 16800 units of width. In cartesian coordinates, the center of the x-y mesh is (0,0). The electrode spreads are kept within the center 40x40 cells, while the remaining cells act as “padding” between the area of interest and the boundaries. The mesh shown in Figure 4.9 represents the x-z or y-z discretization scheme, which is essentially a cross-sectional view of the 3D mesh. For surface surveys, the upper portion of the 3D block is of interest, and hence is discretized more finely than the padding cells which extend to the
Figure 4.7 Illustration of defined parameters for a buried inhomogeneity.
1.) Cross-sectional view illustrating the terminology: x-width, depth extent, depth of burial, and “a” (where “a” refers to the MN spacing or 1/3 AB spacing of a Wenner array.  2.) Plan view illustrating the terms: y-width and x-width.
Figure 4.8 Mesh used for finite difference modeling. Above is the x-y plane for the 3D mesh used to create the results shown in Figures 4.10-4.21.
Figure 4.9 Mesh used for finite difference modeling. Above is the x-z or y-z plane (in this case they are equivalent) of the 3D mesh used to create the results shown in Figures 4.10-4.21.
bottom boundary. The discretized complex conductivity model file and an electrode position file are all the input necessary to run the CR3D forward modeling program.

The results shown in Figures 4.10-4.21 are presented in a format similar to that of Van Nostrand and Cook (1966). The x-axis is in terms of x/a which represents the distance between the plotting point and the center of the inhomogeneity divided by the “a” spacing (MN or 1/3 AB for a Wenner array). For standard (α) Wenner profiles, the plotting point is taken to be at the center of the M and N electrodes. The varied parameters (x-width, y-width, depth extent, depth of burial) are given in terms of the “a” spacing.

Wenner profiles conducted over the center of a block of varying x-width are shown in Figure 4.10. The y-width of the block equals “a”, the depth extent of the block equals “a”, and the depth of burial equals ¼ “a”. As the x-width of the conductive, polarizable inhomogeneity is increased, both the resistivity and phase responses broaden. In the extreme case of the x-width running the length of the model space (simulating infinite strike), both the resistivity and phase profiles have constant values. In Figure 4.10, the computation time for one profile line with 29 current electrode stations was 342 minutes (about 11.8 minutes/current electrode station) on a Pentium II 400 MHz computer. Each current electrode station requires the computation of a forward model.

Figure 4.11 shows the response for Wenner profiles run over the center of a block of varying y-width. The x-width and depth extent of the block are equal to “a”, while the depth of burial is equal to ¼ “a”. The y-width varies from “a” to the entire length of the
Figure 4.10 Wenner profiles at 1.0 Hz over a block with varying x-widths. Y-width, = depth extent = a; depth of burial = 1/4a. The electrical properties of block and background are given in Table 4.2. The computation time for one profile line with 29 current electrode stations was 342 minutes (about 11.8 minutes per current electrode station).
Figure 4.11 Wenner profiles at 1.0 Hz over a block with varying y-widths. X-width = depth extent = a; depth of burial = 1/4a.
model space. As expected, the resistivity decreases and the phase increases with increases in the y-width of the conductive, polarizable block.

Figure 4.12 shows that variations in the depth extent of a block with an x-width and y-width of “a”, and a depth of burial of ¼ “a” do not produce drastic changes in the phase and resistivity profiles. On the contrary, variations in the depth of burial produce dramatic changes in both the resistivity and phase profiles (see Figure 4.13). The x-width, y-width, and depth extent are held constant at “a”, while the depth of burial varies from “a” to zero. The zero case represents an outcropping inhomogeneity and produces the most prominent resistivity and phase anomalies. The block buried at a depth of “a” is scarcely detected.

Figure 4.14 shows the results for Wenner profiles with lines of survey at an offset to the center of the block. The block has dimensions of: x-width = y-width = depth extent = “a”, and is buried at a depth of ¼ “a”. The zero offset profile (i.e. directly over the center of the block) produces the largest resistivity and phase anomalies, while the profile run at an offset of “2a” shows no noticeable resistivity or phase anomaly.

The profiles for a Wenner, collinear dipole-dipole, parallel dipole-dipole, and an “expanding potential” array over a cube of dimensions: x-width = y-width = depth extent = “a”, and buried at a depth of ¼ “a” are shown in Figure 4.15. The collinear dipole-dipole array has an MN = AB = “a”, and an “n” spacing of 1—where “n” spacing refers to the distance between the closest current and potential electrode. The parallel array (see Figure 2.3) in this instance has square dimensions; that is, AB = MN = “a”, and n = 1.
Figure 4.12 Wenner profiles at 1.0 Hz over a block with varying depth extent. X-width = y-width = a; depth of burial = 1/4a.
Figure 4.13 Wenner profiles at 1.0 Hz over a block with varying depths of burial. \( x\)-width = \( y\)-width = depth extent = \( a \).
Figure 4.14 Wenner profiles at 1.0 Hz directly over, and offset from, a block with x-width = y-width = depth of extent = a, buried at a depth 1/4a. The offset profiles are 1a and 2a from the center of the block.
The parallel dipole-dipole profile was run with the potential and current electrode pairs perpendicular to the line of survey. The “expanding potential” array is similar to the expanding potential array described in Chapter 2, and the array used at Hill AFB (see Figure 3.11). The AB spacing = “4a” while the potential pairs have spacings of “2a”, “a”, and “1/2a”. Somewhat like an AB rectangle array, the expanding potential array has two branches parallel to the collinear branch and offset by “3/4a”.

In Figure 4.15, the expanding potential profile (MN = “a”/2) gives the sharpest phase and resistivity anomalies. However, the parallel dipole-dipole profile displays the largest phase anomaly (in terms of breadth of anomaly and largest value). The collinear dipole-dipole array gives an interesting “W”-shaped resistivity anomaly, and “M”-shaped phase anomaly. The Wenner profile produces the smallest phase and resistivity anomalies.

Figures 4.16, 4.17, and 4.18 display the profiles for additional potential electrode pairs for the expanding potential array. Figure 4.16 shows profiles for the three potential pairs that were collinear with the current electrodes. The profile corresponding to the smallest MN spacing gives the largest phase and resistivity anomalies, while the profile for the largest MN gives the smallest phase and resistivity anomalies. Figure 4.17 shows the profiles for the non-collinear or offset branch of the expanding potential array. As with the previous figure, the smallest MN spacing produces the largest phase and
Figure 4.15  Comparison of Wenner, collinear dipole-dipole, parallel dipole-dipole, and expanding potential profiles at 1.0 Hz directly over a block of dimensions x-width = y-width = depth extent = a, buried at a depth of 1/4a.
Figure 4.16  Comparison of expanding potential array profiles at 1.0 Hz for MN = a/2, a, and 2a over a block of dimensions x-width = y-width = depth extent = a buried at a depth 1/4a. The potential electrodes are collinear with the current electrodes. When MN = a/2, the array is similar to a Schlumberger array; when MN = a, it is a Wenner array.
Figure 4.17 Comparison of expanding potential array profiles at 1.0 Hz for MN = a/2, a, and 2a over a block of dimensions x-width = y-width = depth extent = a, buried at a depth 1/4a. The potential electrodes are offset from the current electrode line of survey by 0.75a.
Figure 4.18  Comparison of profiles at 1.0 Hz for the collinear and offset potential electrode (MN = a/2) branches of an expanding potential array. The block is buried at a depth of 1/4a, and has the dimensions: x-width = y-width = depth extent = a.
resistivity anomalies. Figure 4.18 emphasizes the difference in anomaly amplitude between the collinear and offset branches in the expanding potential array.

The effect of frequency on the resistivity and phase profiles for a Wenner profile over a cube with dimensions: \(x\)-width = \(y\)-width = depth extent = \(a\), and buried at a depth of \(\frac{1}{4}\) \(a\) is shown in Figure 4.19. Profiles were produced using frequencies of 0.001, 1.0, and 100.0 Hz. Although the resistivity anomalies are almost identical over frequency, the phase anomalies are quite different. The profile at 1.0 Hz gives a much larger phase anomaly than the profiles collected at 0.001 and 100.0 Hz; this correlates with the phase plot for the cube (Figure 4.5) where the phase maximum occurs near 1.0 Hz. Figure 4.20 shows a close-up view of the phase anomaly; the 0.001 and 100.0 Hz phase anomalies are similar in shape to the 1.0 Hz anomaly, but much smaller (< 2% of the phase maximum).

The final example in this chapter is for a buried cube (\(x\)-width = \(y\)-width = depth extent = \(a\); depth of burial = \(\frac{1}{4}\) \(a\)) whose DC resistivity is equal to that of the surrounding medium. However, the Cole-Cole parameters for the cube are different than the background, and in this case, although the resistivity profile displays a very small anomaly, the phase profile displays a quite clear and distinct anomaly (see Figure 4.21). The Cole-Cole parameters for the background are the same as those shown in Figure 4.4; resistivity and phase plots versus frequency for the cube are displayed in Figure 4.22 (\(\rho_{DC} = 150\) ohm-m, \(m = 0.35\), \(\tau = 0.2\), and \(\alpha = 1.0\)). The profile was performed with a frequency of 1.0 Hz. The above is a case where a DC resistivity survey may not produce...
Figure 4.19 Comparison of Wenner profiles at 0.001, 1.0, and 100.0 Hz over a block buried at a depth of 1/4a with dimensions x-width = y-width = depth extent = a.
Figure 4.20 Close-up of phase plot from Figure 4.19. Comparison of Wenner profiles at 0.001, 1.0, and 100.0 Hz over a block buried at a depth of 1/4a with dimensions x-width = y-width = depth extent = a.
Figure 4.21 Wenner profile at 1.0 Hz over a cube whose $\rho_{dc}$ is the same as the background medium. The cube is buried at $1/4a$ and has the dimension $x$-width $= y$-width $= \text{depth extent} = a$. The background has the Cole-Cole parameters shown in Table 4.2. The cube, however, has an $m = 0.35$, $\tau = 0.2$, $\alpha = 1.0$, and $\rho_{dc} = 150 \text{ ohm-m.}$
Figure 4.22 Resistivity and phase plots versus frequency for the buried cube described in Figure 4.21. The single dispersion has the following Cole-Cole parameters: $m = 0.35$, $\tau = 0.2$, $\alpha = 1.0$ and $\rho_{dc} = 150 \text{ ohm-m}$. 
useful results, whereas a CR survey would produce excellent results. At DC frequency (0 Hz), the cube and background both have resistivities of 150 ohm-m. However, at 1.0 Hz, the buried cube has a resistivity of approximately 120 ohm-m and produces a noticeable phase contrast with the background due primarily to the cube’s high chargeability (m = 0.35) versus the low chargeability of the background (m = 1e-5).

4.4 Discretization Errors

The discretization of the forward model can introduce numerical errors into the calculated potentials. Two important factors in the discretization process are the location of the boundaries with respect to the electrode array, and the number of mesh cells located between the electrodes. Increasing the distance between the model boundary and the nearest electrode will decrease the contribution of the boundary to the calculated potential. Figure 4.23 shows the % error of apparent resistivity versus an analytical solution for a Wenner array (a = 400) over a homogeneous 10 ohm-m half-space. The meshes shown in Figures 4.8 and 4.9 were used for the modeling. When the x and y boundaries are located only 400 mesh units from the nearest electrode, an error of about 5.5% is introduced to the resistivity measurement. At distances of greater than 2300 mesh units for this example, the error introduced by the boundary is less than 1%. A distance of 6200 was selected for the models shown in Figures 4.10-4.21.

In addition to the distance between the electrodes and boundaries, the number of mesh cells between the potential electrodes (or current electrodes in a reciprocal Schlumberger array) is an important factor in the discretization process. Figure 4.24
Figure 4.23 Effect of distance between the boundary and the nearest electrode. The x-axis is in mesh units. The y-axis is the percent error of the resistivity calculated from the modeled data versus an analytical solution. The data are for a Wenner array (a = 400) over a homogeneous 10 ohm-m half-space.
Figure 4.24 Effect of varying the number of mesh cells between the potential electrodes. The x-axis is in mesh units. The y-axis is the percent error of the resistivity calculated from the modeled data versus an analytical solution. The data are for a Wenner array (a = 400) over a homogeneous 10 ohm-m half-space.
illustrates the % error trend in resistivity with respect to the number of mesh cells between the potential electrodes. The response for a Wenner array (a = 400) was modeled over a 10 ohm-m homogeneous half-space. Note the rapid decrease in error between 1 (>17% error), 2 (>6% error), and 4 (2% error) mesh cells. Placing more than 10 mesh cells between the potential electrodes does not significantly change the % error with respect to the analytical solution. Although the low % errors for 10, 12, or 16 mesh cells (<1%) looks quite attractive, such spacings result in very large, cumbersome meshes and correspondingly long computation times. Hence, a compromise is necessary to produce a mesh with relatively low error and a reasonable overall size. The results shown in Figures 4.10-4.22 were modeled with four mesh cells between the potential electrodes.
5.1 Introduction

The CR method was originally developed for and applied to mineral exploration. Interest in CR grew with the demonstration of the applicability of CR to discrimination between various minerals (Pelton et al., 1978). In the last 15 years CR has proven useful for environmental applications as a non-invasive tool to detect chemical reactions in the subsurface—especially clay-organic reactions which often produce large low frequency phase anomalies.

As described in Chapter 2, one of the challenges of conducting field surveys is the selection of a proper array for a particular target and geologic setting. The next section describes an environmental application of CR forward modeling to a site encountered at Hill AFB.

5.1.1 Description of Hill AFB Model

A numerical model was built to simulate a Hill AFB-type environment where an organic contaminant (in this case PCE) is attacking a clay-slurry wall. Such a scenario is of great interest in the environmental world due to the possible ability of some organic contaminants to attack and increase the permeability of clay barrier walls, thus allowing
contamination to pass through. An illustration of the Hill AFB-type model is shown in Figure 5.1. The model was based on the field setting at Hill AFB described in Chapter 3. As opposed to the angled wall that was encountered in the field, only the section of the wall parallel with the strike of the arrays was used for the computer models. One model was run with and without the angled section of the wall, and the difference in the results was minute (simplifying the wall geometry allowed for much more freedom in mesh design). The objective of the modeling in this chapter is to compare CR results for various electrode locations on the earth’s surface with field data. In this chapter, modeled results are presented for three frequencies at two expanding potential array locations and two Wenner array locations.

5.1.2 Laboratory Data

An attempt to simulate the geologic setting at the Hill AFB site was made by basing the Cole-Cole parameters for the natural clay layer, uncontaminated clay-slurry wall, and the clay-slurry wall contaminated with PCE on actual laboratory samples from the field site. The samples were measured using laboratory CR equipment as described in Olhoeft (1979) and Jones (1997). The Cole-Cole parameters were then inverted from the laboratory data using Dan Jones’ ColeCole program (Jones, 1997). The laboratory data for the above materials are presented in Figures 5.2-5.3. The presentation of the laboratory data is the same as that of field data with the exception that an additional box containing %RCD and PCD is present. The %RCD and PCD represent the differences
Figure 5.1 3D block model used for numerical modeling. 1.) Cross-sectional view of model. 2.) Plan view of model. (Note: figure not to scale and the Wenner array is a schematic representation to show orientation).
Figure 5.2 Laboratory data for a core sample taken from a depth between 12.19-12.80 m at Hill AFB, OU2. The sample presumably represents the clay layer at OU2, Hill AFB.
Figure 5.3 Laboratory data for a Hill AFB OU2 clay-slurry containment wall sample with and without added PCE (after Olhoeft and Wardwell, 1998).
between the measured laboratory data and the Cole-Cole fit used to extrapolate the Cole-Cole parameters. The large low frequency dispersion for the PCE-contaminated slurry wall sample in Figure 5.3 is of particular interest since it is quite different from the responses of other materials at the site. The PCE-clay wall signature is the target for the modeled field site.

Although the laboratory data generally shows three dispersions for the OU2 materials, only the two lower frequency dispersions will be considered in the following example (since the modeling program assumes that only low frequencies will be used and EM coupling effects can be ignored). The first example uses the exact Cole-Cole parameters extrapolated from the laboratory data for the clay layer, the PCE-contaminated clay slurry wall, and the uncontaminated clay-slurry wall. The laboratory data for the upper soil layer contained an erroneous data point that could not be inverted with the ColeCole program, thus a value of 10 ohm-m was assigned to the upper layer. The CR3D results for the exact laboratory parameters and the exact electrode array locations for ARRAYS 1 and 2 at Hill AFB (see Figures 3.9 and 3.10) are shown in Figure 5.4. The Cole-Cole parameters are given in Table 5.1. Figure 5.4 illustrates that for the electrode geometry used at Hill AFB, no appreciable phase anomaly exists between a completely uncontaminated and a PCE-contaminated clay-slurry wall. This most likely indicates that the laboratory samples were not truly representative of the actual field site. Factors such as a perched water table, dilution, and geometric effects
Figure 5.4  Resistivity and phase plots versus frequency for an expanding potential array (AB = 32 m, MN = 16 m) of the same dimensions and location as the arrays used at Hill AFB. The exact laboratory data was used as input for the forward model. There is no detectable anomaly for this combination of parameters.
such as current channeling may help explain the discrepancy between the modeled data and field data shown in Figure 5.5.

<table>
<thead>
<tr>
<th></th>
<th>Clay layer</th>
<th>Uncontaminated clay-slurry wall</th>
<th>Contaminated clay-slurry wall</th>
<th>Upper soil layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_1$</td>
<td>0.012</td>
<td>0.0097</td>
<td>0.0086</td>
<td>---</td>
</tr>
<tr>
<td>$\tau_1$</td>
<td>66</td>
<td>1700</td>
<td>23</td>
<td>---</td>
</tr>
<tr>
<td>$\alpha_1$</td>
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<td>0.64</td>
<td>0.97</td>
<td>---</td>
</tr>
<tr>
<td>$m_2$</td>
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<td>0.026</td>
<td>0.031</td>
<td>---</td>
</tr>
<tr>
<td>$\tau_2$</td>
<td>0.00091</td>
<td>0.0012</td>
<td>0.00065</td>
<td>---</td>
</tr>
<tr>
<td>$\alpha_2$</td>
<td>0.65</td>
<td>1.00</td>
<td>0.93</td>
<td>---</td>
</tr>
<tr>
<td>$\rho_{dc}$ ($\Omega \cdot m$)</td>
<td>$\frac{1}{\sigma_{dc}}$</td>
<td>21.43</td>
<td>7.00</td>
<td>7.27</td>
</tr>
</tbody>
</table>

Table 5.1 Input Cole-Cole parameters for Figure 5.4 derived from laboratory data for the clay layer, uncontaminated clay-slurry wall, and PCE-contaminated clay-slurry wall. Note that the upper soil layer was assigned a value of 10 ohm-m and was considered non-polarizable.

To create a large enough phase anomaly to more closely match the field data, the Cole-Cole parameters for the PCE-contaminated slurry wall, the uncontaminated slurry wall, and the upper soil layer were modified for the following examples. The resistivity and phase plots versus frequency for the modeled clay layer, uncontaminated slurry wall,
Figure 5.5  Complex resistivity field data collected at OU2, Hill AFB. The three plotted channels have an MN spacing of 8 m and an AB spacing of 32 m. The low frequency (<0.1 Hz) trend in the data for Channel 9 resembles the laboratory data for PCE reacting with the clay-slurry wall (see Figure 5.3.)
PCE-contaminated slurry wall, and upper soil layer are shown in Figures 5.6. The Cole-Cole parameters for the above materials are given in Table 5.2. The parameters for the modified uncontaminated clay-slurry wall are within the experimental error-bars of the measured laboratory data shown in Figure 5.3. The shape of the frequency-dependence of the modified PCE-contaminated layer was kept the same as the measured laboratory data, but the amplitude (chargeability of the low-frequency dispersion) was increased. If the lab sample had dried-out before the laboratory measurements were performed, the above modification may be reasonable. The modified upper soil layer parameters were derived from a hand-fit match to the laboratory data that could not be modeled with the Cole-Cole inversion program.

An example of field data from the OU2 site is shown in Figure 5.5. Channel 9 (AB = 32 m, MN = 8 m) recorded a much higher low-frequency phase response than the other channels (which correlates to the detection of a PCE-clay slurry wall reaction). As noted in Chapter 3, the CR survey location at OU2 was restricted by heavy construction traffic. Instead of positioning the arrays directly over the containment wall, the positioning of the electrodes was limited to one current electrode and no potential electrodes above the wall. The following modeling exercise was performed to investigate how varying the positioning or type of electrode array would affect the phase response in a setting similar to that at the OU2 site.
Figure 5.6 Phase versus frequency plot for the modeled upper soil layer, clay layer, PCE-contaminated clay-slurry wall, and uncontaminated clay-slurry wall. The Cole-Cole parameters for the modeled materials are given in Table 5.2.
Table 5.2  Input Cole-Cole parameters for the modified uncontaminated clay-slurry wall, PCE-contaminated clay-slurry wall, and upper soil layer. The clay layer is unchanged from the inverted laboratory parameters.

<table>
<thead>
<tr>
<th></th>
<th>Clay layer</th>
<th>Uncontaminated clay-slurry wall</th>
<th>Contaminated clay-slurry wall</th>
<th>Upper soil layer</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.0016</td>
<td>0.39</td>
<td>0.016</td>
</tr>
<tr>
<td>$\tau_1$</td>
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</tr>
<tr>
<td>$\alpha_1$</td>
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<td>0.28</td>
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<td>0.90</td>
</tr>
<tr>
<td>$m_2$</td>
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<td>0.026</td>
<td>0.031</td>
<td>0.20</td>
</tr>
<tr>
<td>$\tau_2$</td>
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</tr>
<tr>
<td>$\alpha_2$</td>
<td>0.65</td>
<td>1.00</td>
<td>0.93</td>
<td>0.65</td>
</tr>
<tr>
<td>$\rho_{dc}(\Omega \cdot m) = \frac{1}{\sigma_{dc}}$</td>
<td>21.43</td>
<td>7.00</td>
<td>7.27</td>
<td>2500</td>
</tr>
</tbody>
</table>

5.1.3 CR3D Models

The first pair of models was run to determine the difference in phase and resistivity responses due to the presence or lack of a section of PCE-contaminated clay slurry wall. The 3D mesh used for the models in this chapter is much larger (80x80x32 nodes = 204800 cells) than the mesh used in Chapter 4 (54x54x21 nodes = 61236 cells). Figures 5.7 and 5.8 show the x-y and y-z planes of the 3D mesh. The computation time for one frequency of one forward model was over 180 minutes (the lengthy time is a
Figure 5.7 Mesh used for finite difference modeling. Above is the x-y plane for the 3D mesh used for all the models presented in Chapter 5. The 3D mesh measured 80x80x32 nodes resulting in 204800 total cells.
Figure 5.8 Mesh used for finite difference modeling. Above is the y-z plane for the 3D mesh used for all the models presented in Chapter 5. The 3D mesh measured 80x80x32 nodes resulting in 204800 total cells.
result of the large mesh size, the very high resistivity contrast, and the lack of a pre-conditioner for the solution of the matrix equations. The expanding potential array (see Figure 3.10 for array geometry) used at Hill AFB was selected for the first modeling example (AB = 32 m). The array was located with only one current electrode over the wall to simulate the same location as ARRAY 1 for the Hill AFB surveys (see Figure 5.9). The modeling results for Channel 9 (MN = 8 m) are shown in Figure 5.10. As expected, the contaminated model produces a greater low-frequency phase peak than the uncontaminated model. In Figure 5.11 the same expanding electrode array is located entirely over the clay-slurry wall (see Figure 5.9). The difference in phase responses at 0.01 Hz between the contaminated and uncontaminated models is nearly 95 mRads. Also, the for the contaminated model the apparent resistivity decreases to a greater extent with increasing frequency (almost 20 ohm-m between 0.001 and 0.1 Hz) than the uncontaminated model (less than 1 ohm-m difference between 0.001 and 0.1 Hz). Figure 5.12 shows the two previous figures on the same plot. The much larger phase anomaly for the array located directly over the wall indicates that positioning the arrays directly over the wall at the Hill AFB site would have resulted in much more distinct phase anomalies resulting from the contaminated wall.

To compare results with the expanding potential array, models for the above locations were run using a Wenner array (AB = 30 m, “a” = 10 m). The modeled results for the first location with one current electrode directly above the wall (see Figure 5.9) are shown in Figure 5.13. As with the expanding potential array the contaminated model
Figure 5.9 Plan view of the two modeled electrode array locations. 1.) The center branch of the array is located directly over the clay-slurry wall. 2.) The array is offset from the wall so that only one current electrode is located directly over the wall. (Note: figure not to scale).
Figure 5.10 Comparison of resistivity and phase plots versus frequency for an expanding potential array (AB = 32 m, MN = 8 m) offset from the containment wall (see Figure 5.9) with and without a PCE-contaminated portion of the wall.
Figure 5.11  Comparison of resistivity and phase plots versus frequency for an expanding potential array (AB = 32 m, MN = 8 m) located directly over the containment wall (see Figure 5.9) with and without a PCE-contaminated portion of the wall.
Figure 5.12 Comparison of resistivity and phase plots versus frequency for an expanding potential array (AB = 32 m, MN = 8 m) located directly over the containment wall and offset from the containment wall (see Figure 5.9). Results for both the contaminated and uncontaminated wall are shown.
Figure 5.13 Comparison of resistivity and phase plots versus frequency for a Wenner array (AB = 30 m, a = 10 m) offset from the containment wall (see Figure 5.9) with and without a PCE-contaminated portion of the wall.
produced a higher phase peak and lower apparent resistivity at 0.01 Hz than the uncontaminated model. Figure 5.14 shows the results for a Wenner array located directly above the clay-slurry wall (see Figure 5.9). The results for the Wenner array and expanding potential array located directly over the clay-slurry wall are compared in Figure 5.15. The phase anomalies for the contaminated model are nearly identical, while the Wenner array produces a slightly lower phase anomaly for the uncontaminated model. The Wenner array produces a higher apparent resistivity at all frequencies for both the uncontaminated and contaminated models compared to the expanding potential array.
Figure 5.14  Comparison of resistivity and phase plots versus frequency for a Wenner array (AB = 30 m, a = 10 m) located directly over the containment wall (see Figure 5.9) with and without a PCE-contaminated portion of the wall.
Figure 5.15 Comparison of resistivity and phase plots versus frequency for a Wenner array (AB = 30 m, a = 10 m) and an expanding potential array (AB = 32 m, MN = 8 m) located directly over the containment wall (see Figure 5.9) Results are shown for an uncontaminated wall and a PCE-contaminated wall.
CHAPTER 6
DISCUSSION AND CONCLUSIONS

6.1 Discussion

In this thesis, complex resistivity laboratory data, field data, and computer modeled data have been presented. Each of the above types of data has strengths and weaknesses with respect to accurately describing the true electrical properties of the subsurface. Laboratory data collection has the advantage of a controlled setting that avoids the logistical unknowns usually found in the field. However, laboratory samples may not be measured under the same conditions (temperature, pressure, moisture content) as in situ material. In addition, laboratory samples (well cores or cuttings for example) may be mislabeled and not actually represent the targeted geologic unit.

Field data collection has the advantage of being a direct, in-situ measurement of the earth’s electrical properties. However, noise, biases, errors, and sources of interference can contaminate CR field data, thus distorting the reality of the representation of the earth’s electrical properties. Also, logistical constraints (time, weather, spatial restrictions) can limit the effectiveness of field data collection.

One of the strengths of computer modeling is the ease with which different electrode geometries can be simulated for a particular field geometry. Also, the logistical constraints and sources of noise for field data collection are not a factor in computer
modeling. However, numerical errors caused by model boundaries or a poor discretization can lead to inaccurate results. Also, to accurately model a field site, the size, extent, and electrical properties of the subsurface materials must be known. Usually laboratory data is relied upon to provide the above information. Unfortunately, one or two samples from a particular layer is not usually enough to accurately establish the electrical properties for the entire layer (i.e. simplifications must be made such as the assumption that the layer is homogeneous and isotropic). Hence, computer modeled data may not provide the best representation of a given field site.

Ultimately, field data, laboratory data, and computer-modeled data should be used in a concerted effort to produce the most likely portrayal of the true properties of the earth’s subsurface.

6.2 Conclusions

For this thesis, a finite-volume computer modeling program capable of producing frequency-dependent forward models for simple (one block) and more complex (Hill AFB example) situations has been developed. For the case history application in Chapter 5, the modeling results show that for the given conditions, locating the array directly above the contaminated wall (collinear with the strike of the wall) will produce a much larger phase anomaly than locating the electrodes only partially over the wall.

The results presented in Chapter 4 show that in relation to the line of survey, varying the x-width of a buried, conductive, polarizable block produces greater variations
in phase responses than does varying the y-width or depth extent. Varying the depth of burial of the block produced the largest range of phase responses.

The forward modeling approaches and tools described in this thesis could potentially prove quite useful in environmental applications of the complex resistivity technique. CR3D could be used prior to field data collection to determine an appropriate array type and orientation depending on the electrical properties, size, and orientation of the target and background medium. Ideally, samples of the target and host medium would be available from a potential survey site prior to field work. This would allow the materials to be characterized through laboratory measurements and would somewhat constrain the input parameters for a forward model. Given the electrical properties for a particular geologic setting, the CR3D code could be used to select the type and orientation of electrode array that would produce a maximum phase.

Although clay-organic reactions are not generally well understood, Olhoeft and King (1991) have demonstrated that laboratory data for the clay-catalyzed polymerization of toluene on montmorillonite strongly correlates with CR field data. As more clay-organic reactions become better understood, it may become possible to not only detect clay-organic reactions in the subsurface using CR, but to determine what type of clay-organic reaction is occurring. Coupled with forward (and inverse) modeling programs for field data, the CR technique could evolve from an anomaly detecting technique into a technique that could determine the type, quantity, and location of contamination. CR
would then become a very attractive technique for environmental applications where the location of quantity of contamination over time is of interest.

6.3 Recommendations For Future Work

The work described in this thesis could provide the basis for some intriguing future studies. First, the forward modeling code could be used as a platform for an inversion program. Weller et al. (1999) and Shi (1998) have both developed inversion routines for complex resistivity modeling. However, neither program is readily available and neither researcher has published work pertaining to the modeling of CR data in relation to a Cole-Cole type model. An efficient CR data inversion scheme could greatly aid in the interpretation of field data, which in turn could increase the interest and popularity of CR as a geophysical technique.

The forward modeling routine could be made applicable to a wider range of field situations if EM coupling effects were taken into account. Instead of being limited to modeling low frequency relaxations (<1.0 Hz), a wider variety of relaxation phenomena could be modeled at higher frequencies. However, accurately modeling the EM coupling for a particular field situation is not a trivial task.

The modeling code developed for this thesis could be greatly improved by adding an efficient pre-conditioner to the solution of the matrix equations. Weller et al. (1996) have shown for their forward modeling code that preconditioning can decrease computation time by a factor of 10 for grids of 100,000 nodes (vs. no pre-conditioning).
REFERENCES CITED


Kunetz, G., 1966, Principles of direct current resistivity prospecting: Geopublication


APPENDIX OUTLINE

A. Modeling code

B. Modeling program instructions and model input files for all figures

C. Field data

D. Laboratory data

E. Diagrams of CSM CR field system

   a. Complete system
   b. Isolation amplifiers
   c. Differential amplifiers
   d. Battery chargers

CD-ROM
APPENDIX A

This appendix contains the Fortran 90 source code for the necessary programs and subroutines to run forward complex resistivity models. For this thesis, the modeling code was run on a PC (Pentium II, 400 MHz, 384 MB RAM) running on a Linux Redhat 5.2 platform using a NAGWare f90 Release 2.2 compiler. The main program is listed first, followed by the necessary subroutines. The subroutines were linked to the NAGWare f90 library.

The source code is essentially the University of British Columbia-Geophysical Inversion Facility’s DC resistivity code that was graciously provided by Dr. Yaoguo Li with the consent of Dr. Doug Oldenburg. The primary modifications are several substitutions of type complex for real or double precision and the addition of a complex conjugate gradient solver.

```
* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
* program dcipf3d
* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
implicit none

integer ncur,i,j,id,ncell,idum,istat,ios
real x0,y0,elev0,dum

real,allocatable:: xa(:),ya(:),za(:),xb(:),yb(:),zb(:),
  & xm(:),ym(:),zm(:),xn(:),yn(:),zn(:)
real,allocatable:: x(:),y(:),z(:),dx(:),dy(:),dz(:)
cc real,allocatable:: cond(:)
complex(kind=2),allocatable:: cond(:),dat(:)
integer,allocatable:: la(:),lb(:),lm(:),ln(:),nobs(:),itopo(:),
  & iptype(:)
```
character*60 meshf,locf,condf,topof
data meshf,locf,condf,topof/'','','',''/
character*200 line
logical datxyz

integer mcell,ndat,mx,my,mz,
   & nnodx,nnody,nnodz,nnode,nband

common /dimen/ mcell,ndat,mx,my,mz
common /blk8/ nnodx,nnody,nnodz,nnode
common /blk9/ nband

*******************************************
*                                         *
*  open output and input files            *
*                                         *
*******************************************
c     open(*,carriagecontrol='LIST')
c     call cputimer(0,6)
c     call banner('DCIPF3D')
c     call getcl(line)
c     read(line,*),iostat=ios) meshf,locf,condf,topof
open(unit=1,file='dcipf3d.inp',status='old')
read(1,'(a)')meshf
read(1,'(a)')locf
read(1,'(a)')condf
read(1,'(a)')topof
close(unit=1)
cc      if (len_trim(line).eq.0.or.len_trim(meshf).eq.0.or.
cc     &    len_trim(locf).eq.0.or.len_trim(condf).eq.0) then
cc         print 1
cc 1       format(/' Usage: dcipf3d dc|ip fdmesh obs3d.loc',
cc     &           ' file.con|const [topo]' )
c   & stop
cc     endif
cc     if (len_trim(topof).eq.0) topof = 'null'

***********************************************************************
*                                                                     *
*  read input data                                                    *
*                                                                     *
***********************************************************************
c
call getdim(meshf,locf,ncur,ndat,mx,my,mz,datxyz)
ncell = mx*my*mz
nnodx = mx+1
nnody = my+1
nnodz = mz+1
allocate (x(nnodx),y(nnody),z(nnodz),cond(ncell),dx(mx),dy(my),
& dz(mz),itopo(mx*my), stat=istat)
if (istat.ne.0) call memerror()
call readmesh(x0,y0,elev0,dx,dy,dz,x,y,z,mx,my,mz)
allocate (xa(ncur),ya(ncur),za(ncur),xb(ncur),yb(ncur),zb(ncur),
& nobs(ncur),xm(ndat),ym(ndat),zm(ndat),xn(ndat),yn(ndat),zn(ndat),
& iptype(ncur),la(ncur),lb(ncur),lm(ndat),ln(ndat), stat=istat)
if (istat.ne.0) call memerror()
if (datxyz) then
call gettopo(itopo,mx,my,mz,mcell,topof)
call readloc(ncur,ndat,xa,ya,za,xb,yb,zb,xm,ym,zm,
& xn,yn,zn,nobs,la,lb,lm,ln,x,y,z,elev0,
& iptype,datxyz,dum,idum,idum)
else
   call readtopo(topof,x,y,z,mx,my,mz,elev0,itopo,
   & ncur,ndat,xa,ya,za,xb,yb,zb,xm,ym,zm,xn,yn,zn,nobs,
   & la,lb,lm,ln,iptype,mcell)
end if
allocate (dat(ndat), stat=istat)
if (istat.ne.0) call memerror()
call readmod(condf,mx,my,mz,cond,.false.,itopo)
call getair(itopo,mx,my,mz,cond)
print*,print*, 'Starting CR forward modelling ...
call dcfors3d(x,y,z,dx,dy,dz,la,lb,lm,ln,
& ncur,nobs,cond,itopo,dat)
call outdat(ncur,ndat,xa,ya,za,xb,yb,zb,nobs,xm,ym,zm,
& xn, yn, zn, dat, .true., iotype, 'dc3d.dat', elev0, datxyz)

print*
c call cputimer(-1,6)stopend

subroutine dcfor3d(x,y,z,dx,dy,dz,la,lb,lm,ln,
& ncur,nobs,cond,itopo,dat)

C Input:
C mx, my, mz - # of cells in x, y & z directions
C x(), y(), z() - node coordinates
C dx(), dy(), dz() - cell widths
C ncur - # of current locations
C ndat - total # of data
C la(), lb() - current electrode node #
C nobs() - # voltage measurements for each current
C lm(), ln() - voltage electrode node #
C cond() - complex conductivity
C itopo() - topography

C Output:
C dat() - forward modelled data

implicit none

integer mcell, ndat, mx, my, mz
integer nnodx, nnody, nnodz, nnode, nband

common /dimen/ mcell, ndat, mx, my, mz
common /blk8/ nnodx, nnody, nnodz, nnode
common /blk9/ nband

integer ncur, nobs(ncur), itopo(mx, my),
& la(ncur), lb(ncur), lm(ndat), ln(ndat)
real*4 x(mx+1), y(my+1), z(mz+1), dx(mx), dy(my), dz(mz)
complex(kind=2) cond(mz, my, mx)
cc real*4 dat(ndat)
cc complex(kind=2) dat(ndat)
cc pointer (pb,b)
double precision, allocatable:: b(:)

integer i, nd, icur, ia, npos(2), istat, ipercnt, ioldper
cc real*4 pot
complex(kind=2) pot
cc pointer (pxmat, xmat)
 double precision, allocatable:: xmat(:)
complex(kind=2), allocatable:: xmat(:)
c arrays for bandx3
 pointer (piam, iam), (pjam, jam), (pamat, amat),
 & (prwork, rwork), (piwork, iwork)
integers, allocatable:: iam(:), jam(:), iwork(:)
nja, lenw, leniw
double precision, allocatable:: amat(:), rwork(:)
complex(kind=2), allocatable:: amat(:), rwork(:)
logical compch
double precision amp
data amp/1.d0/
write(*,*) "i'm in dcfor3d"
write(*,*) "cond=", cond
mem = 0
nnode = nnodx*nnody*nnodz
nband = nnody*nnodz + 1
c allocate bandx3 arrays
 piam = malloc(4*(nnode+1))
pjam = malloc(4*7*nnode)
pamat = malloc(8*7*nnode)
mem = mem + 4*(1 + 8*nnode) + 4*7*nnode
allocate(iam(nnnode+1), jam(7*nnode), amat(7*nnode), stat=istat)
if (istat.ne.0) call memerror()
call setupmat(x, y, z, dx, dy, dz, cond, iam, jam, nja, amat)
c work arrays for dsiccg
 lenw = nja + 5*nnode
 leniw = nja + nnode + 11
 prwork = malloc(8*lenw)
 piwork = malloc(4*leniw)
 pb = malloc(8*nnode)
 pxmat = malloc(8*nnode)
mem = mem + 4*2*nnode
allocate(rwork(lenw), iwork(leniw), b(nnode), xmat(nnode),
 & stat=istat)
if (istat.ne.0) call memerror()
c print*, 'Memory allocated: ', real(mem)/1024., ' kb'
compch = .true.
nd = 0

print*, '% done:'
write(*,10,advance='no') 0
call flush(6)
ioldper = 0

do 1000 icur = 1, ncur
    npos(1) = la(icur)
    do ia = 1, nnode
        b(ia) = 0.d0
    end do
    b(npos(1)) = amp
    if (la(icur).ne.lb(icur)) then
        npos(2) = lb(icur)  !! dipole
        b(npos(2)) = -amp
    else
        npos(2) = 0
    end if

    write(*,'(" Starting current ...",i4)') icur
    call solvemat(b,xmat,iam,jam,amat,nja,
                 & rwork,lenw,iwork,leniw,compch)
    do i = 1, nobs(icur)
        nd=nd+1
        npos(1) = ln(nd)
        pot = xmat(npos(1))
        if (lm(nd).ne.ln(nd)) then
            npos(2) = lm(nd)
            pot = pot-xmat(npos(2))
        else
            npos(2) = 0
        end if
        dat(nd) = pot
    end do

    ipercnt = real(icur)/real(ncur) * 20.
    if (ipercnt.ne.ioldper) then
        if (ipercnt.lt.20) then
            write(*,10,advance='no') ipercnt*5
else
    print 11
end if

call flush(6)
ioldper = ipercnt
end if
10 format(i3)
11 format(' 100. ')

1000 continue

call free(pamat)
call free(pjam)
call free(piam)
call free(pxmat)
call free(pb)
call free(prwork)
call free(piwork)
deallocate(amat,jam,iam,xmat,b,rwork,iwork)

print*, 'Memory freed: ', real(mem)/1024., ' kb'
return
end

subroutine outdat(ncur,ndat,xa,ya,za,xb,yb,zb,nobs,xm,ym,zm,
&                  xn,yn,zn,dat,dcout,iptype,outf,elev0,datxyz)
implicit none

integer ncur,ndat,nobs(ncur),iptype(ncur), i,j,nd
real*4 xa(ncur),ya(ncur),za(ncur),xb(ncur),yb(ncur),zb(ncur),
&                  xm(ndat),ym(ndat),zm(ndat),xn(ndat),yn(ndat),zn(ndat),
&                  elev0
complex(kind=2) dat(ndat)
logical dcout,datxyz
character(*) outf

open(unit=1,file=outf)

if (dcout) then
    write(1,5) '! complex potential data'
    write(1,7) 0
else

write(1,5) 'IP DATA'
write(1,7) iptype(1)
end if

nd=0
do i = 1, ncur
   if (.not.dcout.and.i.gt.1.and.iptype(i).ne.iptype(i-1))
      write(1,7) iptype(i)
      if (datxyz) then
         write(1,10) ya(i),xa(i),elev0-za(i),
                        & yb(i),xb(i),elev0-zb(i), nobs(i)
      else
         write(1,15) ya(i),xa(i), yb(i),xb(i), nobs(i)
      end if
   end if
   do j = 1, nobs(i)
      nd = nd+1
      if (datxyz) then
         write(1,20) yn(nd),xn(nd),elev0-zn(nd),
                        & ym(nd),xm(nd),elev0-zm(nd), dat(nd)
      else
         write(1,25) yn(nd),xn(nd), ym(nd),xm(nd),dat(nd)
      end if
   end do
   write(1,*), ncur
end do

close(1)

5 format(a)
7 format(/'IPTYPE=',i1)
10 format(/,6f10.2,i4)
15 format(/,4f10.2,i4)
20 format(6f10.2,1p,e13.5,e13.5)
cc 21 format(e13.5,e13.5)
25 format(4f10.2,1p,e13.5,e13.5)
return
end

subroutine readmod(modf,mx,my,mz,cond,usetopo,itopo)
C If usetopo is true, cells above topography will not be stored.
implicit none
integer mx,my,mz, itopo(mx,my), ix,iy,iz,icel,k0
cc  real*4 cond(*), const
complex(kind=2) cond(*), const
character(*) modf
logical usetopo

k0 = 0
icel = 0

read(modf,*,err=100) const

C  Model is a constant halfspace
   do ix = 1, mx
      do iy = 1, my
         if (usetopo) k0 = itopo(ix,iy)
         do iz = k0+1, mz
            icel = icel+1
            cond(icel) = const
         end do
      end do
   end do
return

100 continue
C  Read the model file
   open(unit=1,file=modf,status='old',err=902)
   do ix = 1, mx
      do iy = 1, my
         if (usetopo) then
            k0 = itopo(ix,iy)
            do iz = 1, k0
               read(1,*,end=910) const  !! skip "air" cells
            end do
         end if
         do iz = k0+1, mz
            icel = icel+1
            read(1,*,end=910) cond(icel)
         end do
      end do
   end do
close(1)
cc  write(*,*:"cond=", cond(icel)
return
call filerr(modf)
print*, 'Error: Not enough elements in model file ', modf(1:len_trim(modf))
stop
end

subroutine snafu(nnode, b, x, nja, ja, ia, a, tol, itmax)
  integer itmax, nnode, nja
  integer ja(nja), ia(nnode+1)
cc      double precision r(nnode), p(nnode), q(nnode), r0, ad, an, bn,
cc     &                 alpha, beta
cc      complex(kind=2) r(nnode), p(nnode), q(nnode), r0, ad, an, bn,
&        alpha, beta, wk
cc      double precision b(nnode), rms, rnorm, tol
cc      complex(kind=2) a(nja), x(nnode)
  integer nrow, i, it, l
cc    The following code is a modified (changed from real to complex)
cc    excerpt from the "spax" subroutine to compute the product y=Ax
cc    when A is coded in Yale sparse matrix format
cc    (C) COPYRIGHT 1998 UBC-GIF ALL RIGHTS RESERVED
cc    Used with permission from Dr. Yaoguo Li
cc    entering spax
cc    write(*,*) "itmax=", itmax
cc    write(*,*) "I'm in spax"
    do i=1,nrow
      write(*,*) "I'm in the first spax call"
      wk=(0.0,0.0)
      j1=ia(i)
      j2=ia(i+1)-1
      do j=j1, j2
        jj=ja(j)
        wk=wk+a(j)*x(jj)
        write(*,*) "xjj=", x(jj)
      end do
      q(i)=wk
      write(*,*) "q=", q(i)
    end do
The following code is a modified (changed from real to complex) excerpt from the "spax" subroutine to compute the product y=Ax when A is coded in Yale sparse matrix format.

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Used with permission from Dr. Yaoguo Li
do l=1, nnode
   write(*,*) "I'm in iteration=", it
   write(*,*) "l=",  l
   x(l)=x(l)+(alpha*p(l))
   write(*,*) "x=", x(l)
   r(l)=r(l)-(alpha*q(l))
   write(*,*) "r=", r(l)
   bn=bn+(r(l)*r(l))
   rnorm=rnorm+REAL(CONJG(r(l)*r(l)))
   end do
write(*,*) "bn=", bn
write(*,*) "rnorm=", rnorm
rms=SQRT(ABS(bn/r0))
write(*,*) "rms=", rms
rnorm=SQRT(rnorm)
write(*,*) "rnorm2=", rnorm
if (rms .lt. tol) then
   goto 1000
end if
beta=bn/an
end do
write(*,*) "I'm out of the big loop"
1000 continue
write(*,*) "iterations=", it
write(*,*) "final bn=", bn
write(*,*) "final rms=", rms
RETURN
END

C
SUBROUTINE ROW3(A,M,I,L,X,Y,Z,DX,DY,DZ,COND)
C      ----------------------
cc    REAL*4 A(NBAND),COND (NNODZ-1,NNODY-1,NNODX-1), CONDXYZ
cc    COMPLEX(kind=2) A(NBAND),COND (NNODZ-1,NNODY-1,NNODX-1), &
cc    CONDXYZ
REAL*4 X(NNODX), Y(NNODY), Z(NNODZ),
& DX(NNODX-1), DY(NNODY-1), DZ(NNODZ-1)
COMPLEX(kind=2) CNTOP, CNLEFT, CNBOT, CNBACK, CNRGHT, CADD,
& CNCENT, CNFRNT
COMMON /BLK8/ NNODX, NNODY, NNODZ, NNODE
COMMON /BLK9/ NBAND

cc      write(*,*) "i'm in row3 and cond=", cond
NYZ = NNODY*NNODZ
IX  = (I-1)/NYZ + 1
IY  = (I-1-(IX-1)*NYZ)/NNODZ + 1
IZ  = I-(IX-1)*NYZ-(IY-1)*NNODZ
N   = (IX-1)*NNODY*NNODZ+(IY-1)*NNODZ+IZ

IF(IX.LT.NNODX.AND.IY.LT.NNODY.AND.IZ.LT.NNODZ)
& CONDXYZ = COND(IZ,IY,IX)
C  ERROR CONDITION - N = I
IF(N.NE.I) THEN
    PRINT*, 'Error in row3'
cc         IERR = 31
cc         CALL ERTRP3(IERR)
STOP
ENDIF

IF (IX.NE.1.AND.IX.NE.NNODX.AND.IY.NE.1.AND.IY.NE.NNODY.AND.
&   IZ.NE.1.AND.IZ.NE.NNODZ) GOTO 90

XCENTR = (X(1)+X(NNODX))*0.5
YCENTR = (Y(1)+Y(NNODY))*0.5
XTX = ABS(X(IX) - XCENTR)
YTX = ABS(Y(IY) - YCENTR)
R   = SQRT(XTX*XTX + YTX*YTX + Z(IZ)*Z(IZ))

*/////////////////////////////////////////////////////////////////////////////
*  SELECTION OF THE CORNER NODES ON IX = 1 PLANE /
*/////////////////////////////////////////////////////////////////////////////

IF(IX.EQ.1) THEN
    IF(IY.EQ.1.AND.IZ.EQ.1) THEN
        CNTOP   = (0.00,0.00)
        CNLEFT  = (0.00,0.00)
        CNFRNT  = (0.00,0.00)
        CNBOT   = -CONDXYZ*DX(IX)*DY(IY)/
                    (4.0*DZ(IZ))
        CNRGHT  = -CONDXYZ*DY(IY)*DZ(IZ)/
    ENDIF
ENDIF
\[ CNBACK = -\text{CONDXYZ} \cdot \text{DX(IX)} \cdot \text{DZ(IZ)} / (4.0 \cdot \text{DY(IY)}) \]
\[ CADD = -(\text{CNBOT} \cdot Z(IZ) \cdot \text{DZ(IZ)} + \text{CNRGHT} \cdot XTX \cdot \text{DX(IX)} + \text{CNBACK} \cdot YTX \cdot \text{DY(IY)}) / (R \cdot R) \]
\[ \text{CNCENT} = -(\text{CNTOP} + \text{CNBOT} + \text{CNLEFT} + \text{CNRGHT} + \text{CNFRNT} + \text{CNBACK}) + \text{CADD} \]
GOTO 100

ENDIF

***************************************************************
*                                                             *
*  COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES   *
*  AT THE BACK, TOP, LEFT CORNER.                             *
*                                                             *
***************************************************************

IF (IY.EQ.NNODY.AND.IZ.EQ.1) THEN
  \[ CNTOP = (0.00,0.00) \]
  \[ CNLEFT = (0.00,0.00) \]
  \[ CNBACK = (0.00,0.00) \]
  \[ CNBOT = -\text{COND}(IZ, IY-1, IX) \cdot \text{DX(IX)} \cdot \text{DY(IY-1)} / (4.0 \cdot \text{DZ(IZ)}) \]
  \[ CNRGHT = -\text{COND}(IZ, IY-1, IX) \cdot \text{DY(IY-1)} \cdot \text{DZ(IZ)} / (4.0 \cdot \text{DX(IX)}) \]
  \[ CNFRNT = -\text{COND}(IZ, IY-1, IX) \cdot \text{DX(IX)} \cdot \text{DZ(IZ)} / (4.0 \cdot \text{DY(IY-1)}) \]
  \[ CADD = -(\text{CNBOT} \cdot Z(IZ) \cdot \text{DZ(IZ)} + \text{CNRGHT} \cdot XTX \cdot \text{DX(IX)} + \text{CNFRNT} \cdot YTX \cdot \text{DY(IY-1)}) / (R \cdot R) \]
  \[ \text{CNCENT} = -(\text{CNTOP} + \text{CNBOT} + \text{CNLEFT} + \text{CNRGHT} + \text{CNFRNT} + \text{CNBACK}) + \text{CADD} \]
GOTO 100
ENDIF

***************************************************************
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATIONS FOR THE NODES  *
*   AT THE FRONT, BOTTOM, LEFT CORNER                         *
*                                                             *
***************************************************************

C

IF (IY.EQ.1.AND.IZ.EQ.NNODZ) THEN
  \[ CNTOP = -\text{COND}(IZ-1, IY, IX) \cdot \text{DX(IX)} \cdot \text{DY(IY)} / (4.0 \cdot \text{DZ(IZ-1)}) \]
  \[ CNRGHT = -\text{COND}(IZ-1, IY, IX) \cdot \text{DY(IY)} \cdot \text{DZ(IZ-1)} / (4.0 \cdot \text{DX(IX)}) \]
  \[ CNFRNT = -\text{COND}(IZ-1, IY, IX) \cdot \text{DX(IX)} \cdot \text{DZ(IZ-1)} / (4.0 \cdot \text{DY(IY)}) \]
  \[ CADD = -(\text{CNTOP} \cdot Z(IZ) \cdot \text{DZ(IZ-1)} + \text{CNRGHT} \cdot XTX \cdot \text{DX(IX)} + \text{CNFRNT} \cdot YTX \cdot \text{DY(IY)}) / (R \cdot R) \]
  \[ \text{CNCENT} = -(\text{CNTOP} + \text{CNBOT} + \text{CNLEFT} + \text{CNRGHT} + \text{CNFRNT} + \text{CNBACK}) + \text{CADD} \]
GOTO 100
C
**COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES AT THE BACK, BOTTOM, LEFT CORNER**

```
C
IF (IY.EQ.NNODY.AND.IZ.EQ.NNODZ) THEN
  CNBOT   = (0.00,0.00)
  CNLEFT  = (0.00,0.00)
  CNBACK  = (0.00,0.00)
  CNTOP   = -COND(IZ-1,IY-1,IX)*DX(IX)*DY(IY-1)/
            (4.0*DZ(IZ-1))
  CNRGHT = -COND(IZ-1,IY-1,IX)*DY(IY-1)*DZ(IZ-1)/
            (4.0*DX(IX))
  CNFRNT = -COND(IZ-1,IY-1,IX)*DX(IX)*DZ(IZ-1)/
            (4.0*DY(IY-1))
  CADD    = -(CNTOP*Z(IZ)*DZ(IZ-1)+CNRGHT*XTX*DX(IX)
            +CNFRNT*YTX*DY(IY-1))/(R*R)
  CNCENT  = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT
            +CNBACK)+CADD
GOTO 100
ENDIF
C
ENDIF

C
**COEFFICIENTS FOR THE SELF ADJOINT EQUATIONS FOR THE NODES ON THE TOP LEFT EDGE.**

```

```
C
IF (IZ.EQ.1) THEN
  CNTOP   = (0.00,0.00)
  CNLEFT  = (0.00,0.00)
  CNBOT   = -(CONDXYZ*DX(IX)*DY(IY)
              +COND(IZ,IY-1,IX)*DX(IX)*DY(IY-1))/(4.0*DZ(IZ))
  CNRGHT = -(COND(IZ,IY-1,IX)*DY(IY-1)*DZ(IZ)
              +CONDXYZ*DY(IY)*DZ(IZ))/(4.0*DX(IX))
  CNFRNT = -COND(IZ,IY-1,IX)*DX(IX)*DZ(IZ)/(4.0*DY(IY))
  CADD    = -(CNBOT*Z(IZ)*DZ(IZ)+CNRGHT*XTX*DX(IX))
            /(R*R)
  CNCENT  = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT
            +CNBACK)+CADD
GOTO 100
ENDIF
C
```
& +CNBACK)+CADD
GOTO 100
ENDIF
C
********************************************************************
*                                                                  *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATIONS FOR THE NODES ON    *
*   THE BOTTOM,LEFT EDGE.                                           *
*                                                                  *
********************************************************************
C
IF(IZ.EQ.NNODZ) THEN
  CNBOT   = (0.00,0.00)
  CNLEFT  = (0.00,0.00)
  CNTOP   = -(COND(IZ-1,IY,IX)*DX(IX)*DY(IY)
  &    +COND(IZ-1,IY-1,IX)*DX(IX)*DY(IY-1))/
  &    (4.0*DZ(IZ-1))
  CNRGHT = -(COND(IZ-1,IY-1,IX)*DY(IY-1)*DZ(IZ-1)
  &    +COND(IZ-1,IY,IX)*DY(IY)*DZ(IZ-1))/
  &    (4.0*DX(IX))
  CNFRNT = -COND(IZ-1,IY-1,IX)*DX(IX)*DZ(IZ-1)/
  &    (4.0*DY(IY-1))
  &
  CNBACK  = -COND(IZ-1,IY,IX)*DX(IX)*DZ(IZ-1)/
  &    (4.0*DY(IY))
  &
  CADD    = -(CNRGHT*XTX*DX(IX)+CNBACK*YTX*DY(IY))/
  &    (R*R)
  &
  CNCENT  = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT
  &    +CNBACK)+CADD
GOTO 100
ENDIF
C
********************************************************************
*                                                                  *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATIONS FOR THE NODES ON    *
*   THE FRONT,LEFT EDGE.                                           *
*                                                                  *
********************************************************************
C
IF(IY.EQ.1) THEN
  CNLEFT  = (0.00,0.00)
  CNFRNT  = (0.00,0.00)
  CNTOP   = -COND(IZ-1,IY,IX)*DX(IX)*DY(IY)/
  &    (4.0*DZ(IZ-1))
  &
  CNBOT   = -CONDXYZ*DX(IX)*DY(IY)/
  &    (4.0*DZ(IZ))
  CNRGHT = -(COND(IZ-1,IY,IX)*DY(IY)*DZ(IZ-1)
  &    +CONDXYZ*DY(IY)*DZ(IZ))/(4.0*DX(IX))
  &
  CNBACK  = -(COND(IZ-1,IY,IX)*DX(IX)*DZ(IZ-1)
  &    +CONDXYZ*DX(IX)*DZ(IZ))/(4.0*DY(IY))
  &
  CADD    = -(CNRGHT*XTX*DX(IX)+CNBACK*YTX*DY(IY))/
  &    (R*R)
  &
  CNCENT  = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT
  &    +CNBACK)+CADD
(R*R)
  
  \[
  \text{CNCENT} = - \left( \text{CNTOP} + \text{CNBOT} + \text{CNLEFT} + \text{CNRGHT} + \text{CNFRNT} \right) + \text{CADD}
  \]
  
GOTO 100
ENDIF

*******************************************************************
*                                                                 *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATIONS FOR THE NODES ON   *
*   THE BACK LEFT EDGE.                                            *
*                                                                 *
*******************************************************************
C
IF(IY.EQ.NNODY) THEN
  
  CNLEFT  = (0.00,0.00)
  CNBACK  = (0.00,0.00)
  CNTOP   = \(-\text{COND}(IZ-1,IY-1,IX)*DX(IX)*DY(IY-1)/\)
            \((4.0*\text{DZ}(IZ-1))\)
  &
  CNBOT   = \(-\text{COND}(IZ,IY-1,IX)*DX(IX)*DY(IY-1)/\)
            \((4.0*\text{DZ}(IZ))\)
  &
  CNRIGH = \(-\text{COND}(IZ-1,IY-1,IX)*DY(IY-1)*DZ(IZ-1)\)
            \(+\text{COND}(IZ,IY-1,IX)*DY(IY-1)*DZ(IZ))/\)
            \((4.0*DX(\text{IX}))\)
  &
  CNFRNT = \(-\text{COND}(IZ-1,IY-1,IX)*DX(\text{IX})*DZ(IZ-1)\)
            \(+\text{COND}(IZ,IY-1,IX)*DX(\text{IX})*DZ(IZ))/\)
            \((4.0*DY(IY-1))\)
  &
  CADD    = \(-\text{CNRGHT}*\text{XTX}*DX(\text{IX})+\text{CNFRNT}*\text{YTX}*DY(IY-1))/\)
            \((R*R)\)
  &
  CNCENT  = \(-\left(\text{CNTOP} + \text{CNBOT} + \text{CNLEFT} + \text{CNRGHT} + \text{CNFRNT} \right) + \text{CADD}\)
  GOTO 100
ENDIF

*******************************************************************
*                                                                 *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATIONS FOR THE NODES ON   *
*   THE BACK LEFT EDGE.                                            *
*                                                                 *
*******************************************************************
C
IF(IY.EQ.NNODY) THEN
  
  CNLEFT  = (0.00,0.00)
  CNBACK  = (0.00,0.00)
  CNTOP   = \(-\text{COND}(IZ-1,IY-1,IX)*DX(IX)*DY(IY-1)/\)
            \((4.0*\text{DZ}(IZ-1))\)
  &
  CNBOT   = \(-\text{COND}(IZ,IY-1,IX)*DX(IX)*DY(IY-1)/\)
            \((4.0*\text{DZ}(IZ))\)
  &
  CNRIGH = \(-\text{COND}(IZ-1,IY-1,IX)*DY(IY-1)*DZ(IZ-1)\)
            \(+\text{COND}(IZ-1,IY,IX)*DY(IY)*DZ(IZ-1)\)
            \(+\text{COND}(IZ,IY-1,IX)*DY(IY-1)*DZ(IZ)\)
            \(+\text{CONDXYZ})*\)
            \(DY(IY)*DZ(IZ))/\)
            \((4.0*DX(\text{IX}))\)
  &
  CNFRNT = \(-\text{COND}(IZ-1,IY-1,IX)*DX(\text{IX})*DZ(IZ-1)\)
            \(+\text{COND}(IZ,IY-1,IX)*DX(\text{IX})*DZ(IZ))/\)
            \((4.0*DY(IY-1))\)
  &
  CADD    = \(-\text{CNRGHT}*\text{XTX}*DX(\text{IX})+\text{CNFRNT}*\text{YTX}*DY(IY-1))/\)
            \((R*R)\)
  &
  CNCENT  = \(-\left(\text{CNTOP} + \text{CNBOT} + \text{CNLEFT} + \text{CNRGHT} + \text{CNFRNT} \right) + \text{CADD}\)
  GOTO 100
ENDIF
CNBACK = -(COND(IZ-1,IY,IX)*DX(IX)*DZ(IZ-1) + CONDXYZ*DX(IX)*DZ(IZ))/(4.0*DY(IY))
CADD = -CNRGHT*XTX*DX(IX)/(R*R)
CNCENT = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT + CNBACK) + CADD
GOTO 100
ENDIF
C
*-------------------------------------------------------------------------*
*   SELECTION OF THE CORNER NODES ON IX = NNODX PLANE                    *
*-------------------------------------------------------------------------*
C
IF(IX.EQ.NNODX) THEN
C
*********************************************************************
*                                                                     *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES AT THE    *
*   FRONT,TOP,RIGHT CORNER.                                           *
*                                                                     *
*********************************************************************
C
IF(IY.EQ.1.AND.IZ.EQ.1) THEN
CNTOP = (0.00,0.00)
CNRGHT = (0.00,0.00)
CNFRNT = (0.00,0.00)
CNBOT = -COND(IZ,IY,IX-1)*DX(IX-1)*DY(IY)/(4.0*DZ(IZ))
&
CNLEFT = -COND(IZ,IY,IX-1)*DY(IY)*DZ(IZ)/(4.0*DX(IX-1))
&
CNBACK = -COND(IZ,IY,IX-1)*DX(IX-1)*DZ(IZ)/(4.0*DY(IY))
&
CADD = -(CNBOT*Z(IZ)*DZ(IZ)+CNLEFT*XTX*DX(IX-1)+CNBACK*YTX*DY(IY))/(R*R)
&
CNCENT = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT + CNBACK) + CADD
GOTO 100
ENDIF
C
*******************************************************************
*                                                                 *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES AT       *
*   THE BACK,TOP,RIGHT CORNER.                                       *
*                                                                 *
*******************************************************************
C
IF(IY.EQ.NNODY.AND.IZ.EQ.1) THEN
CNTOP = (0.00,0.00)
CNRGHT = (0.00,0.00)
CNBACK = (0.00,0.00)
CNBOT = -COND(IZ,IY-1,IX-1)*DX(IX-1)*DY(IY-1)/
       (4.0*DZ(IZ))
&
CNLEFT = -COND(IZ,IY-1,IX-1)*DY(IY-1)*DZ(IZ)/
       (4.0*DX(IX-1))
&
CNFRNT = -COND(IZ,IY-1,IX-1)*DX(IX-1)*DZ(IZ)/
       (4.0*DY(IY-1))
&
CADD = -(CNBOT*Z(IZ)*DZ(IZ)+CNLEFT*XTX*DX(IX-1)
       +CNFRNT*YTX*DY(IY-1))/(R*R)
&
CNCENT = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT
       +CNBACK)+CADD
GOTO 100
ENDIF
C
*********************************************************************
*                                                                   *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES AT THE *
*   FRONT,BOTTOM,RIGHT CORNER.                                      *
*                                                                   *
*********************************************************************
C
IF(IY.EQ.1.AND.IZ.EQ.NNODZ) THEN
CNBOT = (0.00,0.00)
CNRGHT = (0.00,0.00)
CNFRNT = (0.00,0.00)
CNTOP = -COND(IZ-1,IY,IX-1)*DX(IX-1)*DY(IY)/
       (4.0*DZ(IZ-1))
&
CNLEFT = -COND(IZ-1,IY,IX-1)*DY(IY)*DZ(IZ-1)/
       (4.0*DX(IX-1))
&
CNBACK = -COND(IZ-1,IY,IX-1)*DX(IX-1)*DZ(IZ-1)/
       (4.0*DY(IY))
&
CADD = -(CNTOP*Z(IZ)*DZ(IZ-1)+CNLEFT*XTX*DX(IX-1)
       +CNFRNT*YTX*DY(IY-1))/(R*R)
&
CNCENT = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT
       +CNBACK)+CADD
GOTO 100
ENDIF
C
*********************************************************************
*                                                                   *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATIONS FOR THE NODES AT     *
*   THE BACK,BOTTOM,RIGHT CORNER.                                  *
*                                                                   *
*********************************************************************
C
IF(IY.EQ.NNODY.AND.IZ.EQ.NNODZ) THEN
CNBOT = (0.00,0.00)
CNRGHT = (0.00,0.00)
CNFRNT = (0.00,0.00)
CNTOP = -COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DY(IY-1)/
       (4.0*DZ(IZ-1))
&
CNLEFT = -COND(IZ-1,IY-1,IX-1)*DY(IY-1)*DZ(IZ-1)/
       (4.0*DX(IX-1))
&
CNBACK = -COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DZ(IZ-1)/
       (4.0*DY(IY-1))
&
CADD = -(CNTOP*Z(IZ)*DZ(IZ-1)+CNLEFT*XTX*DX(IX-1)
       +CNFRNT*YTX*DY(IY-1))/(R*R)
&
CNCENT = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT
       +CNBACK)+CADD
GOTO 100
ENDIF
C
*********************************************************************
*                                                                   *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATIONS FOR THE NODES AT     *
*   THE BACK,BOTTOM,RIGHT CORNER.                                  *
*                                                                   *
*********************************************************************
C
IF(IY.EQ.NNODY.AND.IZ.EQ.NNODZ) THEN
CNBOT = (0.00,0.00)
CNRGHT = (0.00,0.00)
CNFRNT = (0.00,0.00)
CNTOP = -COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DY(IY-1)/
& CNLEFT = -COND(IZ-1,IY-1,IX-1)*DY(IY-1)*DZ(IZ-1)/
& (4.0*DX(IX-1))
& CNFRNT = -COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DZ(IZ-1)/
& (4.0*DY(IY-1))
& CADD = -(CNTOP*Z(IZ)*DZ(IZ-1)+CNLEFT*XTX*DX(IX-1)
& +CNFRNT*YTX*DY(IY-1))/(R*R)
& CNCENT = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT
& +CNBACK)+CADD
GOTO 100
ENDIF
C
C
C********************************************************************
*                                                                  *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES ON THE*
*   TOP,RIGHT EDGE.                                                *
*                                                                  *
********************************************************************
C
IF(IZ.EQ.1) THEN
  CNTOP   = (0.00,0.00)
  CNRGHT  = (0.00,0.00)
  CNBOT   = -(COND(IZ,IY,IX-1)*DX(IX-1)*DY(IY)
& +COND(IZ,IY-1,IX-1)*DX(IX-1)*DY(IY-1))/(4.0*DZ(IZ))
  CNLEFT  = -(COND(IZ,IY-1,IX-1)*DY(IY-1)*DZ(IZ)
& +COND(IZ,IY,IX-1)*DY(IY)*DZ(IZ))/(4.0*DX(IX-1))
  CNFRNT  = -COND(IZ,IY-1,IX-1)*DX(IX-1)*DZ(IZ)
& (4.0*DY(IY-1))
  CNBACK  = -COND(IZ,IY,IX-1)*DX(IX-1)*DZ(IZ)/(4.0*DY(IY))
  CADD    = -(CNBOT*Z(IZ)*DZ(IZ)+CNLEFT*XTX*DX(IX-1))
& +CNFRNT/(R*R)
  CNCENT = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT
& +CNBACK)+CADD
GOTO 100
ENDIF
C
C*******************************************************************
*                                                                 *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES ON THE*
*   THE BOTTOM,RIGHT EDGE.                                        *
*                                                                 *
*******************************************************************
C
IF(IZ.EQ.NNODZ) THEN
  CNBOT   = (0.00,0.00)
  CNRGHT  = (0.00,0.00)
  CADD    = -(CNBOT*Z(IZ)*DZ(IZ)+CNLEFT*XTX*DX(IX-1))
& +CNFRNT/(R*R)
  CNCENT = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT
& +CNBACK)+CADD
GOTO 100
ENDIF
C
**********************************************************************
*                                                                  *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES ON THE *
*   THE BOTTOM,RIGHT EDGE.                                        *
*                                                                  *
**********************************************************************
C
IF(IZ.EQ.NNODZ) THEN
  CNBOT   = (0.00,0.00)
  CNRGHT  = (0.00,0.00)
CNFRNT = -COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DZ(IZ-1)/
        (4.0*DZ(IZ-1))
&
CNBACK  = -COND(IZ-1,IY,IX-1)*DX(IX-1)*DZ(IZ-1)/
        (4.0*DZ(IZ))
&
CADD    = -(CNTOP*Z(I)*DZ(IZ-1)+CNLEFT*XTX*DX(IX-1))/
        (R*R)
&
CNCENT  = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT
        +CNBACK)+CADD
GOTO 100
ENDIF
C
******************************************************************
**                                                                 **
**   COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODE ON    **
**   THE FRONT,RIGHT EDGE.                                         **
**                                                                 **
******************************************************************
C
IF(IY.EQ.1) THEN
  CNRGHT = (0.00,0.00)
  CNFRNT = (0.00,0.00)
  CNTOP   = -COND(IZ-1,IY,IX-1)*DX(IX-1)*DY(IY)/
        (4.0*DZ(IZ-1))
&
  CNBOT   = -COND(IZ,IY,IX-1)*DX(IX-1)*DY(IY)/
        (4.0*DZ(IZ))
&
  CNLEFT  = -(COND(IZ-1,IY,IX-1)*DY(IY)*DZ(IZ-1)
        +COND(IZ,IY,IX-1)*DY(IY)*DZ(IZ))/(4.0*DX(IX-1))
&
  CNBACK  = -(COND(IZ-1,IY,IX-1)*DX(IX-1)
        *DZ(IZ-1)+COND(IZ,IY,IX-1)*DX(IX-1)*DZ(IZ))/
        (4.0*DY(I))
&
  CADD    = -(CNLEFT*XTX*DX(IX-1)+CNBACK*YTX*DY(I))/
        (R*R)
&
  CNCENT  = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT
        +CNBACK)+CADD
GOTO 100
ENDIF
C
*********************************************************************
**                                                                   **
**   COEFFICIENTS FOR THE SELF ADJOINT EQUATIONS FOR THE NODES ON    **
**   THE BACK,RIGHT EDGE.                                            **
**                                                                   **
*********************************************************************
C
IF(IY.EQ.NNODY) THEN
CNRGHT = (0.00,0.00)
CNBACK = (0.00,0.00)
CNTOP = -COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DY(IY-1)/(4.0*DZ(IZ-1))
& CNBOT = -COND(IZ,IY-1,IX-1)*DX(IX-1)*DY(IY-1)/(4.0*DZ(IZ))
& CNLEFT = -(COND(IZ-1,IY-1,IX-1)*DY(IY-1)*DZ(IZ-1)+COND(IZ,IY-1,IX-1)*DY(IY-1)*DZ(IZ))/(4.0*DX(IX-1))
& CNFRNT = -(COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DZ(IZ-1)+COND(IZ,IY-1,IX-1)*DX(IX-1)*DZ(IZ))/(4.0*DY(IY-1))
CADD = -(CNLEFT*XTX*DX(IX-1)+CNFRNT*YTX*DY(IY-1))/(R*R)
& CNCIENT = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT+CNBACK)+CADD
GOTO 100
ENDIF
C
*********************************************************************
*                                                                     *
*     COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES ON     *
*     THE RIGHT FACE.                                                 *
*                                                                     *
*********************************************************************
C
CNTOP = -COND(IZ-1,IY,IX-1)*DX(IX-1)*DY(IY)
&   +COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DY(IY-1)/(4.0*DZ(IZ-1))
& CNBOT = -COND(IZ,IY,IX-1)*DX(IX-1)*DY(IY)
&   +COND(IZ,IY-1,IX-1)*DX(IX-1)*DY(IY-1)/(4.0*DZ(IZ))
& CNLEFT = -(COND(IZ-1,IY-1,IX-1)*DY(IY-1)*DZ(IZ-1)+COND(IZ,IY-1,IX-1)*DY(IY-1)*DZ(IZ))
&   +COND(IZ-1,IY,IX-1)*DY(IY)*DZ(IZ-1)
&   +COND(IZ,IY-1,IX-1)*DY(IY-1)*DZ(IZ)+COND(IZ,IY,IX-1)*DY(IY)*DZ(IZ))/(4.0*DX(IX-1))
& CNFRNT = 0.00,0.00)
& CNFRNT = -(COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DZ(IZ-1)
&   +COND(IZ,IY-1,IX-1)*DX(IX-1)*DZ(IZ))/(4.0*DY(IY-1))
& CNBACK = -(COND(IZ-1,IY,IX-1)*DX(IX-1)*DZ(IZ-1)
&   +COND(IZ,IY,IX-1)*DX(IX-1)*DZ(IZ))/(4.0*DY(IY))
CADD = -CNLEFT*XTX*DX(IX-1)/(R*R)
& CNCIENT = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT+CNBACK)+CADD
GOTO 100
ENDIF
C
**//////////////////////////////////////////////////////////////////////////////////////////
* SELECTION OF THE EDGES ON IY = 1 PLANE /
* //**************************************************************************************
C IF(IY.EQ.1) THEN
C
**********************************************************************************************************************************************
* COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES ON THE TOP,FRONT EDGE. 
**********************************************************************************************************************************************
C IF(IZ.EQ.1) THEN
  CNTOP   = (0.00,0.00)
  CNFRNT = (0.00,0.00)
  CNBOT   = -(COND(IZ,IY,IX-1)*DX(IX-1)*DY(IY)
&                  +CONDXYZ*DX(IX)*DY(IY))/(4.0*DZ(IZ))
  CNLEFT  = -COND(IZ,IY,IX-1)*DY(IY)*DZ(IZ)/
&                  (4.0*DX(IX-1))
  CNRght = -CONDXYZ*DY(IY)*DZ(IZ)/(4.0*DX(IX))
  CNBACK  = -(CONDXYZ*DX(IX)*DZ(IZ)
&                  +COND(IZ,IY,IX-1)*DX(IX-1)
&                  *DZ(IZ))/(4.0*DY(IY))
  CADD    = -(CNBOT*Z(IZ)*DZ(IZ)+CNBACK*YTX*DY(IY))/
&                  (R*R)
  CNCENT  = -(CNTOP+CNBOT+CNLEFT+CNRght+CNFRNT
&                  +CNBACK)+CADD
  GOTO 100
ENDIF
C
**********************************************************************************************************************************************
* COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES ON THE FRONT,BOTTOM EDGE. 
**********************************************************************************************************************************************
C IF(IZ.EQ.NNODZ) THEN
  CNBOT   = (0.00,0.00)
  CNFRNT = (0.00,0.00)
  CNTOP   = -(COND(Iz-1,IY,IX-1)*DX(IX-1)*DY(IY)
&                  +COND(IZ-1,IY,IX)*DX(IX)
&                  *DY(IY))/(4.0*DZ(IZ-1))
  CNLEFT  = -COND(IZ-1,IY,IX-1)*DY(IY)*DZ(IZ-1)/
&                  (4.0*DX(IX-1))
  CNRght = -COND(IZ-1,IY,IX)*DY(IY)*DZ(IZ-1)/(4.0*DX(IX))
CNBACK = -(COND(IZ-1,IY,IX-1)*DX(IX-1)*DZ(IZ-1) & DX(IX)*DZ(IZ-1)) / (4.0*DY(IY)) & CADD = -(CNTOP*Z(IZ)*DZ(IZ-1)+CNBACK*YTX*DY(IY)) / (R*R) & CNCENT = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT & +CNBACK)+CADD
GOTO 100
ENDIF
C
C**********************************************************************
*                                                                    *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES ON      *
*   THE FRONT FACE.                                                  *
**********************************************************************
C
CNTOP  = -(COND(IZ-1,IY,IX-1)*DX(IX-1)*DY(IY) & +COND(IZ-1,IY,IX)*DX(IX) & *DY(IY))/(4.0*DZ(IZ-1)) & CNBOT  = -(COND(IZ,IY,IX-1)*DX(IX-1)*DY(IY) & +CONDXYZ*DX(IX) & *DY(IY))/(4.0*DZ(IZ)) & CNLEFT = -(COND(IZ-1,IY,IX)*DY(IY) & *DZ(IZ-1)+COND(IZ,IY,IX-1)*DY(IY) )/ (4.0*DX(IX-1)) & CNRght = -(COND(IZ-1,IY,IX)*DY(IY) & *DZ(IZ-1)+CONDXYZ*DY(IY) & )/ (4.0*DX(IX)) & CNFRNT = (0.00,0.00) & CNBACK = -(COND(IZ-1,IY,IX-1)*DX(IX-1)*DZ(IZ-1) & +COND(IZ-1,IY,IX)* & DX(IX)*DZ(IZ-1)+COND(IZ,IY,IX-1)*DX(IX-1) & *DZ(IZ)+CONDXYZ* & DX(IX)*DZ(IZ))/(4.0*DY(IY)) & CADD  = -CNBACK*YTX*DY(IY)/(R*R) & CNCENT  = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT & +CNBACK)+CADD
GOTO 100
ENDIF
C
C**********************************************************************
*                                                                    *
*   SELECTION OF THE EDGES ON IY = NNODY PLANE                      *
*                                                                    *
**********************************************************************
C
IF(IY.EQ.NNODY) THEN
C
ENDIF
* COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES ON *
* THE TOP, BACK EDGE.                                       *
******************************************************************
C
IF(IZ.EQ.1) THEN
    CNTOP   = (0.00,0.00)
    CNBACK  = (0.00,0.00)
    CNBOT   = -(COND(IZ,IY-1,IX-1)*DX(IX-1)*DY(IY-1)
            &       +COND(IZ,IY-1,IX)*
            &       DX(IX)*DY(IY-1))/(4.0*DZ(IZ))
    CNFRNT  = -(COND(IZ,IY-1,IX-1)*DX(IX-1)*DZ(IZ)
            &       +COND(IZ,IY-1,IX)*
            &       DX(IX)*DZ(IZ))/(4.0*DY(IY-1))
    CNLEFT  = -COND(IZ,IY-1,IX-1)*DY(IY-1)*DZ(IZ)/
            &       (4.0*DX(IX-1))
    CNRHT   = -COND(IZ,IY-1,IX)*DY(IY-1)*DZ(IZ)/
            &       (4.0*DX(IX))
    CADD    = -(CNBOT*Z(IZ)*DZ(IZ)+CNFRNT*YTX*DY(IY-1))/
            &       (R*R)
    CNCENT  = -(CNTOP+CNBOT+CNLEFT+CNRHT+CNFRNT
            &       +CNBACK)+CADD
GOTO 100
ENDIF
C
*********************************************************************
*                                                                   *
*   COEFFICIENTS FOR THE SELG ADJOINT EQUATIONS FOR THE NODES ON    *
*   THE BOTTOM, BACK EDGE.                                           *
*********************************************************************
C
IF(IZ.EQ.NNODZ) THEN
    CNBOT   = (0.00,0.00)
    CNBACK  = (0.00,0.00)
    CNTOP   = -(COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DY(IY-1)
            &       +COND(IZ-1,IY-1,IX)*
            &       DX(IX)*DY(IY-1))/(4.0*DZ(IZ-1))
    CNFRNT  = -(COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DZ(IZ)
            &       +COND(IZ-1,IY-1,IX)*
            &       DX(IX)*DZ(IZ))/(4.0*DY(IY-1))
    CNLEFT  = -COND(IZ-1,IY-1,IX-1)*DY(IY-1)*DZ(IZ)/
            &       (4.0*DX(IX-1))
    CNRHT   = -COND(IZ-1,IY-1,IX)*DY(IY-1)*DZ(IZ)/
            &       (4.0*DX(IX))
    CADD    = -(CNBOT*Z(IZ)*DZ(IZ-1)+CNFRNT*YTX*DY(IY-1))/
            &       (R*R)
    CNCENT  = -(CNTOP+CNBOT+CNLEFT+CNRHT+CNFRNT
            &       +CNBACK)+CADD
GOTO 100
ENDIF
C
*********************************************************************
GOTO 100

ENDIF

C

**********************************************************************
*                                                                    *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES ON      *
*   THE BACK FACE.                                                   *
*                                                                    *
**********************************************************************

C

CNTOP   = -(COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DY(IY-1)
&             +COND(IZ-1,IY-1,IX)*
&             *DX(IX)*DY(IY-1))/(4.0*DZ(IZ-1))
CNBOT   = -(COND(IZ,IY-1,IX-1)*DX(IX-1)*DY(IY-1)
&             +COND(IZ,IY-1,IX)*
&             DX(IX)*DY(IY-1))/(4.0*DZ(IZ))
CNLEFT  = -(COND(IZ-1,IY-1,IX-1)*DY(IY-1)*DZ(IZ-1)
&             +COND(IZ,IY-1,IX-1)
&             *DY(IY-1)*DZ(IZ))/(4.0*DX(IX-1))
CNRGHT  = -(COND(IZ-1,IY-1,IX)*DY(IY-1)*DZ(IZ-1)
&             +COND(IZ,IY-1,IX)
&             *DY(IY-1)*DZ(IZ))/(4.0*DX(IX))
CNFRNT  = -(COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DZ(IZ-1)
&             +COND(IZ,IY-1,IX)
&             )*DX(IX)*DZ(IZ-1)+COND(IZ,IY-1,IX-1)*DX(IX-1)
&             *DZ(IZ)+COND(IZ,IY-1,
&             IX)*DX(IX)*DZ(IZ))/(4.0*DY(IY-1))
CNBACK  = (0.00,0.00)
CADD    = -CNFRNT*YTX*DY(IY-1)/(R*R)
CNCENT  = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT
&             +CNBACK)+CADD
GOTO 100

ENDIF

C

**********************************************************************
*                                                                    *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES ON      *
*   THE TOP FACE.                                                   *
*                                                                    *
**********************************************************************

C

IF(IZ.EQ.1) THEN
CNTOP   = (0.00,0.00)
CNBOT   = -(COND(IY-1,IX-1)*DX(IX-1)*DY(IY)
&             +CONDXYZ*DX(IY)*
&             *DY(IY)+COND(IY-1,IX-1)*DX(IX-1)*DY(IY-1)
&             +COND(IY,IY-1,IX)*DX(IX
&             )*DY(IY-1))/(4.0*DZ(IY))
CNLEFT  = -(COND(IY-1,IX-1)*DY(IY-1)*DZ(IY-1)
&             +COND(IY,IY-1,IX-1)
&             )*DY(IY-1)*DZ(IY))/(4.0*DX(IX))
CNRGHT  = -(COND(IY-1,IX)*DY(IY-1)*DZ(IY-1)
&             +COND(IY,IY-1,IX)
&             *DY(IY-1)*DZ(IY))/(4.0*DX(IX))
CNFRNT  = -(COND(IY-1,IX-1)*DX(IX-1)*DZ(IY-1)
&             +COND(IY-1,IX)
&             )*DX(IX)*DZ(IZ-1)+COND(IY-1,IX-1)*DX(IX-1)
&             *DZ(IZ)+COND(IY,IX-1,
&             IX)*DX(IY)*DZ(IZ))/(4.0*DY(IY))
CNBACK  = (0.00,0.00)
CADD    = -CNFRNT*YTX*DY(IY-1)/(R*R)
CNCENT  = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT
&             +CNBACK)+CADD
ENDIF
\begin{verbatim}
& )*DZ(I2)/(4.0*DX(IX-1))
CNRGHT = -(COND(IZ,IY-1,IX)*DY(IY-1)*DZ(I2)
& +CONDXYZ*DY(IY)
& )*DZ(I2))/(4.0*DX(IX))
CNFRNT = -(COND(IZ,IY-1,IX-1)*DX(IX-1)*DZ(I2)
& +COND(IZ,IY-1,IX)*
& DX(IX)*DZ(I2)))/(4.0*DY(IY-1))
CNBACK = -(COND(IZ,IY,IX-1)*DX(IX-1)*DZ(I2)
& +CONDXYZ*DX(IX)
& *DZ(I2))/(4.0*DY(IY))
CNCENT = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT+CNBACK)
GOTO 100
ENDIF
C
C
**********************************************************************
*                                                                    *
*   COEFFICIENTS FOR THE SELF ADJOINT EQUATION FOR THE NODES ON       *
*   THE BOTTOM FACE.                                                 *
*                                                                    *
**********************************************************************
C
IF(IZ.EQ.NNODZ) THEN
  CNTOP   = -(COND(IZ-1,IY,IX-1)*DX(IX-1)*DY(IY)
  & +COND(IZ-1,IY,IX)*DX(IX)
  & *DY(IY)+COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DY(IY-1)
  & +COND(IZ-1,IY-1,IX)*
  & DX(IX)*DY(IY-1))/(4.0*DZ(IZ-1))
CNRGHT = -(COND(IZ-1,IY-1,IX)*DY(IY-1)*DZ(IZ-1)
  & +COND(IZ-1,IY-1,IX)*
  & *DZ(IZ-1))/(4.0*DX(IX-1))
CNFRNT = -(COND(IZ-1,IY-1,IX)*DY(IY-1)*DZ(IZ-1)
  & +COND(IZ-1,IY-1,IX)*
  & *DX(IX)))/(4.0*DX(IX))
CNBACK = -(COND(IZ-1,IY,IX-1)*DX(IX-1)*DZ(IZ-1)
  & +COND(IZ-1,IY,IX)*
  & DX(IX)*DZ(IZ-1))/(4.0*DY(IY))
CADD = -CNTOP*Z(IZ)*DZ(IZ-1)/(R*R)
CNCENT = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT+CNBACK)+CADD
GOTO 100
ENDIF
C
C
**********************************************************************
*                                                                    *
*   COEFFICIENTS OF THE SELF ADJOINT EQUATION FOR THE NODES AT       *
*                                                                    *
**********************************************************************
C
IF(I.EQ.NNODZ) THEN
  CNTOP = -(COND(I-1,IY,IX-1)*DX(IX-1)*DY(IY)
  & +COND(I-1,IY,IX)*DX(IX)
  & *DY(IY)+COND(I-1,IY-1,IX-1)*DX(IX-1)*DY(IY-1)
  & +COND(I-1,IY-1,IX)*
  & DX(IX)*DY(IY-1))/(4.0*DZ(I-1))
CNFRNT = -(COND(I-1,IY-1,IX)*DY(IY-1)*DZ(I-1)
  & +COND(I-1,IY-1,IX)*
  & *DZ(I-1))/(4.0*DX(I-1))
CNBACK = -(COND(I-1,IY,IX-1)*DX(IX-1)*DZ(I-1)
  & +COND(I-1,IY,IX)*
  & DX(IX)*DZ(I-1))/(4.0*DY(IY))
CADD = -CNTOP*Z(I)*DZ(I-1)/(R*R)
CNCENT = -(CNTOP+CNBOT+CNLEFT+CNRGHT+CNFRNT+CNBACK)+CADD
GOTO 100
ENDIF
C
C
**********************************************************************
*                                                                    *
*   COEFFICIENTS OF THE SELF ADJOINT EQUATION FOR THE NODES AT       *
*                                                                    *
**********************************************************************
C
ENDIF
\end{verbatim}
* ANY INTERIOR LOCATION. *
*                            *
**************************************************************************
C 90  CONTINUE
C   CNTOP = -(COND(IZ-1,IY,IX-1)*DX(IX-1)*DY(IY)+COND(IZ-1,IY,IX)*DX(IX)
      &*DY(IY)+COND(IZ-1,IY-1,IX-1)*DX(IX-1)*DY(IY-1)+COND(IZ-1,IY-1,IX)*
      &DX(IX)*DY(IY-1))/(4.0*DZ(IZ-1))
C   CNBOT = -(COND(IY,IY,IX-1)*DX(IX-1)*DY(IY)+COND(IY,IY-1,IX-1)*
      &DX(IX-1)*DY(IY-1)+CONDXYZ*DX(IX)*DY(IY)+COND(IZ,IY-1,IX)*
      &DX(IX)*DY(IY-1))/(4.0*DZ(IZ))
C   CNLEFT = -(COND(IY-1,IY-1,IX-1)*DY(IY-1)*DZ(IZ-1)+COND(IY-1,IY,IX-1)
      &*DY(IY)*DZ(IZ-1)+COND(IY-1,IX-1)*DY(IY-1)*DZ(IZ)+COND(IZ,IY-1,IX-1)*
      &DY(IY)*DZ(IZ))/(4.0*DX(IX))
C   CNRHT = -(COND(IY-1,IY-1,IX)*DY(IY-1)*DZ(IZ-1)+COND(IY-1,IY,IX)*
      &DY(IY)*DZ(IZ-1)+COND(IY,IX,IX-1)*DY(IY-1)*DZ(IZ)+CONDXYZ*
      &DY(IY)*DZ(IZ))/(4.0*DX(IX))
C   CNFRNT = -(COND(IY-1,IY-1,IX-1)*DX(IX-1)*DZ(IZ-1)+COND(IY-1,IY-1,IX)*
      &DX(IX)*DZ(IZ-1)+COND(IY,IX-1,IX-1)*DX(IX-1)*DZ(IZ)+COND(IY,IX-1,IX-1)*
      &IX)*DX(IX)*DZ(IZ))/(4.0*DY(IY-1))
C   CNBACK = -(COND(IY,IX-1,IX-1)*DX(IX-1)*DZ(IZ-1)+COND(IX-1,IX,IX)*
      &DX(IX)*DZ(IZ-1)+COND(IX,IX,IX)*DX(IX-1)*DZ(IZ)+CONDXYZ*
      &DX(IX)*DZ(IZ))/(4.0*DY(IY))
C   CNCENT = -(CNTOP+CNBOT+CNLEFT+CNRHT+CNFRNT+CNBACK)
C 100  CONTINUE

IF(I.GE.M) THEN
   L = NYZ + 1
   DO IA = 2, L-2
      A(IA) = (0.00, 0.00)
   END DO
   A(1) = CNLEFT
   A(L-NNODZ) = CNFRNT
   A(L-1) = CNTOP
ELSE IF(I.GT.NNODZ.AND.I.LT.M) THEN
   L = NNODZ + 1
   DO IA = 2, L-2
A(IA) = (0.00,0.00)
END DO
A(1) = CNFRNT
A(L-1) = CNTOP
ELSE IF(I.GT.1.AND.I.LE.NNODZ) THEN
  L = 2
  A(1) = CNTOP
ELSE IF(I.EQ.1) THEN
  L = 1
END IF
A(L) = CNCENT
cc     write(*,*) "a(L)=", A(L)
RETURN
END

C
SUBROUTINE SETUPMAT(X,Y,Z,DX,DY,DZ,COND,IAM,JAM,NJA,AMAT)
C     --------------------------
*********************************************************************
*                                                                   *
*            To solve Ax=b using itpack                             *
*                                                                   *
*********************************************************************
REAL*4 X(NNODX),Y(NNODY),Z(NNODZ),
&       DX(NNODX-1),DY(NNODY-1),DZ(NNODZ-1)
COMPLEX(kind=2) COND(NNODZ-1,NNODY-1,NNODX-1)
COMMON /BLK8/ NNODX,NNODY,NNODZ,NNODE
COMMON /BLK9/ NBAND
C
C ARRAYS
cc     POINTER (PA,A)
INTEGER IAM(NNODE+1), JAM(7*NNODE), IBV(3)
c
DOUBLE PRECISION AMAT(7*NNODE)
c
COMPLEX(kind=2) AMAT(7*NNODE)
c
REAL*4 TEMP(7)
c
COMPLEX(kind=2) TEMP(7)
c
REAL,ALLOCATABLE:: A(:)
c
COMPLEX(kind=2),ALLOCATABLE:: A(:)
c
PA = MALLOC(4*NBAND)
c
IF (PA.EQ.0) CALL MEMERROR()
ALLOCATE (A(NBAND), STAT=ISTAT)
IF (ISTAT.NE.0) CALL MEMERROR()

DO I = 1, 7
   TEMP(I)=0.0
END DO
C PRINT *, ' ENTERING BANDX3...

C SET UP SPARSITY PATTERN AND VALUES IN MATRIX
C
cc PRINT *, ' Set up sparsity pattern ...'
NJA=0
IAM(1)=1
C
C FOR EACH ROW OF THE MATRIX CALL ROW3. REMEMBER ROW3 ACTUALLY
C RETURNS THE LOWER TRIANGULAR CAPACITANCE MATRIX SO PULL THE
C UPPER TRIANGULAR VALUES BY NIFFTY ROW3 CALLS ...
C
IBV(1)=1
IBV(2)=NNODZ
IBV(3)=NNODZ*NNODY
DO 800 I=1,NNODE
C THE DIAGONAL ELEMENTS ...
C
   CALL ROW3(A,NBAND,I,L,X,Y,Z,DX,DY,DZ,COND)
cc write(*,'*') 'i'm in setupmat and A=',A(L)
C THE LOWER TRIANGULAR ELEMENTS ...
C
   DO II=1,3
      IF(I.GE.IBV(II)+1) TEMP(II)=A(L-IBV(II))
   ENDDO
C THE UPPER TRIANGULAR ELEMENTS ...
C
   DO II=1,3
      IAMAT=IBV(II)
      IF(IAMAT.LE.NNODE-I) THEN
         CALL ROW3(A,NBAND,I+IAMAT,LL,X,Y,Z,DX,DY,DZ,COND)
         IF(IAMAT-1.LE.LL) TEMP(4+II)=A(LL-IAMAT)
      ENDIF
   ENDDO
C FOR EACH ROW ENTER THE SPARSE MATRIX STORAGE SCHEME ...
C
C THE DIAGONAL ELEMENTS ...
C
NJANJA+1
IAM(I+1)=NJA+1
AMAT(NJA)=TEMP(4)
JAM(NJA)=I

C THE LOWER TRIANGULAR ELEMENTS ...
C
DO II=3,1,-1
    JAMAT=NBAND-IBV(II)
    IF(ABS(TEMP(II)).GT.0.0) THEN
        NJA=NJA+1
        IAM(I+1)=NJA+1
        AMAT(NJA)=TEMP(II)
        write(*,*) "i'm in setupmat 1, amat=", amat
        JAM(NJA)=I+JAMAT-NBAND
    ENDIF
ENDDO
C
C THE UPPER TRIANGULAR ELEMENTS ...
C
DO II=1,3
    JAMAT=NBAND+IBV(II)
    IF(ABS(TEMP(4+II)).GT.0.0.AND.JAMAT.LE.NNODE-I+NBAND) THEN
        NJA=NJA+1
        IAM(I+1)=NJA+1
        AMAT(NJA)=TEMP(4+II)
        JAM(NJA)=I+JAMAT-NBAND
    ENDIF
ENDDO
800 CONTINUE
C
cc      CALL FREE(PA)
DEALLOCATE (A)
cc      write(*,*)"i'm in setupmat and cond=", cond
RETURN
END
C
SUBROUTINE SOLVEMAT(BMAT,XMAT,IAM,JAM,AMAT,nja,
                  &                    rwork,lenw,iwork,leniw,compch)
C
*****************************************************************************
To solve $Ax=b$ using DSICCG

** implicit none **

integer NNODX, NNODY, NNODZ, NNODE
common /BLK8/ NNODX, NNODY, NNODZ, NNODE

integer lenw, leniw, nja, i
double precision BMAT(NNODE)
complex(kind=2) XMAT(NNODE)
logical compch

integer IAM(NNODE+1), JAM(7*NNODE), iwork(leniw), & ierr, iter
double precision err, tol
complex(kind=2) AMAT(7*NNODE), rwork(lenw)

cc      write(*,*)"I'm in solvemat"
cc      do i = 1, nnode
cc          xmat(i) = (0.d0, 0.d0)
cc      end do

tol = 1.d-5

cc      call dsiccg (nnode, bmat, xmat, nja, jam, iam, amat, 0, 1, tol, & 500, iter, err, ierr, 0, rwork, lenw, iwork, leniw, compch)
cc      call snafu (nnode, bmat, xmat, nja, jam, iam, amat, tol, 8000)
cc      if (ierr.gt.0) then
cc          write (*, *) 'DSICCG error code =', ierr
cc      end if
cc      compch = .false.
cc      write (*, *)"i'm about to leave solvemat"

return
end

subroutine memerror()
print *, 'Memory allocation error.'
stop
end

subroutine filerr(file)
character*(*) file
print *, ' File ',file(1:len_trim(file)),' not found.'
print *
stop
end

cc  subroutine ieee_retrospective()
cc  end

subroutine getair(itopo,nx,ny,nz,cond)
  integer nx,ny,nz,itopo(nx,ny),i,j,k
  real*4 cond(nz,ny,nx),air
  cc      write(*,*)"I'm in getair"
cc      nx = nnodx-1
cc      ny = nnody-1

  air = 0.
  do i = 1, nx
    do j = 1, ny
      air = air + log10(cond(itopo(i,j)+1,j,i))
    end do
  end do
  C  air = average log conductivity of the surface cells times 1.e-8
  air = 10**(air/(nx*ny) - 8.)

  do i = 1, nx
    do j = 1, ny
      do k = 1, itopo(i,j)
        cond(k,j,i) = air
      end do
    end do
  end do
return
end

integer function igetnode(x,y,z,nx,ny,nz,itopo,xloc,yloc,zloc,
& elev0)
  implicit none
  integer nx,ny,nz,itopo(nx-1,ny-1)
  real*4 x(nx),y(ny),z(nz), xloc,yloc,zloc,elev0
  integer i,ix,iy,iz
ix=0
iy=0
iz=0

do i = 1, nx
    if (abs(xloc-x(i)).lt..001) then
        ix = i
        goto 10
    end if
end do

10 continue

do i = 1, ny
    if (abs(yloc-y(i)).lt..001) then
        iy = i
        goto 20
    end if
end do

20 continue

do i = 1, nz
    if (abs(zloc-z(i)).lt..001) then
        iz = i
        goto 30
    end if
end do

30 continue

if (ix.eq.0.or.iy.eq.0.or.iz.eq.0) then
    print*, 'Error: Electrode not on a node:', yloc,xloc,elev0-zloc
    stop
end if

if (ix.lt.4.or.ix.gt.nx-3.or.iy.lt.4.or.iy.gt.ny-3) then
    print*, 'Error: Electrode near the edge of the mesh:', yloc,xloc,elev0-zloc
    stop
end if

if (itopo(ix,iy).ge.iz.and.itopo(ix-1,iy).ge.iz.and.
    itopo(ix,iy-1).ge.iz.and.itopo(ix-1,iy-1).ge.iz) then
    print*, 'Error: Electrode above the surface:', yloc,xloc,elev0-zloc
    stop
end if
igetnode = (iy-1)*nz + (ix-1)*ny*nz + iz

return
end

subroutine getdim(meshf,obsf,ncur,ndat,mx,my,mz,datxyz)
C  This routine is used to get the variables for memory allocation.
C  Count the number of source locations, the number of data, and
C  the number of cells.
C  NOTE:  After this routine ends, the files are still open.  After the
C         memory allocation is done in the main program, calls to
C         readloc() and readmesh() should be made.
C
C implicit none
integer ncur,ndat,mx,my,mz,n,lenchar,i,ios
character obsf(*) ,meshf(*) , line*100
logical datxyz, firstread
real x,y,z

i = lenchar(obsf)
i = lenchar(meshf)

firstread = .true.

open(unit=1,file=obsf,status='old',err=900)
c
ncur = 0
ndat = 0

5 format(a)
do while (.true.)
   read(1,5,end=100) line
   do while (line(1:1).eq.'!' .or. len_trim(line).eq.0)
      read(1,5,end=100) line
   end do
   if (line(1:7).ne.'IPTYPE=') then
      if (firstread) then
         read(line,* ,iostat=ios) y,x,z, y,x,z, n
         if (ios.eq.0) then
            datxyz = .true.
         else
            read(line,* ,err=950) y,x, y,x, n
      end if
   else
      firstread = .false.
   end if
end do

datxyz = .false.
end if
firstread = .false.

else
  if (datxyz) then
    read(line,*,err=950) y,x,z, y,x,z, n
  else
    read(line,*,err=950) y,x, y,x, n
  end if
end if

ncur = ncur + 1
do i = 1, n
  call skipcmnts(1,line)
  if (datxyz) then
    read(line,*,err=950) y,x,z, y,x,z
  else
    read(line,*,err=950) y,x, y,x
  end if
end do
ndat = ndat + n
end if
end do

100 continue

open(unit=2,file=meshf,status='old',err=901)
call skipcmnts(2,line)
read(line,*) my,mx,mz

return

900 call filerr(obsf)
901 call filerr(meshf)

950 print*,'Error reading data file ',obsf(1:len_trim(obsf))
stop
end

cc---------------------------------------------------------------
subroutine readloc(ncur,ndat,xa,ya,za,xb,yb,zb,xm,ym,zm,
& xn,yn,zn,nobs,la,lb,lm,ln,x,y,z,elev0,itopo,iptype,
& datxyz,zint,nxi,nyi)
C  Read in the electrode locations


implicit none
integer ncur,ndat,nobs(ncur),iptype(ncur),ic,id,iddat,iflag, &
nnodx,nnody,nnodz,nnode,itopo(nnodx-1,nnody-1),
&
la(ncur),lb(ncur),lm(ndat),ln(ndat),igetnode,
&
nxi,nyi
real*4 xa(ncur),ya(ncur),za(ncur),xb(ncur),yb(ncur),zb(ncur), &
xm(ndat),ym(ndat),zm(ndat),xn(ndat),yn(ndat),zn(ndat), &
x(nnodx),y(nnody),z(nnodz),elev0,zint(nxi,nyi),getznode
integer icmid,idmid
real*4 xmid,ymid,xplot,yplot,zplot,dist,distmin
character line*100
logical datxyz
common /blk8/ nnodx,nnody,nnodz,nnode
common /middat/ icmid,idmid

rewind(1)
iflag = 0
id = 0
if (.not.datxyz) open(unit=3,file='obs.loc')

do ic = 1, ncur
   call skipcmts(1,line)
   if (line(1:7).eq.'IPTYPE=') then
      read(line(8:20),*) iflag
      call skipcmts(1,line)
   end if
   iptype(ic) = iflag
   if (datxyz) then
      read(line,*) ya(ic),xa(ic),za(ic), &
yb(ic),xb(ic),zb(ic), nobs(ic)
   else
      read(line,*) ya(ic),xa(ic), &
yb(ic),xb(ic), nobs(ic)
      za(ic) = getznode(xa(ic),ya(ic),x,y,z,nnodx,nnody,nnodz, &
itopo,elev0,zint,nxi,nyi)
      zb(ic) = getznode(xb(ic),yb(ic),x,y,z,nnodx,nnody,nnodz, &
itopo,elev0,zint,nxi,nyi)
      write(3,10) ya(ic),xa(ic),za(ic),yb(ic),xb(ic),zb(ic), &
nobs(ic)
   end if
   za(ic) = elev0 - za(ic)
   zb(ic) = elev0 - zb(ic)

10 format(20f10.6,i5)
end do
la(ic) = igetnode(x, y, z, nnodx, nnody, nnodz, itopo,
  xa(ic), ya(ic), za(ic), elev0)
&
lb(ic) = igetnode(x, y, z, nnodx, nnody, nnodz, itopo,
  xb(ic), yb(ic), zb(ic), elev0)
&
do idat = 1, nobs(ic)
  call skipcmnts(1, line)
  id = id+1

  if (datxyz) then
    read(line,*) yn(id), xn(id), zn(id), ym(id), xm(id), zm(id)
  else
    read(line,*) yn(id), xn(id), ym(id), xm(id)

    zn(id) = getznode(xn(id), yn(id), x, y, z, nnodx, nnody, nnodz,
      itopo, elev0, zint, nxi, nyi)
&
    zm(id) = getznode(xm(id), ym(id), x, y, z, nnodx, nnody, nnodz,
      itopo, elev0, zint, nxi, nyi)
&
    write(3,15) yn(id), xn(id), zn(id), ym(id), xm(id), zm(id)
    end if

    zn(id) = elev0 - zn(id)
    zm(id) = elev0 - zm(id)

    lm(id) = igetnode(x, y, z, nnodx, nnody, nnodz, itopo,
      xm(id), ym(id), zm(id), elev0)
&
    ln(id) = igetnode(x, y, z, nnodx, nnody, nnodz, itopo,
      xn(id), yn(id), zn(id), elev0)
&
    if (lm(id).eq.la(ic).or.lm(id).eq.lb(ic).or.
      ln(id).eq.la(ic).or.ln(id).eq.lb(ic)) then
      print*, 'Error: source and receiver electrodes cannot',
      ' be in the same location.'
      stop
    end if
  end do
end do

10 format(/, 6f10.2, i5)
15 format(6f10.2)

close(1)
if (.not.datxyz) close(3)
C Find the data nearest the mesh's centre
    xmid = (x(1) + x(nnodx))*0.5
    ymid = (y(1) + y(nnody))*0.5
    print *, 'Middle of mesh: ', ymid, xmid
    distmin = 1.e+20
    id = 0
    do ic = 1, ncur
        do idat = 1, nobs(ic)
            id = id + 1
            xplot = (xa(ic)+xb(ic) + xm(id)+xn(id))*0.25
            yplot = (ya(ic)+yb(ic) + ym(id)+yn(id))*0.25
            zplot = sqrt((xplot-(xa(ic)+xb(ic))*0.5)**2 +
                        (yplot-(ya(ic)+yb(ic))*0.5)**2)
            dist = sqrt((xplot-xmid)**2 + (yplot-ymid)**2 + zplot**2)
            if (dist.lt.distmin) then
                distmin = dist
                icmid = ic
                idmid = id
            end if
        end do
    end do
    print*, 'Data nearest centre at: ',
    & ya(icmid),xa(icmid), yb(icmid),xb(icmid),
    & yn(idmid),xn(idmid), ym(idmid),xm(idmid)
    return
end

---------------------------------------------------------------
subroutine readmesh(x0,y0,elev0,dx,dy,dz,x,y,z,mx,my,mz)
implicit none
integer mx,my,mz, i
real*4 x0,y0,elev0,dx(mx),dy(my),dz(mz),x(mx+1),y(my+1),z(mz+1)

read(2,*,err=950) y0,x0,elev0
read(2,*,err=950) (dy(i),i=1,my)
read(2,*,err=950) (dx(i),i=1,mx)
read(2,*,err=950) (dz(i),i=1,mz)
close(2)
c scale node separations
\begin{verbatim}
x(1)=x0
  do i = 2, mx+1
    x(i) = x(i-1) + dx(i-1)
  end do
y(1)=y0
  do i = 2, my+1
    y(i) = y(i-1) + dy(i-1)
  end do
z(1)=0.
  do i = 2, mz+1
    z(i) = z(i-1) + dz(i-1)
  end do

return

950  print*, 'Error reading mesh file.'
stop
end

C
C  (C) COPYRIGHT 1998 UBC-GIF  ALL RIGHTS RESERVED
C-----------------------------------------------
    subroutine gettopo(itopo,mx,my,mz,mcell,topof)
    cc    read in the surface topographic index
    cc    for each column, the index gives the number of
    cc    cells, from the top of the mesh, that are above
    cc    the actual surface
    cc-----------------------------------------------
    implicit none
    integer
      mx,my,mz,itopo(mx,my),mcell,i,j,iwk,nx,ny,ncol,icol,iline,
      &    lenchar
    character*(*) topof
    character line*60

    mcell = mx*my*mz
    i = lenchar(topof)

    if (topof(1:4).eq.'null'.or.topof(1:4).eq.'NULL') then
      do j=1, my
        do i=1, mx
          itopo(i,j)=0
        enddo
      enddo
    else
      ncell = mcell
      call readfile(ncell, line)
      do j=1, my
        do i=1, mx
          k = (i-1)*my+j
          itopo(i,j) = scan(line(k), 0, iwk)
        enddo
      enddo
    endif
    itopo = itopo - 1

end
\end{verbatim}
else
    open(unit=3,file=topof,status='old',err=900)
call skipcmts(3,line)
read(line,*,err=90) ny,nx
if (nx.ne.mx.or.ny.ne.my) then
    print *, ' Input error in file ',
    & topof, ', line', 1, ' :
    print *, ' dimension(s) incorrect.'
goto 100
endif
ncol=mx*my
do icol=1, ncol
    read(3,*,err=90)j,i,iwk
    if (iwk.lt.0.or.iwk.gt.mz) then
        iline=icol+1
        print *, ' Input error in file ',
        & topof, ', line', iline, ' :
        print *, ' vertical index out of range. '
goto 100
    endif
    if (i.lt.1.or.i.gt.mx.or.j.lt.1.or.j.gt.my) then
        iline=icol+1
        print *, ' Input error in file ',
        & topof, ', line', iline, ' :
        print *, ' horizontal indeces out of range. '
goto 100
    endif
    itopo(i,j)=iwk
    mcell = mcell - iwk
endo
    close(3)
endif
return

90   print*,'Error reading ',topof
100   continue
    print *, ' Program terminated.'
    print *
    stop
900   call filerr(topof)
end
integer function lenchar(char)

get the length of the file name,
comment in the input is marked by '!!'
the comments are stripped upon exit

character*60 char

len=0
do while (len.lt.60.and.char(len+1:len+1).ne.'!!')
   len=len+1
endo

doi=len,1,-1
   if (char(i:i).ne.' ') then
      n=i
      lenchar=n
      if (n.gt.0) char=char(1:n)//''
      return
   endif
endo

return
end

subroutine readtopo(topof,xnode,ynode,znode,nx,ny,nz,elev0,ito,
&   ncur,ndat,xa,ya,za,xb,yb,zb,xm,ym,zm,xn,yn,zn,nobs,
&   la,lb,lm,ln,iptype,mcell)

implicit none

integer nx,ny,nz,ncur,ndat,ito(nx,ny),nobs(ncur),iptype(ncur),
&          la(ncur),lb(ncur),lm(ndat),ln(ndat),mcell
real*4  xnode(nx+1),ynode(ny+1),znode(nz+1),elev0,
&         xa(ncur),ya(ncur),za(ncur),xb(ncur),yb(ncur),zb(ncur),
&         xm(ndat),ym(ndat),zm(ndat),xn(ndat),yn(ndat),zn(ndat)
character  topos(*)

cc      pointer (pxloc,xloc),(pyloc,yloc),(pzloc,zloc),(piend,iend),
cc     &        (piadj,iadj),(pxint,xint),(pyint,yint),(pzint,zint),
cc     &        (ptopo,topo)
real,allocatable::  xloc(:),yloc(:),zloc(:),
&         xint(:),yint(:),zint(:),topo(:)
real  xmin,xmax,ymin,ymax,arearatio,areaqtpl,del
real*4  dist,d00,d10,d01,d11,z00,z10,z11,adist,x1,x2,y1,y2
integer,allocatable::  iend(:),iadj(:)
integer  npt,i,j,ier,ist,ind,lenchar, nxi,nyi,ios
real*4  ovp
parameter (ovp=0.3)

adist(x1,y1,x2,y2) = sqrt((x2-x1)**2 + (y2-y1)**2)

nxi = 2*nx+1
nyi = 2*ny+1

cc      pzint = malloc(4*nxi*nyi)
allocate (zint(nxi*nyi))
i = lenchar(topof)
mcell = nx*ny*nz

if (topof(1:4).eq.'null'.or.topof(1:4).eq.'NULL') then
  do j=1, ny
    do i=1, nx
      itopo(i,j)=0
    enddo
  enddo
  do i = 1, nxi*nyi
    zint(i) = elev0
  end do
else   !! descretize topography

open(unit=3,file=topof,status='old',err=901)
  format(a)
read(3,5) buf
  do while(buf(1:1).eq.'!')
    read(3,5) buf
  end do

read(buf,*,iostat=ios) npt, i
if (ios.ne.0) then
   print*, 'Error: topography file in topo.idx format.'
   goto 950
end if

read(buf,*,err=950) npt
cc      pxloc = malloc(4*(npt+4))
cc      pyloc = malloc(4*(npt+4))
cc      pzloc = malloc(4*(npt+4))
cc      piend = malloc(4*(npt+4))
cc      piadj = malloc(4*(6*(npt+4)-9))
cc      pxint = malloc(4*nxi)
cc      pyint = malloc(4*nyi)
cc      ptopo = malloc(4*nx*ny)
allocate(xloc(npt+4),yloc(npt+4),zloc(npt+4),iend(npt+4), & iadj(6*(npt+4)-9),xint(nxi),yint(nyi),topo(nx*ny))
xmin = 1.e+5
xmax =-1.e+5
ymin = 1.e+5
ymax =-1.e+5

d00 = 1.e+5
d10 = 1.e+5
d01 = 1.e+5
d11 = 1.e+5

do i = 1, npt
   read(3,*,err=950) yloc(i), xloc(i), zloc(i)
   xmin = amin1(xmin, xloc(i))
   xmax = amax1(xmax, xloc(i))
   ymin = amin1(ymin, yloc(i))
   ymax = amax1(ymax, yloc(i))

   dist = adist(xnode(1),ynode(1),xloc(i),yloc(i))
   if (dist.lt.d00) then
      d00 = dist
      z00 = zloc(i)
   end if

   dist = adist(xnode(nx+1),ynode(1),xloc(i),yloc(i))
   if (dist.lt.d10) then
      d10 = dist
      z10 = zloc(i)
   end if
```
    dist = adist(xnode(1), ynode(ny+1), xloc(i), yloc(i))
    if (dist.lt.d01) then
        d01 = dist
        z01 = zloc(i)
    end if

    dist = adist(xnode(nx+1), ynode(ny+1), xloc(i), yloc(i))
    if (dist.lt.d11) then
        d11 = dist
        z11 = zloc(i)
    end if

end do
close(3)

areaovlp = (amin1(xmax, xnode(nx+1)) - amax1(xmin, xnode(1)))*
          & (amin1(ymax, ynode(ny+1)) - amax1(ymin, ynode(1)))*
arearatio = areaovlp/((xnode(nx+1)-xnode(1))*(ynode(ny+1)-ynode(1)))*

if (xmin.ge.xnode(nx+1).or.xmax.le.xnode(1).or. &
    ymin.ge.ynode(ny+1).or.ymax.le.ynode(1)) then
    print*, 'Error: Topography is outside the mesh.'
    stop
else if (arearatio.lt.ovp) then
    print*, 'Warning: Topography region is not large enough.'
end if

del = amin1(xnode(2)-xnode(1), ynode(2)-ynode(1))* .25
if (d00.gt.del) then
    npt = npt+1
    xloc(npt) = xnode(1)
    yloc(npt) = ynode(1)
    zloc(npt) = z00
end if
if (d10.gt.del) then
    npt = npt+1
    xloc(npt) = xnode(nx+1)
    yloc(npt) = ynode(1)
    zloc(npt) = z10
end if
if (d01.gt.del) then
    npt = npt+1
    xloc(npt) = xnode(1)
    yloc(npt) = ynode(ny+1)
    zloc(npt) = z01
end if
```
if (d11.gt.del) then
    npt = npt+1
    xloc(npt) = xnode(nx+1)
    yloc(npt) = ynode(ny+1)
    zloc(npt) = z11
end if

C (xint,yint) = centre, edges and corners of cells.
do i = 1, nx
    xint(2*i-1) = xnode(i)
    xint(2*i) = (xnode(i)+xnode(i+1))*0.5
  end do
xint(nxi) = xnode(nx+1)
do j = 1, ny
    yint(2*j-1) = ynode(j)
    yint(2*j) = (ynode(j)+ynode(j+1))*0.5
  end do
yint(nyi) = ynode(ny+1)

C--------
call reordr(npt,3,xloc,yloc,zloc,iend)
call trmesh(npt,xloc,yloc,iadj,iend,ier)
if (ier.eq.2) then
  print*,'Error: Points in the topography file are collinear.'
  stop
end if

ist = 1
ind = 1
do j = 1, nyi
  do i = 1, nxi
    call intrc0(npt,xint(i),yint(j),xloc,yloc,zloc,iadj,iend,
&                  ist,zint(ind),ier)
    ind = ind+1
  end do
end do

call toposet(zint,nxi,nyi,topo,znode,nx,ny,nz,elev0,itopo)

open(unit=3,file='topo.idx')
write(3,'(2i5)') ny, nx
do j = 1, ny
    do i = 1, nx
        write(3,10) j, i, itopo(i, j)
        mcell = mcell - itopo(i, j)
    end do
end do
close(3)

10 format(3i4)

cc write(11,*) nyi, nxi, 0
cc do j = 1, nyi
cc    do i = 1, nxi
cc        write(11,*) yint(j), xint(i), zint((j-1)*nxi+i)
cc    end do
cc end do
cc end do

call free(pxloc)
call free(pyloc)
call free(pzloc)
call free(piend)
call free(piadj)
call free(pxint)
call free(pyint)
call free(ptopo)
deallocate(xloc, yloc, zloc, iend, iadj, xint, yint, topo)
end if

call readloc(ncur, ndat, xa, ya, za, xb, yb, zb, xm, ym, zm, xn, yn, zn, 
&   nobs, la, lb, lm, ln, xnode, ynode, znode, elev0, itopo, iptype, 
&   .false., zint, nxi, nyi)

call free(pxint)
deallocate(zint)

return

901 call filerr(topof)
950 print*, 'Error reading ', topos stop
end
real function getznode(xa, ya, xnode, ynode, znode, nx, ny, nz, itopo, &     elev0, zint, nxi, nyi)
  implicit none
  integer nx, ny, nz, nxi, nyi, itopo(nx-1, ny-1)
  real xa, ya, xnode(nx), ynode(ny), znode(nz), zint(nxi, nyi), &     elev0

  integer i, ix, iy, mintp, maxtp
  real ztr, za, delmn, del

  ix=0
  iy=0

  do i = 1, nx
    if (abs(xa-xnode(i)).lt.1.e-03) then
      ix = i
      goto 10
    end if
  end do

10   continue

  do i = 1, ny
    if (abs(ya-ynode(i)).lt.1.e-03) then
      iy = i
      goto 20
    end if
  end do

20   continue

  if (ix.eq.0.or.iy.eq.0) then
    print*, 'Error: Electrode not on a node:', ya, xa
    stop
  end if

  ztr = elev0 - zint(2*ix-1, 2*iy-1)

  mintp = min(itopo(ix, iy), itopo(ix, iy-1), &     itopo(ix-1, iy), &     itopo(ix-1, iy-1)) +1
  maxtp = max(itopo(ix, iy), itopo(ix, iy-1), itopo(ix-1, iy), &     itopo(ix-1, iy-1)) +1

  delmn = 1.e+20

  do i = mintp, maxtp
    del = abs(znode(i) - ztr)
    if (del .lt. delmn) then
      delmn = del
      za = znode(i)
    end if
end do

cc     do j = iy-1, iy
cc          do i = ix-1, ix
cc             del = abs(znode(itopo(i,j)+1) - ztr)
cc
cc             if (del .lt. delmn) then
cc                delmn = del
cc                za = znode(itopo(i,j)+1)
cc           end if
cc       end do
cc     end do

getznode = elev0 - za

return
end

cc----------------------------------------------------------
subroutine toposet(zint,nxi,nyi,topo,znod,nx,ny,nz,znot,itop)
cc
cc    toposet finds the discretized surface in the mesh
cc----------------------------------------------------------
implicit none
integer nxi,nyi,nx,ny,nz,itop(nx,ny)
real*4 zint(nxi,nyi),topo(nx,ny),znod(nz+1),znot
integer i,j,ii,jj,k,indz
real sum,zsurf

do j = 1, ny
jj = 2*j
  do i = 1, nx
ii = 2*i

        sum = 4*zint(ii,jj) +
        &  2*(zint(ii-1,jj)+zint(ii+1,jj)+zint(ii,jj-1)+
        &    zint(ii,jj+1)) +
        &  zint(ii-1,jj-1)+zint(ii+1,jj-1)+zint(ii-1,jj+1)+
        &  zint(ii+1,jj+1)
topo(i,j) = sum/16.

cc            sum = zint(ii,jj) +
cc            &  zint(ii-1,jj)+zint(ii+1,jj)+zint(ii,jj-1)+
cc            &  zint(ii,jj+1) +
cc            &  zint(ii-1,jj-1)+zint(ii+1,jj-1)+zint(ii-1,jj+1)+
cc            &  zint(ii+1,jj+1)
topo(i,j) = sum/9.
cc----begin to match the topo-surface with the mesh
cc first convert the depth to elevation

do i=1, nz+1
    znod(i)=znot - znod(i)
enddo

do j= 1, ny
    do i= 1, nx
        zsurf=topo(i,j)
        k=indz(znod,zsurf,nz)
        if (k.eq.0) then
            itop(i,j)=0
        else if (k.gt.nz) then
            itop(i,j)=nz
        else
            itop(i,j)=k
        endif
    enddo
endo
endo

C Convert znod to its original values.

do i=1, nz+1
    znod(i)=znot - znod(i)
endo

return
end

integer function indz(z,zsurf,n)
integer n
real*4 z(n+1),zsurf

if (zsurf.ge.z(1)) then
    indz=0
else if (zsurf.lt.z(n+1)) then
    indz=n+1
else
    do i=1, n
        if (zsurf.le.z(i).and.zsurf.ge.z(i+1)) then
            if (z(i)-zsurf .lt. zsurf-z(i+1)) then
                indz = i-1
            endif
        endif
    enddo

end
else
    indz=i
end if
return
endif
enddo
endif
return
end

subroutine skipcmnts(iu,line)
C Skip lines that start with '!' or are empty.
implicit none
integer iu
character line*(*)
5     format(a)
read(iu,5) line
  do while (line(1:1).eq.'!'.or.len_trim(line).eq.0)
    read(iu,5) line
  end do
return
end

*======================================================================
*NIST Guide to Available Math Software.
*Fullsource for module 624 from package TOMS.
*Retrieved from NETLIB on Thu Sep 25 20:00:14 1997.
*======================================================================
C     ALGORITHM 624 COLLECTED ALGORITHMS FROM ACM.
C     ALGORITHM APPEARED IN ACM-TRANS. MATH. SOFTWARE, VOL.10, NO. 4,
C     DEC., 1984, P. 453.
SUBROUTINE ADNODE (KK,X,Y, IADJ,IEND, IER)
integer KK, IADJ(1), IEND(KK), IER
C***********************************************************
C
C                                               ROBERT RENKA
C                                       OAK RIDGE NATL. LAB.
THIS ROUTINE ADDS NODE KK TO A TRIANGULATION OF A SET OF POINTS IN THE PLANE PRODUCING A NEW TRIANGULATION. A SEQUENCE OF EDGE SWAPS IS THEN APPLIED TO THE MESH, RESULTING IN AN OPTIMAL TRIANGULATION. ADNODE IS PART OF AN INTERPOLATION PACKAGE WHICH ALSO PROVIDES ROUTINES TO INITIALIZE THE DATA STRUCTURE, PLOT THE MESH, AND DELETE ARCS.

INPUT PARAMETERS -   KK - INDEX OF THE NODE TO BE ADDED TO THE MESH. KK .GE. 4.

X,Y - VECTORS OF COORDINATES OF THE NODES IN THE MESH. (X(I),Y(I)) DEFINES NODE I FOR I = 1,...,KK.

IADJ - SET OF ADJACENCY LISTS OF NODES 1,...,KK-1.

IEND - POINTERS TO THE ENDS OF ADJACENCY LISTS IN IADJ FOR EACH NODE IN THE MESH.

IADJ AND IEND MAY BE CREATED BY TRMESH.

KK, X, AND Y ARE NOT ALTERED BY THIS ROUTINE.

OUTPUT PARAMETERS - IADJ,IEND - UPDATED WITH THE ADDITION OF NODE KK AS THE LAST ENTRY.

IER - ERROR INDICATOR
    IER = 0 IF NO ERRORS WERE ENCOUNTERED.
    IER = 1 IF ALL NODES (INCLUDING KK) ARE COLLINEAR.

MODULES REFERENCED BY ADNODE - TRFIND, INTADD, BDYADD, SHIFTD, INDEX, SWPTST, SWAP

INTEGER K, KM1, I1, I2, I3, INDKF, INDKL, NABOR1,
    I01, IO2, IN1, INDK1, IND2F, IND21
REAL XK, YK

LOCAL PARAMETERS -
C K = LOCAL COPY OF KK
C KM1 = K - 1
C I1, I2, I3 = VERTICES OF A TRIANGLE CONTAINING K
C INDFK = IADJ INDEX OF THE FIRST NEIGHBOR OF K
C INDKL = IADJ INDEX OF THE LAST NEIGHBOR OF K
C NABOR1 = FIRST NEIGHBOR OF K BEFORE ANY SWAPS OCCUR
C IO1, IO2 = ADJACENT NEIGHBORS OF K DEFINING AN ARC TO
C BE TESTED FOR A SWAP
C IN1 = VERTEX OPPOSITE K -- FIRST NEIGHBOR OF IO2
C WHICH PRECEDES IO1. IN1, IO1, IO2 ARE IN
C COUNTERCLOCKWISE ORDER.
C INDK1 = INDEX OF IO1 IN THE ADJACENCY LIST FOR K
C INDF2 = INDEX OF THE FIRST NEIGHBOR OF IO2
C IND21 = INDEX OF IO1 IN THE ADJACENCY LIST FOR IO2
C XK, YK = X(K), Y(K)
C
IER = 0
K = KK

C INITIALIZATION
C
KM1 = K - 1
XK = X(K)
YK = Y(K)

C ADD NODE K TO THE MESH
C
CALL TRFIND(KM1, XK, YK, X, Y, IADJ, IEND, I1, I2, I3)
IF (I1 .EQ. 0) GO TO 5
IF (I3 .EQ. 0) CALL BDYADD(K, I1, I2, IADJ, IEND)
IF (I3 .NE. 0) CALL INTADD(K, I1, I2, I3, IADJ, IEND)

C INITIALIZE VARIABLES FOR OPTIMIZATION OF THE MESH
C
INDFK = IEND(KM1) + 1
INDKL = IEND(K)
NABOR1 = IADJ(INDFK)
IO2 = NABOR1
INDK1 = INDFK + 1
IO1 = IADJ(INDK1)

C BEGIN LOOP -- FIND THE VERTEX OPPOSITE K
C
1 IND2F = 1
IF (IO2 .NE. 1) IND2F = IEND(IO2 - 1) + 1
IND21 = INDEX(IO2, IO1, IADJ, IEND)
IF (IND2F .EQ. IND21) GO TO 2
IN1 = IADJ(IND21 - 1)
GO TO 3
C
C IN1 IS THE LAST NEIGHBOR OF IO2
C
2 IND21 = IEND(IO2)
   IN1 = IADJ(IND21)
   IF (IN1 .EQ. 0) GO TO 4
C
C SWAP TEST -- IF A SWAP OCCURS, TWO NEW ARCS ARE OPPOSITE K
C              AND MUST BE TESTED. INDK1 AND INDKF MUST BE
C              DECREMENTED.
C
3 IF ( .NOT. SWPTST(IN1,K,IO1,IO2,X,Y) ) GO TO 4
   CALL SWAP(IN1,K,IO1,IO2, IADJ,IEND )
   IO1 = IN1
   INDK1 = INDK1 - 1
   INDKF = INDKF - 1
   GO TO 1
C
C NO SWAP OCCURRED.  RESET IO2 AND IO1, AND TEST FOR
C   TERMINATION.
C
4 IF (IO1 .EQ. NABOR1) RETURN
   IO2 = IO1
   INDK1 = INDK1 + 1
   IF (INDK1 .GT. INDKL) INDK1 = INDKF
   IO1 = IADJ(INDK1)
   IF (IO1 .NE. 0) GO TO 1
RETURN
C
C ALL NODES ARE COLLINEAR
C
5 IER = 1
RETURN
END
SUBROUTINE BDYADD (KK,I1,I2, IADJ,IEND )
INTEGER KK, I1, I2, IADJ(1), IEND(KK)

C***********************************************************************

C ROBERT RENKA
C OAK RIDGE NATL. LAB.
C (615) 576-5139
C
C THIS ROUTINE ADDS A BOUNDARY NODE TO A TRIANGULATION
C OF A SET OF KK-1 POINTS IN THE PLANE. IADJ AND IEND ARE
C UPDATED WITH THE INSERTION OF NODE KK.
C
C INPUT PARAMETERS - KK - INDEX OF AN EXTERIOR NODE TO BE
C ADDED. KK .GE. 4.
I1 - FIRST (RIGHTMOST AS VIEWED FROM KK) BOUNDARY NODE IN THE MESH WHICH IS VISIBLE FROM KK - THE LINE SEGMENT KK-I1 INTERSECTS NO ARCS.

I2 - LAST (LEFTMOST) BOUNDARY NODE WHICH IS VISIBLE FROM KK.

IADJ - SET OF ADJACENCY LISTS OF NODES IN THE MESH.

IEND - POINTERS TO THE ENDS OF ADJACENCY LISTS IN IADJ FOR EACH NODE IN THE MESH.

IADJ AND IEND MAY BE CREATED BY TRMESH AND MUST CONTAIN THE VERTICES I1 AND I2. I1 AND I2 MAY BE DETERMINED BY TRFIND.

KK, I1, AND I2 ARE NOT ALTERED BY THIS ROUTINE.

OUTPUT PARAMETERS - IADJ, IEND - UPDATED WITH THE ADDITION OF NODE KK AS THE LAST ENTRY. NODE KK WILL BE CONNECTED TO I1, I2, AND ALL BOUNDARY NODES BETWEEN THEM. NO OPTIMIZATION OF THE MESH IS PERFORMED.

MODULE REFERENCED BY BDYADD - SHIFTD

INTRINSIC FUNCTIONS CALLED BY BDYADD - MIN0, MAX0

************************************************************

INTEGER K, KM1, NRIGHT, NLEFT, NF, NL, N1, N2, I, IMIN, IMAX, KEND, NEXT, INDX

LOCAL PARAMETERS -

K = LOCAL COPY OF KK
KM1 = K - 1
NRIGHT, NLEFT = LOCAL COPIES OF I1, I2
NF, NL = INDICES OF IADJ BOUNDING THE PORTION OF THE ARRAY TO BE SHIFTED
N1 = IADJ INDEX OF THE FIRST NEIGHBOR OF NLEFT
N2 = IADJ INDEX OF THE LAST NEIGHBOR OF NRIGHT
I = DO-LOOP INDEX
IMIN, IMAX = BOUNDS ON DO-LOOP INDEX -- FIRST AND LAST
C ELEMENTS OF IEND TO BE INCREMENTED
C KEND = POINTER TO THE LAST NEIGHBOR OF K IN IADJ
C NEXT = NEXT BOUNDARY NODE TO BE CONNECTED TO KK
C INDX = INDEX FOR IADJ
C
K = KK
KM1 = K - 1
NRIGHT = I1
NLEFT = I2
C
C INITIALIZE VARIABLES
C
NL = IEND(KM1)
N1 = 1
IF (NLEFT .NE. 1) N1 = IEND(NLEFT-1) + 1
N2 = IEND(NRIGHT)
NF = MAX0(N1,N2)
C
C INSERT K AS A NEIGHBOR OF MAX(NRIGHT,NLEFT)
C
CALL SHIFTD(NF,NL,2, IADJ )
IADJ(NF+1) = K
IMIN = MAX0(NRIGHT,NLEFT)
DO 1 I = IMIN,KM1
   IEND(I) = IEND(I) + 2
1   CONTINUE
C
C INITIALIZE KEND AND INSERT K AS A NEIGHBOR OF
C MIN(NRIGHT,NLEFT)
C
KEND = NL + 3
NL = NF - 1
NF = MIN0(N1,N2)
CALL SHIFTD(NF,NL,1, IADJ )
IADJ(NF) = K
IMAX = IMIN - 1
IMIN = MIN0(NRIGHT,NLEFT)
DO 2 I = IMIN,IMAX
   IEND(I) = IEND(I) + 1
2   CONTINUE
C
C INSERT NRIGHT AS THE FIRST NEIGHBOR OF K
C
IADJ(KEND) = NRIGHT
C
C INITIALIZE INDX FOR LOOP ON BOUNDARY NODES BETWEEN NRIGHT
C AND NLEFT
C
INDX = IEND(NRIGHT) - 2
3 NEXT = IADJ(INDX)
IF (NEXT .EQ. NLEFT) GO TO 4

C CONNECT NEXT AND K

KEND = KEND + 1
IADJ(KEND) = NEXT
INDX = IEND(NEXT)
IADJ(INDX) = K
INDX = INDX - 1
GO TO 3

C INSERT NLEFT AND 0 AS THE LAST NEIGHBORS OF K

4 IADJ(KEND+1) = NLEFT
KEND = KEND + 2
IADJ(KEND) = 0
IEND(K) = KEND
RETURN

END

SUBROUTINE COORDS (X,Y,X1,X2,X3,Y1,Y2,Y3, R,IER)

INTEGER IER
REAL    X, Y, X1, X2, X3, Y1, Y2, Y3, R(3)

C***********************************************************
C
C                                               ROBERT RENKA
C                                       OAK RIDGE NATL. LAB.
C                                             (615) 576-5139
C
C   THIS ROUTINE COMPUTES THE THREE BARYCENTRIC COORDINATES
C OF A POINT IN THE PLANE FOR A GIVEN TRIANGLE.
C
C INPUT PARAMETERS - X,Y - X AND Y COORDINATES OF THE POINT
C WHOSE BARYCENTRIC COORDINATES ARE
C DESIRED.
C
C X1,X2,X3,Y1,Y2,Y3 - COORDINATES OF THE VERTICES OF
C THE TRIANGLE.
C
C INPUT PARAMETERS ARE NOT ALTERED BY THIS ROUTINE.
C
C OUTPUT PARAMETERS - R - 3-VECTOR OF BARYCENTRIC COORDI-
NATES UNLESS IER = 1. NOTE THAT
C R(I) .LT. 0. IFF (X,Y) IS TO THE
C RIGHT OF THE VECTOR FROM VERTEX
C I+1 TO VERTEX I+2 (CYCLICAL
C ARITHMETIC).
C
C IER - ERROR INDICATOR
C IER = 0 IF NO ERRORS WERE
ENCOUNTERED.

IER = 1 IF THE VERTICES OF THE
TRIANGLE ARE COLLINEAR.

MODULES REFERENCED BY COORDS - NONE

***********************************************************

REAL U(3), V(3), AREA, XP, YP

LOCAL PARAMETERS -

U(K),V(K) = X AND Y COMPONENTS OF THE VECTOR REPRESENTING
THE SIDE OPPOSITE VERTEX K FOR K = 1,2,3.
AREA = TWICE THE AREA OF THE TRIANGLE.
XP,YP = X-X1, Y-Y1

U(1) = X3-X2
U(2) = X1-X3
U(3) = X2-X1

V(1) = Y3-Y2
V(2) = Y1-Y3
V(3) = Y2-Y1

AREA = 3-1 X 3-2

AREA = U(1)*V(2) - U(2)*V(1)
IF (AREA .EQ. 0.) GO TO 1

R(1) = (2-3 X 2-(X,Y))/AREA, R(2) = (1-(X,Y) X 1-3)/AREA,
R(3) = (1-2 X 1-(X,Y))/AREA

R(1) = (U(1)*(Y-Y2) - V(1)*(X-X2))/AREA
XP = X - X1
YP = Y - Y1
R(2) = (U(2)*YP - V(2)*XP)/AREA
R(3) = (U(3)*YP - V(3)*XP)/AREA
IER = 0
RETURN

VERTICES ARE COLLINEAR

1 IER = 1
RETURN
END

INTEGER FUNCTION INDEX (NVERTX,NABOR,IADJ,IEND)
INTEGER NVERTX, NABOR, IADJ(1), IEND(1)

***********************************************************
THIS FUNCTION RETURNS THE INDEX OF NABOR IN THE
ADJACENCY LIST FOR NVERTX.

INPUT PARAMETERS - NVERTX - NODE WHOSE ADJACENCY LIST IS
      TO BE SEARCHED.
NABOR - NODE WHOSE INDEX IS TO BE RETURNED. NABOR MUST BE
      CONNECTED TO NVERTX.
IADJ - SET OF ADJACENCY LISTS.
IEND - POINTERS TO THE ENDS OF ADJACENCY LISTS IN IADJ.

INPUT PARAMETERS ARE NOT ALTERED BY THIS FUNCTION.

OUTPUT PARAMETER - INDEX - IADJ(INDEX) = NABOR.

MODULES REFERENCED BY INDEX - NONE

********************************************************************

INTEGER NB, INDX

LOCAL PARAMETERS -

NB = LOCAL COPY OF NABOR
INDX = INDEX FOR IADJ

NB = NABOR

INITIALIZATION

INDX = IEND(NVERTX) + 1

SEARCH THE LIST OF NVERTX NEIGHBORS FOR NB

1  INDX = INDX - 1
   IF (IADJ(INDX) .NE. NB) GO TO 1

INDEX = INDX
RETURN
END

SUBROUTINE INTADD (KK,I1,I2,I3, IADJ,IEND )
INTEGER KK, I1, I2, I3, IADJ(1), IEND(KK)

C***********************************************************
C
C                                               ROBERT RENKA
C                                       OAK RIDGE NATL. LAB.
(615) 576-5139
C
C THIS ROUTINE ADDS AN INTERIOR NODE TO A TRIANGULATION
C OF A SET OF KK-1 POINTS IN THE PLANE. IADJ AND IEND ARE
C UPDATED WITH THE INSERTION OF NODE KK IN THE TRIANGLE
C WHOSE VERTICES ARE I1, I2, AND I3.
C
C INPUT PARAMETERS -        KK - INDEX OF NODE TO BE
C                                INSERTED. KK .GE. 4.
C
C                     I1,I2,I3 - INDICES OF THE VERTICES OF
C                                A TRIANGLE CONTAINING NODE
C                                KK -- IN COUNTERCLOCKWISE
C                                ORDER.
C
C                         IADJ - SET OF ADJACENCY LISTS
C                                OF NODES IN THE MESH.
C
C                         IEND - POINTERS TO THE ENDS OF
C                                ADJACENCY LISTS IN IADJ FOR
C                                EACH NODE IN THE MESH.
C
C IADJ AND IEND MAY BE CREATED BY TRMESH AND MUST CONTAIN
C THE VERTICES I1, I2, AND I3. I1,I2,I3 MAY BE DETERMINED
C BY TRFIND.
C
C KK, I1, I2, AND I3 ARE NOT ALTERED BY THIS ROUTINE.
C
C OUTPUT PARAMETERS - IADJ,IEND - UPDATED WITH THE ADDITION
C OF NODE KK AS THE LAST
C ENTRY. NODE KK WILL BE
C CONNECTED TO NODES I1, I2,
C AND I3. NO OPTIMIZATION
C OF THE MESH IS PERFORMED.
C
C MODULE REFERENCED BY INTADD - SHIFTD
C
C INTRINSIC FUNCTION CALLED BY INTADD - MOD
C
C***********************************************************
C
C LOCAL PARAMETERS -
C
C K = LOCAL COPY OF KK
C KM1 = K - 1
C N = VECTOR CONTAINING I1, I2, I3
C NFT = POINTERS TO THE TOPS OF THE 3 SETS OF IADJ
C ELEMENTS TO BE SHIFTED DOWNWARD
C IP1, IP2, IP3 = PERMUTATION INDICES FOR N AND NFT
C INDX = INDEX FOR IADJ AND N
C NF, NL = INDICES OF FIRST AND LAST ENTRIES IN IADJ
C TO BE SHIFTED DOWN
C N1, N2 = FIRST 2 VERTICES OF A NEW TRIANGLE --
C (N1, N2, KK)
C IMIN, IMAX = BOUNDS ON DO-LOOP INDEX -- FIRST AND LAST
C ELEMENTS OF IEND TO BE INCREMENTED
C I = DO-LOOP INDEX
C ITEMP = TEMPORARY STORAGE LOCATION
C
K = KK
C
C INITIALIZATION
C
N(1) = I1
N(2) = I2
N(3) = I3
C
C SET UP NFT
C
DO 2 I = 1, 3
   N1 = N(I)
   INDX = MOD(I, 3) + 1
   N2 = N(INDX)
   INDX = IEND(N1) + 1
2 CONTINUE
C
C FIND THE INDEX OF N2 AS A NEIGHBOR OF N1
C
1   INDX = INDX - 1
   IF (IADJ(INDX) .NE. N2) GO TO 1
   NFT(I) = INDX + 1
2 CONTINUE
C
C ORDER THE VERTICES BY DECREASING MAGNITUDE.
C N(IP(I+1)) PRECEDES N(IP(I)) IN IEND FOR
C I = 1, 2.
C
   IP1 = 1
   IP2 = 2
   IP3 = 3
   IF (N(2) .LE. N(1)) GO TO 3
   IP1 = 2
IP2 = 1
3 IF ( N(3) .LE. N(IP1) ) GO TO 4
   IP3 = IP1
   IP1 = 3
4 IF ( N(IP3) .LE. N(IP2) ) GO TO 5
   ITEMP = IP2
   IP2 = IP3
   IP3 = ITEMP
C
C ADD NODE K TO THE ADJACENCY LISTS OF EACH VERTEX AND
C UPDATE IEND. FOR EACH VERTEX, A SET OF IADJ ELEMENTS
C IS SHIFTED DOWNWARD AND K IS INSERTED. SHIFTING STARTS
C AT THE END OF THE ARRAY.
C
5 KM1 = K - 1
   NL = IEND(KM1)
   NF = NFT(IP1)
   IF ( NF .LE. NL ) CALL SHIFTD(NF,NL,3, IADJ )
   IADJ(NF+2) = K
   IMIN = N(IP1)
   IMAX = KM1
   DO 6 I = IMIN,IMAX
       IEND(I) = IEND(I) + 3
   6 CONTINUE
C
   NL = NF - 1
   NF = NFT(IP2)
   CALL SHIFTD(NF,NL,2, IADJ )
   IADJ(NF+1) = K
   IMAX = IMIN - 1
   IMIN = N(IP2)
   DO 7 I = IMIN,IMAX
       IEND(I) = IEND(I) + 2
   7 CONTINUE
C
   NL = NF - 1
   NF = NFT(IP3)
   CALL SHIFTD(NF,NL,1, IADJ )
   IADJ(NF) = K
   IMAX = IMIN - 1
   IMIN = N(IP3)
   DO 8 I = IMIN,IMAX
       IEND(I) = IEND(I) + 1
   8 CONTINUE
C
C ADD NODE K TO IEND AND ITS NEIGHBORS TO IADJ
C
   INDX = IEND(KM1)
   IEND(K) = INDX + 3
   DO 9 I = 1,3
INDX = INDX + 1
IADJ(INDX) = N(I)
9 CONTINUE
RETURN
END
SUBROUTINE INTRC0 (N,PX,PY,X,Y,Z,IADJ,IEND, IST, PZ, IER)
INTEGER N, IADJ(1), IEND(N), IST, IER
REAL PX, PY, X(N), Y(N), Z(N), PZ

C***********************************************************
C
C                                               ROBERT RENKA
C                                       OAK RIDGE NATL. LAB.
C                                             (615) 576-5139
C
C GIVEN A TRIANGULATION OF A SET OF POINTS IN THE PLANE,
C THIS ROUTINE COMPUTES THE VALUE AT (PX,PY) OF A PIECEWISE
C LINEAR SURFACE WHICH INTERPOLATES DATA VALUES AT THE
C VERTICES OF THE TRIANGLES. THE SURFACE IS EXTENDED IN A
C CONTINUOUS FASHION BEYOND THE BOUNDARY OF THE TRIANGULAR
C MESH, ALLOWING EXTRAPOLATION. INTRC0 IS PART OF AN
C INTERPOLATION PACKAGE WHICH PROVIDES ROUTINES TO GENERATE,
C UPDATE, AND PLOT THE MESH.
C
C INPUT PARAMETERS -     N - NUMBER OF NODES IN THE MESH.
C                   N .GE. 3.
C
C            PX,PY - POINT AT WHICH THE INTERPOLATED
C               VALUE IS DESIRED.
C
C            X,Y  - VECTORS OF COORDINATES OF THE
C               NODES IN THE MESH.
C
C            Z  - VECTOR OF DATA VALUES AT THE
C               NODES.
C
C            IADJ  - SET OF ADJACENCY LISTS OF NODES
C               IN THE MESH.
C
C            IEND  - POINTERS TO THE ENDS OF
C               ADJACENCY LISTS IN IADJ FOR
C               EACH NODE IN THE MESH.
C
C            IST  - INDEX OF THE STARTING NODE IN
C               THE SEARCH FOR A TRIANGLE CON-
C               TAINING (PX,PY).  1 .LE. IST
C               .LE. N.  THE OUTPUT VALUE OF
C               IST FROM A PREVIOUS CALL MAY
C               BE A GOOD CHOICE.
C IADJ AND IEND MAY BE CREATED BY TRMESH.
C
C INPUT PARAMETERS OTHER THAN IST ARE NOT ALTERED BY THIS
C ROUTINE.
C
C OUTPUT PARAMETERS - IST - INDEX OF ONE OF THE VERTICES OF
C THE TRIANGLE CONTAINING (PX,PY)
C UNLESS IER .LT. 0.
C
C PZ - VALUE OF THE INTERPOLATORY
C SURFACE AT (PX,PY) OR ZERO
C IF IER .LT. 0.
C
C IER - ERROR INDICATOR
C IER = 0 IF NO ERRORS WERE
C ENCOUNTERED.
C IER = 1 IF NO ERRORS WERE EN-
C COUNTED AND EXTRAPRO-
C LATION WAS PERFORMED.
C IER = -1 IF N OR IST IS OUT OF
C RANGE.
C IER = -2 IF THE NODES ARE COL-
C LINEAR.
C
C MODULES REFERENCED BY INTRC0 - TRFIND, COORDS
C
C***********************************************************
C
INTEGER I1, I2, I3, N1, N2, INDX
REAL XP, YP, R(3), X1, Y1, X2, Y2, DP
C
C LOCAL PARAMETERS -
C
C I1,I2,I3 = VERTEX INDICES RETURNED BY TRFIND
C N1,N2 = ENDPOINTS OF THE CLOSEST BOUNDARY EDGE TO P
C WHEN P IS OUTSIDE OF THE MESH BOUNDARY
C INDX = IADJ INDEX OF N1 AS A NEIGHBOR OF N2
C XP,YP = LOCAL COPIES OF THE COORDINATES OF P=(PX,PY)
C R = BARYCENTRIC COORDINATES
C X1,Y1 = X,Y COORDINATES OF N1
C X2,Y2 = X,Y COORDINATES OF N2
C DP = INNER PRODUCT OF N1-N2 AND P-N2
C
IF (N .LT. 3 .OR. IST .LT. 1 .OR. IST .GT. N)
   GO TO 5
XP = PX
YP = PY
C
C FIND A TRIANGLE CONTAINING P IF P IS WITHIN THE MESH
BOUNDARY

CALL TRFIND(IST,XP,YP,X,Y,IADJ,IEND, I1,I2,I3)
IF (I1 .EQ. 0) GO TO 6
IST = I1
IF (I3 .EQ. 0) GO TO 1

CALL COORDS(XP,YP,X(I1),X(I2),X(I3),Y(I1),Y(I2),
   Y(I3), R,IER)
IF (IER .NE. 0) GO TO 6
PZ = R(1)*Z(I1) + R(2)*Z(I2) + R(3)*Z(I3)
RETURN

P IS OUTSIDE OF THE MESH BOUNDARY. EXTRAPOLATE TO P BY
EXTENDING THE INTERPOLATORY SURFACE AS A CONSTANT
BEYOND THE BOUNDARY. THUS PZ IS THE SURFACE FUNCTION
VALUE AT Q WHERE Q IS THE CLOSEST BOUNDARY POINT TO P.

DETERMINE Q BY TRAVERSING THE BOUNDARY STARTING FROM THE
RIGHTMOST VISIBLE NODE I1.

1 N2 = I1

SET N1 TO THE LAST NONZERO NEIGHBOR OF N2 AND COMPUTE DP

2 INDX = IEND(N2) - 1
   N1 = IADJ(INDX)
   X1 = X(N1)
   Y1 = Y(N1)
   X2 = X(N2)
   Y2 = Y(N2)
   DP = (X1-X2)*(XP-X2) + (Y1-Y2)*(YP-Y2)
   IF (DP .LE. 0.) GO TO 3
   IF ((XP-X1)*(X2-X1) + (YP-Y1)*(Y2-Y1) .GT. 0.) GO TO 4
   N2 = N1
   GO TO 2

N2 IS THE CLOSEST BOUNDARY POINT TO P

3 PZ = Z(N2)
   IER = 1
   RETURN

THE CLOSEST BOUNDARY POINT TO P LIES ON N2-N1. COMPUTE
ITS COORDINATES WITH RESPECT TO N2-N1.

4 R(1) = DP/((X2-X1)**2 + (Y2-Y1)**2 )
   R(2) = 1. - R(1)
PZ = R(1)*Z(N1) + R(2)*Z(N2)
IER = 1
RETURN

C
N .LT. 3 OR IST IS OUT OF RANGE
C
5 PZ = 0.
IER = -1
RETURN
C
NODES ARE COLLINEAR
C
6 PZ = 0.
IER = -2
RETURN
END
SUBROUTINE PERMUT (NN, IP, A)
INTEGER NN, IP (NN)
REAL A(NN)
C
C***********************************************************
C
C                                               ROBERT RENKA
C                                       OAK RIDGE NATL. LAB.
C                                             (615) 576-5139
C
C   THIS ROUTINE APPLIES A SET OF PERMUTATIONS TO A VECTOR.
C
C INPUT PARAMETERS - NN - LENGTH OF A AND IP.
C
C                    IP - VECTOR CONTAINING THE SEQUENCE OF
C                         INTEGERS 1,...,NN PERMUTED IN THE
C                         SAME FASHION THAT A IS TO BE PER-
C                         MUTED.
C
C                     A - VECTOR TO BE PERMUTED.
C
C NN AND IP ARE NOT ALTERED BY THIS ROUTINE.
C
C OUTPUT PARAMETERS - A - REORDERED VECTOR REFLECTING THE
C PERMUTATIONS DEFINED BY IP.
C
C MODULES REFERENCED BY PERMUT - NONE
C
C***********************************************************
C
INTEGER N, K, J, IPJ
REAL TEMP
C
C LOCAL PARAMETERS -
C
N = LOCAL COPY OF NN
C K = INDEX FOR IP AND FOR THE FIRST ELEMENT OF A IN A
C PERMUTATION
C J = INDEX FOR IP AND A, J .GE. K
C IPJ = IP(J)
C TEMP = TEMPORARY STORAGE FOR A(K)
C
N = NN
IF (N .LT. 2) RETURN
K = 1
C
C LOOP ON PERMUTATIONS
C
1 J = K
TEMP = A(K)
C
C APPLY PERMUTATION TO A. IP(J) IS MARKED (MADE NEGATIVE)
C AS BEING INCLUDED IN THE PERMUTATION.
C
2 IPJ = IP(J)
IP(J) = -IPJ
IF (IPJ .EQ. K) GO TO 3
A(J) = A(IPJ)
J = IPJ
GO TO 2
3 A(J) = TEMP
C
C SEARCH FOR AN UNMARKED ELEMENT OF IP
C
4 K = K + 1
IF (K .GT. N) GO TO 5
IF (IP(K) .GT. 0) GO TO 1
GO TO 4
C
C ALL PERMUTATIONS HAVE BEEN APPLIED. UNMARK IP.
C
5 DO 6 K = 1,N
IP(K) = -IP(K)
6 CONTINUE
RETURN
END

SUBROUTINE QSORT (N,X, IND)
INTEGER N, IND(N)
REAL X(N)
C
C******************************************************************************
C
C
C ROBERT RENKA
C
C OAK RIDGE NATL. LAB.
C
C******************************************************************************
THIS SUBROUTINE USES AN ORDER $N \cdot \log(N)$ QUICK SORT TO
SORT THE REAL ARRAY $X$ INTO INCREASING ORDER. THE ALGORITHM IS AS FOLLOWS. $IND$ IS INITIALIZED TO THE ORDERED
SEQUENCE OF INDICES $1, \ldots, N$, AND ALL INTERCHANGES ARE
APPLIED TO $IND$. $X$ IS DIVIDED INTO TWO PORTIONS BY PICKING
A CENTRAL ELEMENT $T$. THE FIRST AND LAST ELEMENTS ARE COM-
PARED WITH $T$, AND INTERCHANGES ARE APPLIED AS NECESSARY SO
THAT THE THREE VALUES ARE IN ASCENDING ORDER. INTER-
CHANGES ARE THEN APPLIED SO THAT ALL ELEMENTS GREATER THAN
$T$ ARE IN THE UPPER PORTION OF THE ARRAY AND ALL ELEMENTS
LESS THAN $T$ ARE IN THE LOWER PORTION. THE UPPER AND LOWER
INDICES OF ONE OF THE PORTIONS ARE SAVED IN LOCAL ARRAYS,
AND THE PROCESS IS REPEATED ITERATIVELY ON THE OTHER
PORTION. WHEN A PORTION IS COMPLETELY SORTED, THE PROCESS
BEGIN AGAIN BY RETRIEVING THE INDICES BOUNDING ANOTHER
UNSORTED PORTION.

INPUT PARAMETERS - $N$ - LENGTH OF THE ARRAY $X$.

$X$ - VECTOR OF LENGTH $N$ TO BE SORTED.

$IND$ - VECTOR OF LENGTH $\geq N$.

$N$ AND $X$ ARE NOT ALTERED BY THIS ROUTINE.

OUTPUT PARAMETER - $IND$ - SEQUENCE OF INDICES $1, \ldots, N$
PERMUTED IN THE SAME FASHION AS $X$
WOULD BE. THUS, THE ORDERING ON
$X$ IS DEFINED BY $Y(I) = X(IND(I))$.

MODULES REFERENCED BY QSORT - NONE

INTRINSIC FUNCTIONS CALLED BY QSORT - IFIX, FLOAT

NOTE -- $IU$ AND $IL$ MUST BE DIMENSIONED $\geq \log(N)$ WHERE
$\log$ HAS BASE 2.

IU,IL = TEMPORARY STORAGE FOR THE UPPER AND LOWER
INDICES OF PORTIONS OF THE ARRAY X

M = INDEX FOR IU AND IL
I,J = LOWER AND UPPER INDICES OF A PORTION OF X
K,L = INDICES IN THE RANGE I,...,J
IJ = RANDOMLY CHOSEN INDEX BETWEEN I AND J
IT,ITT = TEMPORARY STORAGE FOR INTERCHANGES IN IND
INDX = TEMPORARY INDEX FOR X
R = PSEUDO RANDOM NUMBER FOR GENERATING IJ
T = CENTRAL ELEMENT OF X

IF (N .LE. 0) RETURN

DO 1 I = 1,N
    IND(I) = I
  1 CONTINUE
M = 1
I = 1
J = N
R = .375

TOP OF LOOP

IF (I .GE. J) GO TO 10
IF (R .GT. .5898437) GO TO 3
R = R + .0390625
GO TO 4
3 R = R - .21875

INITIALIZE K

K = I

SELECT A CENTRAL ELEMENT OF X AND SAVE IT IN T

IJ = I + IFIX(R*FLOAT(J-I))
IT = IND(IJ)
T = X(IT)

IF THE FIRST ELEMENT OF THE ARRAY IS GREATER THAN T,
INTERCHANGE IT WITH T

INDX = IND(I)
IF (X(INDX) .LE. T) GO TO 5
IND(IJ) = INDX
IND(I) = IT
IT = INDX
T = X(IT)
C INITIALIZE L

C 5 L = J

C IF THE LAST ELEMENT OF THE ARRAY IS LESS THAN T, INTERCHANGE IT WITH T

C INDX = IND(J)
IF (X(INDX) .GE. T) GO TO 7
IND(IJ) = INDX
IND(J) = IT
IT = INDX
T = X(IT)

C IF THE FIRST ELEMENT OF THE ARRAY IS GREATER THAN T, INTERCHANGE IT WITH T

C INDX = IND(I)
IF (X(INDX) .LE. T) GO TO 7
IND(IJ) = INDX
IND(I) = IT
IT = INDX
T = X(IT)
GO TO 7

C INTERCHANGE ELEMENTS K AND L

C 6 ITT = IND(L)
IND(L) = IND(K)
IND(K) = ITT

C FIND AN ELEMENT IN THE UPPER PART OF THE ARRAY WHICH IS NOT LARGER THAN T

C 7 L = L - 1
INDX = IND(L)
IF (X(INDX) .GT. T) GO TO 7

C FIND AN ELEMENT IN THE LOWER PART OF THE ARRAY WHICH IS NOT SMALLER THAN T

C 8 K = K + 1
INDX = IND(K)
IF (X(INDX) .LT. T) GO TO 8

C IF K .LE. L, INTERCHANGE ELEMENTS K AND L

C IF (K .LE. L) GO TO 6

C SAVE THE UPPER AND LOWER SUBSCRIPTS OF THE PORTION OF THE
C ARRAY YET TO BE SORTED
C
IF (L-I .LE. J-K) GO TO 9
IL(M) = I
IU(M) = L
I = K
M = M + 1
GO TO 11
C
9 IL(M) = K
IU(M) = J
J = L
M = M + 1
GO TO 11
C
C BEGIN AGAIN ON ANOTHER UNSORTED PORTION OF THE ARRAY
C
10 M = M - 1
IF (M .EQ. 0) RETURN
I = IL(M)
J = IU(M)
C
11 IF (J-I .GE. 11) GO TO 4
IF (I .EQ. 1) GO TO 2
I = I - 1
C
C SORT ELEMENTS I+1, ..., J. NOTE THAT 1 .LE. I .LT. J AND
C J-I .LT. 11.
C
12 I = I + 1
IF (I .EQ. J) GO TO 10
INDX = IND(I+1)
T = X(INDX)
IT = INDX
INDX = IND(I)
IF (X(INDX) .LE. T) GO TO 12
K = I
C
13 IND(K+1) = IND(K)
K = K - 1
INDX = IND(K)
IF (T .LT. X(INDX)) GO TO 13
IND(K+1) = IT
GO TO 12
END
SUBROUTINE REORDR (N,IFLAG, A,B,C, IND)
INTEGER N, IFLAG, IND(N)
REAL A(N), B(N), C(N)
C
C************************************************************************
THIS SUBROUTINE USES AN ORDER $N \times \log(N)$ QUICK SORT TO
REORDER THE REAL ARRAY $A$ INTO INCREASING ORDER. A RECORD
OF THE PERMUTATIONS APPLIED TO $A$ IS STORED IN $IND$, AND
THES$E$ PERMUTATIONS MAY BE APPLIED TO ONE OR TWO ADDITIONAL
VECTORS BY THIS ROUTINE. ANY OTHER VECTOR $V$ MAY BE PER-
MUTED IN THE SAME FASHION BY CALLING SUBROUTINE $PERMUT$
WITH $N$, $IND$, AND $V$ AS PARAMETERS.
A SET OF NODES $(X(I), Y(I))$ AND DATA VALUES $Z(I)$ MAY BE
PREPROCESSED BY $REORDR$ FOR INCREASED EFFICIENCY IN THE
TRIANGULATION ROUTINE $TRMESH$. EFFICIENCY IS INCREASED BY
A FACTOR OF APPROXIMATELY $\sqrt{N}/6$ FOR RANDOMLY DISTRIBUTED
NODES, AND THE PREPROCESSING IS ALSO USEFUL FOR
DETECTING DUPLICATE NODES. EITHER $X$ OR $Y$ MAY BE USED AS
THE SORT KEY (ASSOCIATED WITH $A$).

INPUT PARAMETERS - $N$ - NUMBER OF NODES.

IFLAG - NUMBER OF VECTORS TO BE PERMUTED.
IFLAG .LE. 0 IF $A$, $B$, AND $C$ ARE TO
REMAIN UNALTERED.
IFLAG .EQ. 1 IF ONLY $A$ IS TO BE
PERMUTED.
IFLAG .EQ. 2 IF $A$ AND $B$ ARE TO BE
PERMUTED.
IFLAG .GE. 3 IF $A$, $B$, AND $C$ ARE TO
BE PERMUTED.

$A, B, C$ - VECTORS OF LENGTH $N$ TO BE SORTED
(ON THE COMPONENTS OF $A$), OR DUMMY
PARAMETERS, DEPENDING ON IFLAG.

IND - VECTOR OF LENGTH .GE. $N$.

$N$, IFLAG, AND ANY DUMMY PARAMETERS ARE NOT ALTERED BY THIS
ROUTINE.

OUTPUT PARAMETERS - $A, B, C$ - SORTED OR UNALTERED VECTORS.

IND - SEQUENCE OF INDICES $1, \ldots, N$
PERMUTED IN THE SAME FASHION
AS THE REAL VECTORS. THUS,
THE ORDERING MAY BE APPLIED TO
A REAL VECTOR $V$ AND STORED IN
$W$ BY SETTING $W(I) = V(IND(I))$, OR $V$ MAY BE OVERWRITTEN WITH
THE ORDERING BY A CALL TO PERMUT.

MODULES REFERENCED BY REORDR – QSORT, PERMUT

*******************************************************************

INTEGER NN, NV

LOCAL PARAMETERS –

NN = LOCAL COPY OF N
NV = LOCAL COPY OF IFLAG

NN = N
NV = IFLAG
CALL QSORT(NN,A, IND)
IF (NV .LE. 0) RETURN
CALL PERMUT(NN,IND, A )
IF (NV .EQ. 1) RETURN
CALL PERMUT(NN,IND, B )
IF (NV .EQ. 2) RETURN
CALL PERMUT(NN,IND, C )
RETURN
END

SUBROUTINE SHIFTD (NFRST,NLAST,KK, IARR )
INTEGER NFRST, NLAST, KK, IARR(1)

*******************************************************************

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THIS ROUTINE SHIFTS A SET OF CONTIGUOUS ELEMENTS OF AN
INTEGER ARRAY KK POSITIONS DOWNWARD (UPWARD IF KK .LT. 0).
THE LOOPS ARE UNROLLED IN ORDER TO INCREASE EFFICIENCY.

INPUT PARAMETERS – NFRST,NLAST – BOUNDS ON THE PORTION OF
IARR TO BE SHIFTED. ALL ELEMENTS BETWEEN AND INCLUDING THE BOUNDS ARE
SHIFTED UNLESS NFRST .GT. NLAST, IN WHICH CASE NO SHIFT OCCURS.

KK – NUMBER OF POSITIONS EACH ELEMENT IS TO BE SHIFTED.
IF KK .LT. 0 SHIFT UP.
IF KK .GT. 0 SHIFT DOWN.
C
C       IARR - INTEGER ARRAY OF LENGTH .GE. NLAST + MAX(KK,0).
C
C NFRST, NLAST, AND KK ARE NOT ALTERED BY THIS ROUTINE.
C
C OUTPUT PARAMETER -    IARR - SHIFTED ARRAY.
C
C MODULES REFERENCED BY SHIFTD - NONE
C
C***************************************************************************
C
INTEGER INC, K, NF, NL, NLP1, NS, NSL, I, IBAK, INDX, IMAX
DATA INC/5/

C
C LOCAL PARAMETERS -
C
C INC = DO-LOOP INCREMENT (UNROLLING FACTOR) -- IF INC IS
C       CHANGED, STATEMENTS MUST BE ADDED TO OR DELETED
C FROM THE DO-LOOPS
C K = LOCAL COPY OF KK
C NF = LOCAL COPY OF NFRST
C NL = LOCAL COPY OF NLAST
C NLP1 = NL + 1
C NS = NUMBER OF SHIFTS
C NSL = NUMBER OF SHIFTS DONE IN UNROLLED DO-LOOP (MULTIPLE
C       OF INC)
C I = DO-LOOP INDEX AND INDEX FOR IARR
C IBAK = INDEX FOR DOWNWARD SHIFT OF IARR
C INDX = INDEX FOR IARR
C IMAX = BOUND ON DO-LOOP INDEX
C
K = KK
NF = NFRST
NL = NLAST
IF (NF .GT. NL  .OR.  K .EQ. 0) RETURN
NLP1 = NL + 1
NS = NLP1 - NF
NSL = INC*(NS/INC)
IF ( K .LT. 0) GO TO 4

C
C SHIFT DOWNWARD STARTING FROM THE BOTTOM
C
IF (NSL .LE. 0) GO TO 2
DO 1 I = 1,NSL,INC
   IBAK = NLP1 - I
   INDX = IBAK + K
   IARR(INDX) = IARR(IBAK)
   IARR(INDX-1) = IARR(IBAK-1)
1 CONTINUE

C
C***************************************************************************
IARR(INDX-2) = IARR(IBAK-2)
IARR(INDX-3) = IARR(IBAK-3)
IARR(INDX-4) = IARR(IBAK-4)
1 CONTINUE
C
C PERFORM THE REMAINING NS-NSL SHIFTS ONE AT A TIME
C
2 IBAK = NLP1 - NSL
3 IF (IBAK .LE. NF) RETURN
   IBAK = IBAK - 1
   INDX = IBAK + K
   IARR(INDX) = IARR(IBAK)
   GO TO 3
C
C SHIFT UPWARD STARTING FROM THE TOP
C
4 IF (NSL .LE. 0) GO TO 6
   IMAX = NLP1 - INC
   DO 5 I = NF,IMAX,INC
      INDX = I + K
      IARR(INDX) = IARR(I)
      IARR(INDX+1) = IARR(I+1)
      IARR(INDX+2) = IARR(I+2)
      IARR(INDX+3) = IARR(I+3)
      IARR(INDX+4) = IARR(I+4)
   5 CONTINUE
C
C PERFORM THE REMAINING NS-NSL SHIFTS ONE AT A TIME
C
6 I = NSL + NF
7 IF (I .GT. NL) RETURN
   INDX = I + K
   IARR(INDX) = IARR(I)
   I = I + 1
   GO TO 7
END
SUBROUTINE SWAP (NIN1,NIN2,NOUT1,NOUT2, IADJ,IEND )
INTEGER NIN1, NIN2, NOUT1, NOUT2, IADJ(1), IEND(1)
EXTERNAL INDEX
C
C********************************************************************
C
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C (615) 576-5139
C
C THIS SUBROUTINE SWAPS THE DIAGONALS IN A CONVEX QUADRI-
C LATERAL.
C
C INPUT PARAMETERS -  NIN1,NIN2,NOUT1,NOUT2 - NODAL INDICES
OF A PAIR OF ADJACENT TRIANGLES

WHICH FORM A CONVEX QUADRILATERAL. NOUT1 AND NOUT2 ARE CONNECTED BY AN ARC WHICH IS TO BE REPLACED BY THE ARC NIN1-NIN2. (NIN1,NOUT1,NOUT2) MUST BE TRIANGLE VERTICES IN COUNTERCLOCKWISE ORDER.

THE ABOVE PARAMETERS ARE NOT ALTERED BY THIS ROUTINE.

IADJ,IEND - TRIANGULATION DATA STRUCTURE (SEE SUBROUTINE TRMESH).

OUTPUT PARAMETERS - IADJ,IEND - UPDATED WITH THE ARC REPLACEMENT.

MODULES REFERENCED BY SWAP - INDEX, SHIFTD

***********************************************************

INTEGER IN(2), IO(2), IP1, IP2, J, K, NF, NL, I, .
  IMIN, IMAX

LOCAL PARAMETERS -

IN = NIN1 AND NIN2 ORDERED BY INCREASING MAGNITUDE (THE NEIGHBORS OF IN(1) PRECEDE THOSE OF IN(2) IN IADJ)

IO = NOUT1 AND NOUT2 IN INCREASING ORDER

IP1,IP2 = PERMUTATION OF (1,2) SUCH THAT IO(IP1)

J,K = PERMUTATION OF (1,2) USED AS INDICES OF IN AND IO

NF,NL = IADJ INDICES BOUNDARY A PORTION OF THE ARRAY TO BE SHIFTED

I = IEND INDEX

IMIN,IMAX = BOUNDS ON THE PORTION OF IEND TO BE INCREASED OR DECREASED

IN(1) = NIN1
IN(2) = NIN2
IO(1) = NOUT1
IO(2) = NOUT2
IP1 = 1

ORDER THE INDICES SO THAT IN(1) LT. IN(2) AND IO(1) LT. IO(2), AND CHOOSE IP1 AND IP2 SUCH THAT (IN(1),IO(IP1), IO(IP2)) FORMS A TRIANGLE.
IF (IN(1) .LT. IN(2)) GO TO 1
IN(1) = IN(2)
IN(2) = NIN1
IP1 = 2
1 IF (IO(1) .LT. IO(2)) GO TO 2
IO(1) = IO(2)
IO(2) = NOUT1
IP1 = 3 - IP1
2 IP2 = 3 - IP1
IF (IO(2) .LT. IN(1)) GO TO 8
IF (IN(2) .LT. IO(1)) GO TO 12
C
IN(1) AND IO(1) PRECEDE IN(2) AND IO(2). FOR (J,K) =
(1,2) AND (2,1), DELETE IO(K) AS A NEIGHBOR OF IO(J)
BY SHIFTING A PORTION OF IADJ EITHER UP OR DOWN AND
INSERT IN(K) AS A NEIGHBOR OF IN(J).
C
DO 7 J = 1,2
   K = 3 - J
   IF (IN(J) .GT. IO(J)) GO TO 4
C
C   THE NEIGHBORS OF IN(J) PRECEDE THOSE OF IO(J) -- SHIFT
C   DOWN BY 1
C
   NF = 1 + INDEX(IN(J),IO(IP1),IADJ,IEND)
   NL = -1 + INDEX(IO(J),IO(K),IADJ,IEND)
   IF (NF .LE. NL) CALL SHIFTD(NF,NL,1, IADJ )
   IADJ(NF) = IN(K)
   IMIN = IN(J)
   IMAX = IO(J)-1
   DO 3 I = IMIN,IMAX
      IEND(I) = IEND(I) + 1
      GO TO 6
C
C   THE NEIGHBORS OF IO(J) PRECEDE THOSE OF IN(J) -- SHIFT
C   UP BY 1
C
   4 NF = 1 + INDEX(IO(J),IO(KP),IADJ,IEND)
   NL = -1 + INDEX(IN(J),IO(IP2),IADJ,IEND)
   IF (NF .LE. NL) CALL SHIFTD(NF,NL,-1, IADJ )
   IADJ(NL) = IN(K)
   IMIN = IO(J)
   IMAX = IN(J) - 1
   DO 5 I = IMIN,IMAX
      IEND(I) = IEND(I) - 1
      GO TO 6
C
C   REVERSE (IP1,IP2) FOR (J,K) = (2,1)
C
6 IP1 = IP2
   IP2 = 3 - IP1
7    CONTINUE
     RETURN
C
C THE VERTICES ARE ORDERED (IO(1),IO(2),IN(1),IN(2)).
C DELETE IO(2) BY SHIFTING UP BY 1
C
8  NF = 1 + INDEX(IO(1),IO(2),IADJ,IEND)
   NL = -1 + INDEX(IO(2),IO(1),IADJ,IEND)
   IF (NF .LE. NL) CALL SHIFTD(NF,NL,-1, IADJ )
   IMIN = IO(1)
   IMAX = IO(2)-1
   DO 9 I = IMIN,IMAX
9    IEND(I) = IEND(I) - 1
C
C THE VERTICES ARE ORDERED (IO(1),IO(2),IN(1),IN(2)).
C DELETE IO(1) BY SHIFTING UP BY 2 AND INSERT IN(2)
C
10  NF = NL + 2
    NL = -1 + INDEX(IN(1),IO(IP2),IADJ,IEND)
    IF (NF .LE. NL) CALL SHIFTD(NF,NL,-2, IADJ )
    IADJ(NL-1) = IN(2)
    IMIN = IO(2)
    IMAX = IN(1)-1
    DO 10 I = IMIN,IMAX
11   IEND(I) = IEND(I) - 2
     RETURN
C
C THE VERTICES ARE ORDERED (IN(1),IN(2),IO(1),IO(2)).
C DELETE IO(1) BY SHIFTING DOWN BY 1
C
12  NF = 1 + INDEX(IO(1),IO(2),IADJ,IEND)
    NL = -1 + INDEX(IO(2),IO(1),IADJ,IEND)
    IF (NF .LE. NL) CALL SHIFTD(NF,NL, 1, IADJ )
    IMIN = IO(1)
    IMAX = IO(2) - 1
    DO 13 I = IMIN,IMAX
13   IEND(I) = IEND(I) + 1
     RETURN
C
C THE VERTICES ARE ORDERED (IN(1),IN(2),IO(1),IO(2)).
C DELETE IO(2) BY SHIFTING DOWN BY 2 AND INSERT IN(1)
C
14  NF = 1 + INDEX(IO(1),IO(2),IADJ,IEND)
    NL = -1 + INDEX(IO(2),IO(1),IADJ,IEND)
    IF (NF .LE. NL) CALL SHIFTD(NF,NL, 1, IADJ )
    IMIN = IO(1)
    IMAX = IO(2) - 1
    DO 15 I = IMIN,IMAX
15   IEND(I) = IEND(I) + 1
     RETURN
NL = NF - 2
NF = 1 + INDEX(IN(2), IO(IP2), IADJ, IEND)
IF (NF .LE. NL) CALL SHIFTD(NF, NL, 2, IADJ)
IADJ(NF+1) = IN(1)
IMIN = IN(2)
IMAX = IO(1) - 1
DO 14 I = IMIN, IMAX
    IEND(I) = IEND(I) + 2
14   IADJ(NF+1) = IN(1)
C
C   SHIFT DOWN BY 1 AND INSERT IN(2)
C
NL = NF - 1
NF = 1 + INDEX(IN(1), IO(IP1), IADJ, IEND)
CALL SHIFTD(NF, NL, 1, IADJ)
IADJ(NF) = IN(2)
IMIN = IN(1)
IMAX = IN(2) - 1
DO 15 I = IMIN, IMAX
    IEND(I) = IEND(I) + 1
15   IEND(I) = IEND(I) + 1
RETURN
END
LOGICAL FUNCTION SWPTST(IN1, IN2, IO1, IO2, X, Y)
INTEGER IN1, IN2, IO1, IO2
REAL X(1), Y(1)
C
C***********************************************************
C
C                                               ROBERT RENKA
C                                       OAK RIDGE NATL. LAB.
C                                             (615) 576-5139
C
C   THIS FUNCTION DECIDES WHETHER OR NOT TO REPLACE A
C DIAGONAL ARC IN A QUADRILATERAL WITH THE OTHER DIAGONAL.
C THE DETERMINATION IS BASED ON THE SIZES OF THE ANGLES
C CONTAINED IN THE 2 TRIANGLES DEFINED BY THE DIAGONAL.
C THE DIAGONAL IS CHOSEN TO MAXIMIZE THE SMALLEST OF THE
C SIX ANGLES OVER THE TWO PAIRS OF TRIANGLES.
C
C INPUT PARAMETERS -  IN1, IN2, IO1, IO2 - NODE INDICES OF THE
C FOUR POINTS DEFINING THE
C QUADRILATERAL.  IO1 AND IO2
C ARE CURRENTLY CONNECTED BY A
C DIAGONAL ARC.  THIS ARC
C SHOULD BE REPLACED BY AN ARC
C CONNECTING IN1, IN2 IF THE
C DECISION IS MADE TO SWAP.
C IN1, IO1, IO2 MUST BE IN
C COUNTERCLOCKWISE ORDER.
C
C X, Y - VECTORS OF NODAL COORDINATES.
(X(I),Y(I)) are the coordinates of node I for I = IN1, IN2, IO1, or IO2.

None of the input parameters are altered by this routine.

Output parameter - SWPTST - .TRUE. iff the arc connecting IO1 and IO2 is to be replaced.

Modules referenced by SWPTST - None

***********************************************************

REAL DX11, DX12, DX22, DX21, DY11, DY12, DY22, DY21,
   . SIN1, SIN2, COS1, COS2, SIN12

LOCAL PARAMETERS -

DX11, DY11 = X,Y coordinates of the vector IN1-IO1
DX12, DY12 = X,Y coordinates of the vector IN1-IO2
DX22, DY22 = X,Y coordinates of the vector IN2-IO2
DX21, DY21 = X,Y coordinates of the vector IN2-IO1

SIN1 = cross product of the vectors IN1-IO1 and IN1-IO2 -- proportional to sin(T1) where T1 is the angle at IN1 formed by the vectors.
COS1 = inner product of the vectors IN1-IO1 and IN1-IO2 -- proportional to cos(T1)
SIN2 = cross product of the vectors IN2-IO2 and IN2-IO1 -- proportional to sin(T2) where T2 is the angle at IN2 formed by the vectors.
COS2 = inner product of the vectors IN2-IO2 and IN2-IO1 -- proportional to cos(T2)
SIN12 = SIN1*COS2 + COS1*SIN2 -- proportional to sin(T1+T2)

SWPTST = .FALSE.

Compute the vectors containing the angles T1, T2

DX11 = X(IO1) - X(IN1)
DX12 = X(IO2) - X(IN1)
DX22 = X(IO2) - X(IN2)
DX21 = X(IO1) - X(IN2)

DY11 = Y(IO1) - Y(IN1)
DY12 = Y(IO2) - Y(IN1)
DY22 = Y(IO2) - Y(IN2)
DY21 = Y(IO1) - Y(IN2)

Compute inner products
C

\[ \cos_1 = DX_{11} \cdot DX_{12} + DY_{11} \cdot DY_{12} \]
\[ \cos_2 = DX_{22} \cdot DX_{21} + DY_{22} \cdot DY_{21} \]
C

THE DIAGONALS SHOULD BE SWAPPED IFF \((T_1+T_2) \geq 180\) DEGREES. THE FOLLOWING TWO TESTS INSURE NUMERICAL STABILITY.
C

\[
\text{IF } (\cos_1 \geq 0. \text{ AND } \cos_2 \geq 0.) \text{ RETURN}
\]
\[
\text{IF } (\cos_1 \lt 0. \text{ AND } \cos_2 \lt 0.) \text{ GO TO 1}
\]
C

COMPUTE VECTOR CROSS PRODUCTS
C

\[ \sin_1 = DX_{11} \cdot DY_{12} - DX_{12} \cdot DY_{11} \]
\[ \sin_2 = DX_{22} \cdot DY_{21} - DX_{21} \cdot DY_{22} \]
\[ \sin_{12} = \sin_1 \cdot \cos_2 + \cos_1 \cdot \sin_2 \]
\[
\text{IF } (\sin_{12} \geq 0.) \text{ RETURN}
\]
1

SWPTST = .TRUE.
RETURN
END

SUBROUTINE TRFIND (NST, PX, PY, X, Y, IADJ, IEND, I1, I2, I3)
INTEGER NST, IADJ(1), IEND(1), I1, I2, I3
REAL PX, PY, X(1), Y(1)
C
C***********************************************************
C
C                                               ROBERT RENKA
C                                       OAK RIDGE NATL. LAB.
C                                             (615) 576-5139
C
C   THIS ROUTINE LOCATES A POINT P IN A THIESSEN TRIANGU-
C LATION, RETURNING THE VERTEX INDICES OF A TRIANGLE WHICH
C CONTAINS P. TRFIND IS PART OF AN INTERPOLATION PACKAGE
C WHICH PROVIDES SUBROUTINES FOR CREATING THE MESH.
C
C INPUT PARAMETERS -    NST - INDEX OF NODE AT WHICH TRFIND
C                       BEGINS SEARCH. SEARCH TIME
C                       DEPENDS ON THE PROXIMITY OF
C                       NST TO P.
C
C                       PX, PY - X AND Y-COORDINATES OF THE
C                       POINT TO BE LOCATED.
C
C                       X, Y - VECTORS OF COORDINATES OF
C                       NODES IN THE MESH. \((X(I), Y(I))\)
C                       DEFINES NODE I FOR I = 1, \ldots, N
C                       WHERE N \geq 3.
C
C                       IADJ - SET OF ADJACENCY LISTS OF
C                       NODES IN THE MESH.
IEND - POINTERS TO THE ENDS OF
ADJACENCY LISTS IN IADJ FOR
EACH NODE IN THE MESH.

IADJ AND IEND MAY BE CREATED BY TRMESH.

INPUT PARAMETERS ARE NOT ALTERED BY THIS ROUTINE.

OUTPUT PARAMETERS - I1, I2, I3 - VERTEX INDICES IN COUNTER-
CLOCKWISE ORDER - VERTICES
OF A TRIANGLE CONTAINING P
IF P IS AN INTERIOR NODE.
IF P IS OUTSIDE OF THE
BOUNDARY OF THE MESH, I1
AND I2 ARE THE FIRST (RIGHT-
MOST) AND LAST (LEFTMOST)
NODES WHICH ARE VISIBLE
FROM P, AND I3 = 0. IF P
AND ALL OF THE NODES LIE ON
A SINGLE LINE THEN I1 = I2
= I3 = 0.

MODULES REFERENCED BY TRFIND - NONE

INTRINSIC FUNCTION CALLED BY TRFIND - MAX0

************************************************************

INTEGER N0, N1, N2, N3, N4, INDX, IND, NF,
   .   .   NL, NEXT
REAL XP, YP
LOGICAL LEFT

LOCAL PARAMETERS -

XP,YP = LOCAL VARIABLES CONTAINING PX AND PY
N0,N1,N2 = NODES IN COUNTERCLOCKWISE ORDER DEFINING A
   .   . CONE (WITH VERTEX N0) CONTAINING P
N3,N4 = NODES OPPOSITE N1-N2 AND N2-N1, RESPECTIVELY
INDX,IND = INDICES FOR IADJ
NF,NL = FIRST AND LAST NEIGHBORS OF N0 IN IADJ, OR
   .   . FIRST (RIGHTMOST) AND LAST (LEFTMOST) NODES
   .   . VISIBLE FROM P WHEN P IS OUTSIDE THE
   .   . BOUNDARY
NEXT = CANDIDATE FOR I1 OR I2 WHEN P IS OUTSIDE OF
   .   . THE BOUNDARY
LEFT = STATEMENT FUNCTION WHICH COMPUTES THE SIGN OF
   .   . A CROSS PRODUCT (Z-COMPONENT). LEFT(X1,...,
   .   . Y0) = .TRUE. IFF (X0,Y0) IS ON OR TO THE
LEFT(X1,Y1,X2,Y2,X0,Y0) = (X2-X1)*(Y0-Y1) .GE. (X0-X1)*(Y2-Y1)

XP = PX
YP = PY

C INITIALIZE VARIABLES AND FIND A CONE CONTAINING P

N0 = MAX0(NST,1)
1 INDX = IEND(N0)
NL = IADJ(INDX)
INDX = 1
IF (N0 .NE. 1) INDX = IEND(N0-1) + 1
NF = IADJ(INDX)
N1 = NF
IF (NL .NE. 0) GO TO 3

C N0 IS A BOUNDARY NODE. SET NL TO THE LAST NONZERO NEIGHBOR OF N0.

IND = IEND(N0) - 1
NL = IADJ(IND)
IF ( LEFT(X(N0),Y(N0),X(NF),Y(NF),XP,YP) ) GO TO 2

C P IS OUTSIDE THE BOUNDARY

NL = N0
GO TO 16
2 IF ( LEFT(X(NL),Y(NL),X(N0),Y(N0),XP,YP) ) GO TO 4

C P IS OUTSIDE THE BOUNDARY AND N0 IS THE RIGHTMOST VISIBLE BOUNDARY NODE

I1 = N0
GO TO 18

C N0 IS AN INTERIOR NODE. FIND N1.

3 IF ( LEFT(X(N0),Y(N0),X(N1),Y(N1),XP,YP) ) GO TO 4
INDX = INDX + 1
N1 = IADJ(INDX)
IF (N1 .EQ. NL) GO TO 7
GO TO 3

C P IS TO THE LEFT OF ARC N0-N1. INITIALIZE N2 TO THE NEXT NEIGHBOR OF N0.

4 INDX = INDX + 1
N2 = IADJ(INDX)
IF (.NOT. LEFT(X(N0),Y(N0),X(N2),Y(N2),XP,YP) )  
   GO TO 8
N1 = N2
IF (N1 .NE. NL) GO TO 4
IF (.NOT. LEFT(X(N0),Y(N0),X(NF),Y(NF),XP,YP) )  
   GO TO 7
IF (XP .EQ. X(N0) .AND. YP .EQ. Y(N0)) GO TO 6

C P IS LEFT OF OR ON ARCS N0-NB FOR ALL NEIGHBORS NB OF N0.
C ALL POINTS ARE COLLINEAR IFF P IS LEFT OF NB-N0 FOR ALL NEIGHBORS NB OF N0. SEARCH THE NEIGHBORS OF N0 IN REVERSE ORDER. NOTE -- N1 = NL AND INDX POINTS TO NL.

5 IF (.NOT. LEFT(X(N1),Y(N1),X(N0),Y(N0),XP,YP) )  
   GO TO 6
   IF (N1 .EQ. NF) GO TO 20
   INDX = INDX - 1
   N1 = IADJ(INDX)
   GO TO 5

C P IS TO THE RIGHT OF N1-N0, OR P=N0. SET N0 TO N1 AND START OVER.

6 N0 = N1
   GO TO 1

C P IS BETWEEN ARCS N0-N1 AND N0-NF
C
7 N2 = NF
C P IS CONTAINED IN A CONE DEFINED BY LINE SEGMENTS N0-N1 AND N0-N2 WHERE N1 IS ADJACENT TO N2
C
8 N3 = N0
   9 IF ( LEFT(X(N1),Y(N1),X(N2),Y(N2),XP,YP) ) GO TO 13
C SET N4 TO THE FIRST NEIGHBOR OF N2 FOLLOWING N1
C
   INDX = IEND(N2)
   IF (IADJ(INDX) .NE. N1) GO TO 10
C N1 IS THE LAST NEIGHBOR OF N2.
C SET N4 TO THE FIRST NEIGHBOR.
C
   INDX = 1
   IF (N2 .NE. 1) INDX = IEND(N2-1) + 1
   N4 = IADJ(INDX)
   GO TO 11
C  N1 IS NOT THE LAST NEIGHBOR OF N2
C
10  INDX = INDX-1
   IF (IADJ(INDX) .NE. N1) GO TO 10
      N4 = IADJ(INDX+1)
   IF (N4 .NE. 0) GO TO 11
C  P IS OUTSIDE THE BOUNDARY
C
      NF = N2
      NL = N1
      GO TO 16
C  DEFINE A NEW ARC N1-N2 WHICH INTERSECTS THE LINE
C   SEGMENT N0-P
C
11  IF ( LEFT(X(N0),Y(N0),X(N4),Y(N4),XP,YP) ) GO TO 12
      N3 = N2
      N2 = N4
      GO TO 9
12  N3 = N1
      N1 = N4
      GO TO 9
C  P IS IN THE TRIANGLE (N1,N2,N3) AND NOT ON N2-N3. IF
C   N3-N1 OR N1-N2 IS A BOUNDARY ARC CONTAINING P, TREAT P
C   AS EXTERIOR.
C
13  INDX = IEND(N1)
   IF (IADJ(INDX) .NE. 0) GO TO 15
C
      N1 IS A BOUNDARY NODE. N3-N1 IS A BOUNDARY ARC IFF N3
C      IS THE LAST NONZERO NEIGHBOR OF N1.
C      IF (N3 .NE. IADJ(INDX-1)) GO TO 14
C
      N3-N1 IS A BOUNDARY ARC
C
      IF ( .NOT. LEFT(X(N1),Y(N1),X(N3),Y(N3),XP,YP) )
         GO TO 14
C
      P LIES ON N1-N3
C
      I1 = N1
      I2 = N3
      I3 = 0
      RETURN
C
      N3-N1 IS NOT A BOUNDARY ARC CONTAINING P. N1-N2 IS A
BOUNDARY ARC IFF N2 IS THE FIRST NEIGHBOR OF N1.

INDX = 1
IF (N1 .NE. 1) INDX = IEND(N1-1) + 1
IF (N2 .NE. IADJ(INDX)) GO TO 15

N1-N2 IS A BOUNDARY ARC

IF ( .NOT. LEFT(X(N2),Y(N2),X(N1),Y(N1),XP,YP) )
   GO TO 15
P LIES ON N1-N2
I1 = N2
I2 = N1
I3 = 0
RETURN

P DOES NOT LIE ON A BOUNDARY ARC.
I1 = N1
I2 = N2
I3 = N3
RETURN

NF AND NL ARE ADJACENT BOUNDARY NODES WHICH ARE VISIBLE
FROM P. FIND THE FIRST VISIBLE BOUNDARY NODE.
SET NEXT TO THE FIRST NEIGHBOR OF NF.

INDX = 1
IF (NF .NE. 1) INDX = IEND(NF-1) + 1
NEXT = IADJ(INDX)
IF ( LEFT(X(NF),Y(NF),X(NEXT),Y(NEXT),XP,YP) )
   GO TO 17
NF = NEXT
GO TO 16

NF IS THE FIRST (RIGHTMOST) VISIBLE BOUNDARY NODE
I1 = NF
FIND THE LAST VISIBLE BOUNDARY NODE. NL IS THE FIRST
CANDIDATE FOR I2.
SET NEXT TO THE LAST NEIGHBOR OF NL.

INDX = IEND(NL) - 1
NEXT = IADJ(INDX)
IF ( LEFT(X(NEXT),Y(NEXT),X(NL),Y(NL),XP,YP) )
   GO TO 19
NL = NEXT
GO TO 18
C NL IS THE LAST (LEFTMOST) VISIBLE BOUNDARY NODE
C
19 I2 = NL
I3 = 0
RETURN
C ALL POINTS ARE COLLINEAR
C
20 I1 = 0
I2 = 0
I3 = 0
RETURN
END
SUBROUTINE TRMESH (N,X,Y, IADJ,IEND,IER)
INTEGER N, IADJ(1), IEND(N), IER
REAL X(N), Y(N)
C***********************************************************
C
C                                               ROBERT RENKA
C                                       OAK RIDGE NATL. LAB.
C                                             (615) 576-5139
C
C   THIS ROUTINE CREATES A THIESSEN TRIANGULATION OF N
C ARBITRARILY SPACED POINTS IN THE PLANE REFERRED TO AS
C NODES. THE TRIANGULATION IS OPTIMAL IN THE SENSE THAT IT
C IS AS NEARLY EQUIANGULAR AS POSSIBLE. TRMESH IS PART OF
C AN INTERPOLATION PACKAGE WHICH ALSO PROVIDES SUBROUTINES
C TO REORDER THE NODES, ADD A NEW NODE, DELETE AN ARC, PLOT
C THE MESH, AND PRINT THE DATA STRUCTURE.
C UNLESS THE NODES ARE ALREADY ORDERED IN SOME REASONABLE
C FASHION, THEY SHOULD BE REORDERED BY SUBROUTINE REORDR FOR
C INCREASED EFFICIENCY BEFORE CALLING TRMESH.
C
C INPUT PARAMETERS - N - NUMBER OF NODES IN THE MESH.
N .GE. 3.
C X,Y - N-VECTORS OF COORDINATES.
(X(I),Y(I)) DEFINES NODE I.
C IADJ - VECTOR OF LENGTH .GE. 6*N-9.
C IEND - VECTOR OF LENGTH .GE. N.
C N, X, AND Y ARE NOT ALTERED BY THIS ROUTINE.
C
C OUTPUT PARAMETERS - IADJ - ADJACENCY LISTS OF NEIGHBORS IN
C COUNTERCLOCKWISE ORDER. THE
LIST FOR NODE I+1 FOLLOWS THAT FOR NODE I WHERE X AND Y DEFINE THE ORDER. THE VALUE 0 DENOTES THE BOUNDARY (OR A PSEUDO-NODE AT INFINITY) AND IS ALWAYS THE LAST NEIGHBOR OF A BOUNDARY NODE. IADJ IS UNCHANGED IF IER .NE. 0.

IEND - POINTERS TO THE ENDS OF ADJACENCY LISTS (SETS OF NEIGHBORS) IN IADJ. THE NEIGHBORS OF NODE 1 BEGIN IN IADJ(1). FOR K .GT. 1, THE NEIGHBORS OF NODE K BEGIN IN IADJ(IEND(K-1)+1) AND K HAS IEND(K) - IEND(K-1) NEIGHBORS INCLUDING (POSSIBLY) THE BOUNDARY. IADJ(IEND(K)) .EQ. 0 IFF NODE K IS ON THE BOUNDARY. IEND IS UNCHANGED IF IER = 1. IF IER = 2 IEND CONTAINS THE INDICES OF A SEQUENCE OF N NODES ORDERED FROM LEFT TO RIGHT WHERE LEFT AND RIGHT ARE DEFINED BY ASSUMING NODE 1 IS TO THE LEFT OF NODE 2.

IER - ERROR INDICATOR
IER = 0 IF NO ERRORS WERE ENCOUNTERED.
IER = 1 IF N .LT. 3.
IER = 2 IF N .GE. 3 AND ALL NODES ARE COLLINEAR.

MODULES REFERENCED BY TRMESH - SHIFTD, ADNODE, TRFIND, INTADD, BDLADD, SWPTST, SWAP, INDEX

***************************************************************************

INTEGER NN, K, KM1, NL, NR, IND, INDX, N0, ITEMP, 
      . IERR, KM1D2, KMI, I, KMIN
REAL XL, YL, XR, YR, DXR, DYR, XK, YK, DXK, DYK, 
      . CPROD, SPROD

LOCAL PARAMETERS -

C NN = LOCAL COPY OF N
C K = NODE (INDEX) TO BE INSERTED INTO IEND
C KM1 = K-1 - (VARIABLE) LENGTH OF IEND
C NL,NR = IEND(1), IEND(KM1) -- LEFTMOST AND RIGHTMOST
C NODES IN IEND AS VIEWED FROM THE RIGHT OF 1-2 WHEN IEND CONTAINS THE INITIAL ORDERED SET OF NODAL INDICES
C XL,YL,XR,YR = X AND Y COORDINATES OF NL AND NR
C DXR,DYR = XR-XL, YR-YL
C XK,YK = X AND Y COORDINATES OF NODE K
C DXK,DYK = XK-XL, YK-YL
C CPROD = VECTOR CROSS PRODUCT OF NL-NR AND NL-K --
C USED TO DETERMINE THE POSITION OF NODE K WITH RESPECT TO THE LINE DEFINED BY THE NODES IN IEND
C SPROD = SCALAR PRODUCT USED TO DETERMINE THE INTERVAL CONTAINING NODE K WHEN K IS ON THE LINE DEFINED BY THE NODES IN IEND
C IND,INDX = INDICES FOR IEND AND IADJ, RESPECTIVELY
C N0,ITEMP = TEMPORARY NODES (INDICES)
C IERR = DUMMY PARAMETER FOR CALL TO ADNODE
C KM1D2,KMI,I = KM1/2, K-I, DO-LOOP INDEX -- USED IN IEND REORDERING LOOP
C KMIN = FIRST NODE INDEX SENT TO ADNODE
C
NN = N
IER = 1
IF (NN .LT. 3) RETURN
IER = 0
C INITIALIZE IEND, NL, NR, AND K
C
IEND(1) = 1
IEND(2) = 2
XL = X(1)
YL = Y(1)
XR = X(2)
YR = Y(2)
K = 2
C
C BEGIN LOOP ON NODES 3,4,...
C
1 DXR = XR-XL
   Dyr = YR-YL
C
C NEXT LOOP BEGINS HERE IF NL AND NR ARE UNCHANGED
C
2 IF (K .EQ. NN) GO TO 13
   KM1 = K
   K = KM1 + 1
   XK = X(K)
   YK = Y(K)
DXK = XK-XL
DYK = YK-YL
CPROD = DXR*DYK - DXK*DYR
IF (CPROD .GT. 0.) GO TO 6
IF (CPROD .LT. 0.) GO TO 8

C
C NODE K LIES ON THE LINE CONTAINING NODES 1,2,...,K-1.
C SET SPROD TO (NL-NR,NL-K).
C
SPROD = DXR*DXK + DYR*DYK
IF (SPROD .GT. 0.) GO TO 3

C
C NODE K IS TO THE LEFT OF NL. INSERT K AS THE FIRST
C (LEFTMOST) NODE IN IEND AND SET NL TO K.
C
CALL SHIFTD(1,KM1,1, IEND )
IEND(1) = K
XL = XK
YL = YK
GO TO 1

C
C NODE K IS TO THE RIGHT OF NL. FIND THE LEFTMOST NODE
C NO WHICH LIES TO THE RIGHT OF K.
C SET SPROD TO (N0-NL,N0-K).
C
3 DO 4 IND = 2,KM1
   N0 = IEND(IND)
   SPROD = (XL-X(N0))*(XK-X(N0)) +
   (YL-Y(N0))*(YK-Y(N0))
   IF (SPROD .GE. 0.) GO TO 5
4 CONTINUE

C
C NODE K IS TO THE RIGHT OF NR. INSERT K AS THE LAST
C (RIGHTMOST) NODE IN IEND AND SET NR TO K.
C
IEND(K) = K
XR = XK
YR = YK
GO TO 1

C
C NODE K LIES BETWEEN IEND(IND-1) AND IEND(IND). INSERT K
C IN IEND.
C
5 CALL SHIFTD(IND,KM1,1, IEND )
IEND(IND) = K
GO TO 2

C
C NODE K IS TO THE LEFT OF NL-NR. REORDER IEND SO THAT NL
C IS THE LEFTMOST NODE AS VIEWED FROM K.
C
6 KM1D2 = KM1/2
DO 7 I = 1,KM1D2
   KMI = K-I
   ITEMP = IEND(I)
   IEND(I) = IEND(KMI)
   IEND(KMI) = ITEMP
7 CONTINUE

C
C NODE K IS TO THE RIGHT OF NL-NR. CREATE A TRIANGULATION
C CONSISTING OF NODES 1,2,...,K.
C
8 NL = IEND(1)
   NR = IEND(KM1)
C
C CREATE THE ADJACENCY LISTS FOR THE FIRST K-1 NODES.
C INSERT NEIGHBORS IN REVERSE ORDER. EACH NODE HAS FOUR
C NEIGHBORS EXCEPT NL AND NR WHICH HAVE THREE.
C
DO 9 IND = 1,KM1
   N0 = IEND(IND)
   INDX = 4*N0
   IF (N0 .GE. NL) INDX = INDX-1
   IF (N0 .GE. NR) INDX = INDX-1
   IADJ(INDX) = 0
   INDX = INDX-1
   IF (IND .LT. KM1) IADJ(INDX) = IEND(IND+1)
   IF (IND .LT. KM1) INDX = INDX-1
   IADJ(INDX) = K
   IF (IND .EQ. 1) GO TO 9
   IADJ(INDX-1) = IEND(IND-1)
9 CONTINUE

C
C CREATE THE ADJACENCY LIST FOR NODE K
C
   INDX = 5*KM1 - 1
   IADJ(INDX) = 0
   DO 10 IND = 1,KM1
      INDX = INDX-1
      IADJ(INDX) = IEND(IND)
10 CONTINUE

C
C REPLACE IEND ELEMENTS WITH POINTERS TO IADJ
C
   INDX = 0
   DO 11 IND = 1,KM1
      INDX = INDX + 4
      IF (IND .EQ. NL .OR. IND .EQ. NR) INDX = INDX-1
      IEND(IND) = INDX
11 CONTINUE

   INDX = INDX + K
IEND(K) = INDX
C
C ADD THE REMAINING NODES TO THE TRIANGULATION
C
IF (K .EQ. NN) RETURN
KMIN = K+1
DO 12 K = KMIN,NN
   CALL ADNODE(K,X,Y, IADJ,IEND, IERR)
12   CONTINUE
RETURN
C
C ALL NODES ARE COLLINEAR
C
13 IER = 2
RETURN
END