High Performance Computing Applications for Material Physics

Matthew Johnson
REMSPEC REU Program
Summer 2011

Advisor: Dr. Timothy Kaiser
Director, Golden Energy Computing Organization

Siesta
- Powerful Modeling Tool
  - Spanish Initiative for Electronic Simulations with Thousands of Atoms.
  - Analyses the electronic-dynamics of a molecule or solid.
  - Can evaluate the photoelectric characteristics of N-body systems, like Si diode QD’s.

Applications in Renewable Energy Materials
- Siesta has two solvers for finding Eigenvalues.
- Default solver chosen based on the number of atoms in the molecule or solid being characterized.
- Order-N Solver -- default solver for problems with more than 1000 atoms.
- Diag Solver -- standard diagonalization algorithm.

Multi-Solution Methods
- SIESTA can be used to characterize the electrical properties of many different molecular structures.
- By offering multiple solution algorithms SIESTA is able to efficiently characterize molecules of many different sizes.
- This allows SIESTA to be scaled based on the size of the molecule it is characterizing.

Communication with MPI
- Used to pass messages between processors on parallel systems.
- Contains many commonly used parallel communication routines, considered a staple on HPC systems.
- Open source and platform/compiler specific distributions are available.
- MPI was designed with an emphasis on minimizing the overhead required for communication.

Types of Operations
- Passing data between processing elements i.e. send, and receive.
- Dissemination of data across groups of processing elements i.e. broadcast, scatter.
- Data reductions, combinations, and simplifications i.e. summations, products, locating maxima and minima, logical operations (AND, OR, XOR, NOT).
- Most complex operations are simply combinations of the simpler send/receive operations and other system operations.

Scalability and Communication
- Scalability is the measure of a computer programs ability to improve its performance as more resources (CPUs, GPUs, RAM, etc) are allocated to a problem.
- Many factors can affect a programs scalability, including: hardware, operating system, programming language.
- Information about a programs scalability is particularly important on HPC systems where resources are both indispensable and costly.

Anatomy of an MPI_AllReduce Call

MPI_AllReduce is a global data reduction operation
- Step 1: Each processor in the specified communicator calls MPI_AllReduce, with its portion of the data. The specified operation is performed on the data and the result is sent to the processor which has been designated root.
- Step 2: The processor designated as root performs the specified reduction operation on the data sent from the individual processors.
- Step 3: The result of the reduction operation performed in step 2 is disseminated across the communicator by a call to MPI_Broadcast.

Use in SIESTA
- An analysis of SIESTA’s runtime behavior was performed using Tuning and Analysis Utilities (TAU).
- The results show that SIESTA spends significantly more time in two communication routines than it does in other portions of the program. The offending routines were: MPI_AllReduce and MPI_Broadcast.
- Examination of SIESTA’s source code revealed that two specific routines were calling MPI_AllReduce more frequently than necessary.
- Below are two examples of how to use MPI_AllReduce to find the sum of two numbers.

Fixed SIESTA Source Code

```

```

Results
- The data collected from the Si 57 and Si 20 quantum dots suggests that the optimal number of processors is higher for the version of SIESTA which uses the more efficient MPI_AllReduce calls.
- In the case of the Si 20 quantum dot the optimal number of processors was doubled.
- For the Si 57 quantum dot, the maximum number of processors increased to 166% of the initial maximum number.

Overall Performance Improvements
- In addition to improving the scalability of SIESTA, more efficient use of MPI_AllReduce also improved SIESTA’s overall runtime.
- For the Si 57 quantum dot overall runtime was approximately 83% of the initial (unmodified) value.
- The Si 20 quantum dot runtime showed the greatest improvement, running in approximately 25% of the time required to run the same model on an unmodified version of SIESTA.