

FY11 JOULE Codes

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- *(SC GG 3.1/2.5.2) Improve computational science capabilities, defined as the average annual percentage increase in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of application codes. Efficiency measure: X% (FY11, x=100)*

Strong Scaling

“simulating the same problem in less time”

- Algorithm, machine strong scaling :
 - Q4 problem := Q2 problem
 - Q4 algorithm := Q2 algorithm
 - Q4 machine $\sim k * \text{Q2 machine}$
 - Q4 time $\sim 1/k * \text{Q2 time}$
 - Algorithm enhancements, performance optimizations:
 - Q4 problem := Q2 problem
 - Q4 algorithm $\sim \text{enhanced Q2 algorithm}$
 - Q4 machine := Q2 machine
 - Q4 time $\sim 1/k * \text{Q2 time}$
- *Could consider other variations: algorithm and machine are varied to achieve reduction of compute time

Weak Scaling

“simulating a larger problem in same time”

- Algorithm, machine weak scaling (defined as 100%):
 - Q4 problem $\sim k * Q2$ problem
 - Q4 algorithm := Q2 algorithm
 - Q4 machine $\sim k * Q2$ machine
 - Q4 time := Q2 time
 - Algorithm enhancements, performance optimizations:
 - Q4 problem $\sim k * Q2$ problem
 - Q4 algorithm \sim enhanced Q2 algorithm
 - Q4 machine := Q2 machine
 - Q4 time := Q2 time
- *Could consider other variations: problem, algorithm and the machine are varied to achieve fixed time assertion

- Four science applications are recommended for ASCAC's consideration for the FY11 Joule metric:
 - OMEN,
 - LAMMPS,
 - COMPASS, and
 - STOMP.

Application Domain: Nanoelectronics

Application Code: OMEN

Target Platform: Jaguar Cray XT5 (OLCF)

Contact: Gerhard Klimeck (gekco@purdue.edu)

References: <http://cobweb.ecn.purdue.edu/~gekco/omen/index.html>

- OMEN is a one-, two-, and three-dimensional quantum transport solver based on the nearest-neighbor tight-binding method and dedicated to the simulation of the next generation transistors like ultra-thin body, nanowire, and band-to-band tunneling field-effect transistors.
- OMEN has already scaled up to 222,720 cores on the Jaguar Cray XT5 at the OLCF with a sustained performance of 860 TFlop/s (about 37% of the peak).
- At the end of the project, it will be possible to investigate novel nanoelectronic devices at unprecedented levels of physical complexity and to directly compare the simulation results to available experimental data. The OMEN research group is actively interacting with two experimental groups to validate the physical correctness of the model and to drive the design of the experiments.

Application Domain: Bioscience

Application Code: LAMMPS

Contact: Steve Plimpton (sjplimp@sandia.gov)

References: <http://lammps.sandia.gov/>

- LAMMPS is a classical molecular dynamics code that models an ensemble of particles in a liquid, solid, or gaseous state. It can model atomic, polymeric, biological, metallic, semiconductor, granular, and coarse-grained or mesoscale or particle-based continuum systems using a variety of force fields and boundary conditions.
- LAMMPS can model systems with only a few particles up to millions or billions, and has run large problems scalably on up to 64K processors of current-generation parallel machines.
- LAMMPS is a freely-available open-source code, distributed under the terms of the GNU Public License. In the last 5 years it has been downloaded roughly 50,000 times. In 2009, approximately 250 papers citing LAMMPS were published.

Application Domain: Accelerator Design

Application Code: COMPASS

Contact: Panagiotis Spentzouris (spentz@fnal.gov)

References: <https://compass.fnal.gov>

- The Community Petascale for Accelerator Science and Simulation (COMPASS) SciDAC2 project is developing a comprehensive computational infrastructure for accelerator modeling and optimization, to advance accelerator computational capabilities from the terascale to the petascale in support of DOE priorities for the next decade and beyond.
- The simulation suite contains a comprehensive set of interoperable components for beam dynamics, electromagnetics, electron cooling, and advanced accelerator modeling. Beam dynamics studies will enhance the understanding of lifetime limits from beam collisions in colliders. Electromagnetics modeling can be used to optimize cavity shapes for increasing the acceleration gradient of beam current. Electron cooling computations can be used to determine the configuration of cooling systems needed for mitigating beam-beam effects.

Application Domain: Carbon Sequestration

Application Code: STOMP

Contact: Tim Scheibe (tim.scheibe@pnl.gov)

References: <http://stomp.pnl.gov/>

- STOMP is a subsurface multfluid flow and reactive transport simulation capability for addressing DOE missions in environmental restoration of nuclear production legacy waste sites, geologic sequestration of CO₂, and the development of alternative energy resources (e.g., methane hydrates, oil shales).
- The STOMP simulator solves the partial-differential equations that describe the conservation of mass or energy quantities by employing integrated-volume finite-difference discretization to the physical domain and backward Euler discretization to the time domain.
- STOMP was recently re-engineered for extreme scale computing with the componentization of grid services and the implementation of the Global Array toolkit (GA) to parallelize the isothermal, variably saturated flow operational mode with high resolution transport (3rd order TVD) and reactions.