Virtual Simulator: An Infrastructure for Design and Performance-Prediction of Massively Parallel Codes*

Kalyan S. Perumalla[†], Richard Fujimoto[‡], Santosh Pande[‡], Homa Karimabadi[§], Jonathan Driscoll[§], Yuri Omelchenko[§]

Large parallel/distributed scientific simulations are very complex, and their dynamic behavior is hard to predict. Efficient development of massively parallel codes remains a computational challenge. For example, almost none of the kinetic codes in use in space physics today have dynamic load balancing capability. Here we present a new infrastructure for design and prediction of parallel codes. Performance prediction is useful to analyze, understand and experiment with different partitioning schemes, multiple modeling alternatives and so on, without having to run the application on supercomputers. Instrumentation of the model (with least perturbance to performance) is useful to glean key metrics and understand application-level behavior. Unfortunately, traditional approaches to virtual execution and instrumentation are limited by either slow execution speed or low resolution or both. We present a new framework that provides a high-resolution framework that provides a virtual CPU abstraction (with a full thread context per CPU), yet scales to thousands of virtual CPUs. The tool, called PDES2, presents different levels of modeling interfaces, from general purpose parallel simulations to parallel grid-based particle-in-cell (PIC) codes. The tool itself runs on multiple processors in order to accommodate the high-resolution by distributing the virtual execution across processors. Validation experiments of PIC models in the framework using a 1-D hybrid shock application show close agreement of results from virtual executions with results from actual supercomputer runs. The utility of this tool is further illustrated through an application to a parallel global hybrid code.

---

* Appeared in Eos Transactions, American Geophysical Union 86(2), Fall Meeting Supplement, December 2005, Abstract SM13A-0322

† Oak Ridge National Laboratory, Oak Ridge, TN
‡ Georgia Institute of Technology, Atlanta, GA
§ SciberQuest Inc., Solana Beach, CA