Three-dimensional Particle-In-Cell plasma simulation on heterogeneous computing systems

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Plasma simulation via the Particle-In-Cell (PIC) method on computer clusters is one of the most effective ways of theoretical research in many areas of state-of-the-art plasma physics, including studies of high power laser applications. The proliferation of graphics processing units (GPUs) as alternative computational devices and their use in hybrid (heterogeneous) clusters dramatically increase the importance of developing hybrid programs that are able to employ both CPUs and GPUs for parallel simulations. The work describes the current state of Picador, a parallel heterogeneous PIC implementation under development.

Picador is being created in order to employ heterogeneous clusters/supercomputers for research on interactions of high intensity laser pulses with various targets in the context of currently important applications, including generation of radiation with tailored properties and laser-driven acceleration of electrons, protons and light ions.

A distinguishing feature of Picador is its ability to use all computational resources available on a node, that is, both traditional and graphics processors, for three-dimensional simulation.

Other notable features of Picador:

- It can simulate a Perfectly Matched Layer (PML).
- It can simulate externally originating electromagnetic waves.
- It supports arbitrary initial and periodic boundary conditions.
- It is written in C and C++ in a fairly portable way; supports building under Windows and Linux (and potentially under other POSIX-compliant systems).
- It supports operation on cluster systems that offer an MPI implementation, as well as parallel execution within a node via the OpenMP (on CPUs) and OpenCL (on GPUs) programming interfaces.
- It is extensible; in particular, it allows to plug in an alternative message passing mechanism (instead of MPI), as well as an alternative implementation of the main computational algorithm.
- It embeds a scripting language that is used to define simulation problems.

Picador has been tested on basic problems (cold plasma oscillations, etc.). Picador scales onto 1000 cores with at least 70% efficiency. The presentation will contain an overview of the software, the method for parallel execution on CPUs and GPUs, a performance analysis and plans for the future.

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