Framework for advanced plasma simulations on GPUs and many-core HPC Clusters

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Introduction:
We have created a fluid modeling code called WARPM to utilize modern many-core compute devices—namely GPUs. Fusion plasma simulation has much in common with computational fluid dynamics (CFD), but adds the complexities of modeling the electromagnetic interactions of the charged plasma species, confinement fields, and heating fields. Modeling involves elaborate codes with computational demands that limit achievable approximation of real-world behavior. WARPM is designed to both minimize data movement and maximize data-parallel computation.

The code is a hybrid combination of OpenCL for parallel computation, MPI for communication between nodes, and threads for task parallelism. WARPM uses Message Passing Interface (MPI) to distribute computation across multiple nodes of a cluster and for parallel file I/O. The OpenCL standard is central to the new code. GPU(s) and/or multi-core CPUs are utilized simultaneously to compute updates to the system of fluid equations.

WARPM

- C-x development: Relies heavily on object-oriented structures and templates.
- Uses coordinated combination of OpenCL, threads, and MPI for different levels of parallelism.
- Primarily uses Finite Volume method for hyperbolic problems on structured grids.
- WARPM is innovative in its flexibility to solve an arbitrarily sized system of equations using solvers specified at run-time, using GPUs and other many-core devices.
- Targets heterogeneous computational resource and multi-level domain decomposition.
- A “typical” simulation might use 128 nodes for >1000 core hours.

Example System of two-fluid plasma hyperbolic equations:
- Electron and ion continuity
- Electron and ion momentum
- Electron and ion state
- Electron and ion pressure
- Faraday’s Law
- Ampere’s Law
- Current density definition

In total, 11 equations (incl. 5 vector equations)

WARPM Framework orchestrates computational kernels, memory movement, and disk I/O based on user specified dependencies

Performance and Energy Impact of Data Movement

Current Hardware Performance Illustrates Need for Careful Consideration for Data Movement.
- PCIe x16 – 8 GB/h host to GPU
- Used NVIDIA Tesla K20c/gpu10/gpu20/gpus
- Peak performance: 515 Gflops/DP
- 515 Gflops/1 B GB/s + 8 bytes/double
- 515 floating point operations needed per operand transferred between GPU and host to hide PCIe bottleneck
- Memory bandwidth: 348 GB/s/16 cores
- 28 floating point operations needed per operand transferred between GPU GRAM and core to hide memory interface bottleneck
- Energy requirements for a FLOP around 50 pJ.

In Future Computing Roadmaps, this problem only becomes more severe.

Designed to Minimize and Hide Data Movement

- Working with block structured grids, data space resident on one node is further subdivided into patches.
- Patches are small enough for multiple to fit in GPU memory so that GPU-Host memory transfer can overlap with GPU computation.
- Patch processing is sequenced so that extraneous patches on a node are computed first. MPI ghost cell updates can then occur in parallel with interior patch computation—hiding the MPI communication.
- All computational steps are grouped into a single kernel so that data need only be transferred from GPU memory to the core once per step.

Users supply the computational model and evaluation sequence.

Performance Improvement:
- Initial performance testing conducted comparing WARPM to single-threaded WARPX code performance for 2D wave propagation on a single node.
- WARPM achieves twice the computational performance of WARPX on the same machine (12-core CPU) execution.
- Performance gains due to primarily eliminating MPI overhead on same node and establishing predictable compile-time execution sequence.
- Performance improvement margin grows up with more complex fluid problems because these are more numerically intensive. (i.e. more floating point operations per data element). This better utilizes the GPU capability.

Performance Study:

Energetic-Particle-Induced Geodesic Acoustic Mode in Tokamaks

- Original PIC
- WARPM Continuous

Physics Study: Energetic-Particle-Induced Geodesic Acoustic Mode in Tokamaks

Energetic particles such as those produced by neutral beam injection can excite a mode similar to Geodesic Acoustic Mode via free energy associated with velocity space gradient in energetic particle distribution. EGAM has been demonstrated by Particle-in-Cell simulations to date. We develop a continuum kinetic model that is more suitable for our many-core computing framework and future architectures. Simulations aim to reproduce the behavior demonstrated by PIC codes including non-linear ‘bursting’ in the radial electric field.

Physical Model

- Drift-kinetic treatment with static magnetic field.
- Delta-f method utilized for hot particles’ deviation from an initial single streaming distribution.

Summary and Upcoming Work

WARPM has proven to be an effective new scientific computing framework that is well suited for emerging computing architectures. Development will continue.

WARPM provides a framework that can be readily utilized by users to solve their own computational models.
- Initial EGAM simulations in continuum kinetic formulation show some similar dynamics to PIC code results, but parameters to give non-linear bursting still need to be identified.
- For physical investigation, we have a priority support general geometry problems.
- We are working to create kernels that are dynamically assembled at run-time based on the specific physics problem and numerical method chosen by the user.

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