Leveraging Charm++ for meshless fluid simulations on distributed memory architectures

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Objective

Design and develop a smoothed particle hydrodynamics (SPH) engine using the Charm++ object-oriented asynchronous message passing parallel programming paradigm.

The Charm++ Programming Paradigm

- Object-Oriented: Chare Objects.
- Overdecomposition

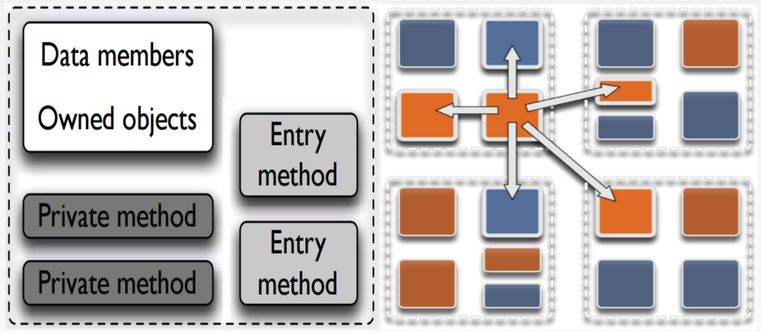

Figure 1: Single Chare Object (left). Overdecomposition; multiple chares in each execution unit exchanging data (right).

- Migratability
- Asynchrony: Message-driven execution.

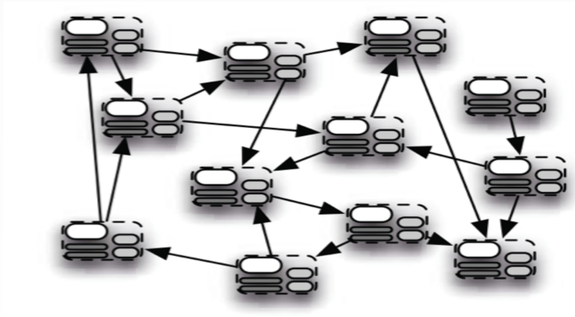

Figure 2: Programmers view of a collection of interacting chares.

Why Charm++ for SPH? Why not CUDA or MPI?

- Adaptive Runtime System: Dynamic load-balancing, communication optimization, fault-tolerance, etc.
- Proven success in molecular dynamics with NaMD. Runs on 500,000+ cores at Blue Waters.
- CUDA is SIMD vs. Charm++ can be MIMD.
- CUDA is a shared memory model.
- Example: Naive Domain decomposition

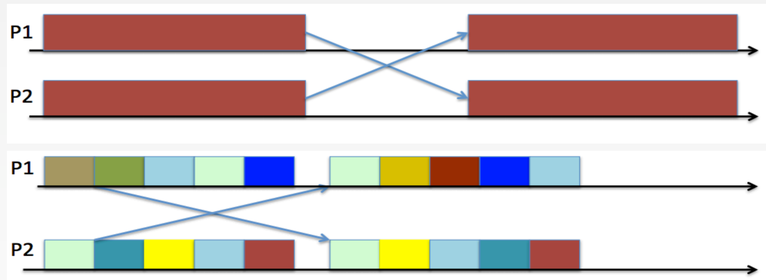

Figure 3: Compute idle time in MPI (top). Reduced idle times due to overdecomposition (bottom).

Charm-based SPH Engine Design

- SPH: Particle-based meshless approach.
- Hybrid decomposition: Spatial + Force decomposition. NaMD inspired.
- **Cell /Bin Chare:** Contains data. Takes care of force reduction, time integration and particle migration to neighbor cells.
- **Compute Chare:** Compute interactions within a Cell or between neighbor cells.

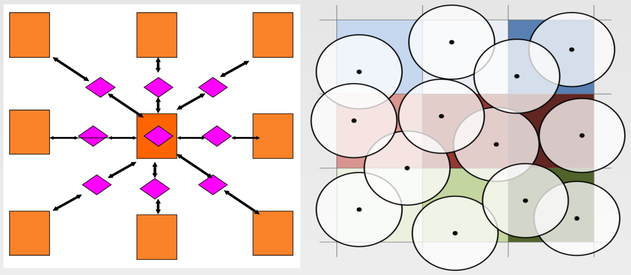

Figure 4: Hybrid decomposition: cell chares (orange) and compute chares (pink) (left). Particle grouped by cell, showing the interaction radius (right).

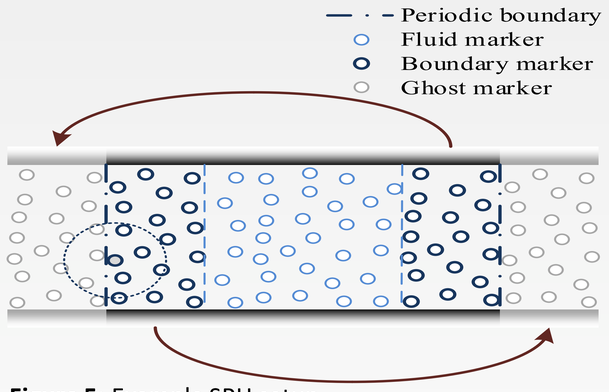

Figure 5: Example SPH setup.

References

[1] PPL at UIUC. "Charm++". http://charmplusplus.org.

[2] N. Jain. "LeanMD". http://charm.cs.illinois.edu/gerrit/benchmarks/leanmd.git

[3] L. Kale, et al. "Charm++ for productivity and performance". PPL Technical Report, 2011.

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