Implementations of Particle-Particle and Fast Hierarchical Methods over N-body problem on Heterogeneous platforms

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N-Body Introduction

- Determine the motion of particles over the time due to the forces from the other particles
  - Calculate forces ($\vec{F_i}$) using the potential function
  - Update velocities i.e., $\vec{v_{i+1}} = \vec{v_i} + \Delta t \times \vec{F_i}$
  - Compute new position as $\vec{x_{i+1}} = \vec{x_i} + \Delta t \times \vec{v_i}$

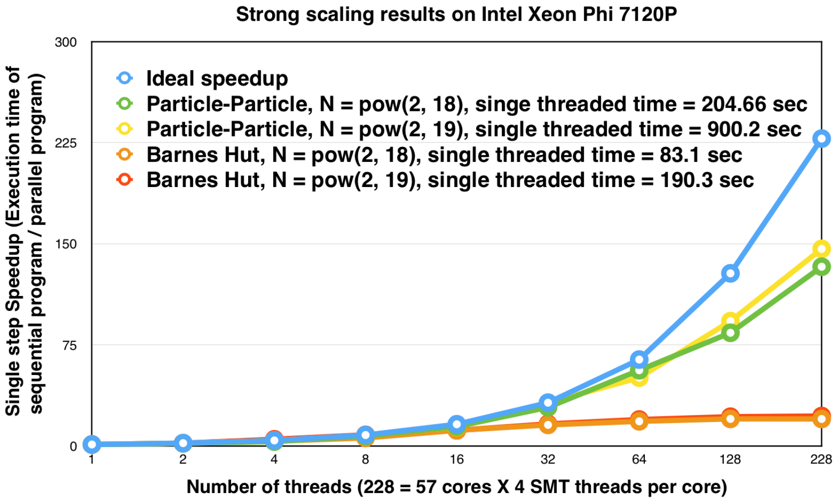
- Various applications in Astronomy, Molecular dynamics, Fluid dynamics etc.

- History of algorithms
  - Exact : Particle-Particle - $O(n^2)$, where n is number of particles
  - Approximation: Mesh based methods - $O(nlogn)$
  - Approximation: Tree based methods - $O(nlogn)$

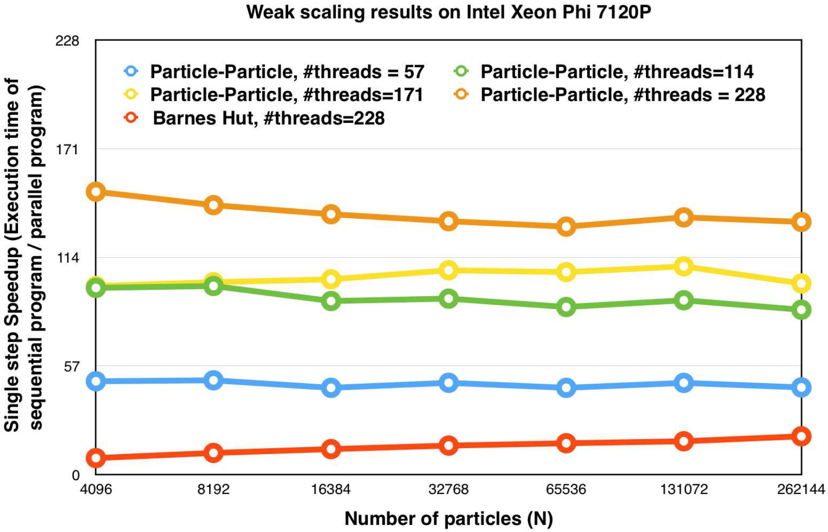
N-Body implementations on Xeon Phi 7120P

- Xeon Phi Co-Processor (Intel Knights Landing) with 57 cores (4 SMT threads per each core) and 512 bit SIMD Instruction set per each core
  - Particle-Particle based approach - Optimization's
    - Array of structures to Structure of Arrays for better vectorization
    - Loop tiling to enhance temporal locality
    - Array expansion to make outermost tile loop parallel
  - Barnes Hut approach (Approximate approach)
    - Idea: When a set of particles are too far away from current particle, we can approximate force to the center of mass of particles rather than calculating for each particle.
    - Enabled OpenMP task-based parallelism to traverse quad tree to compute forces with approximation

Experiments on Intel Xeon Phi for strong scaling - Single step



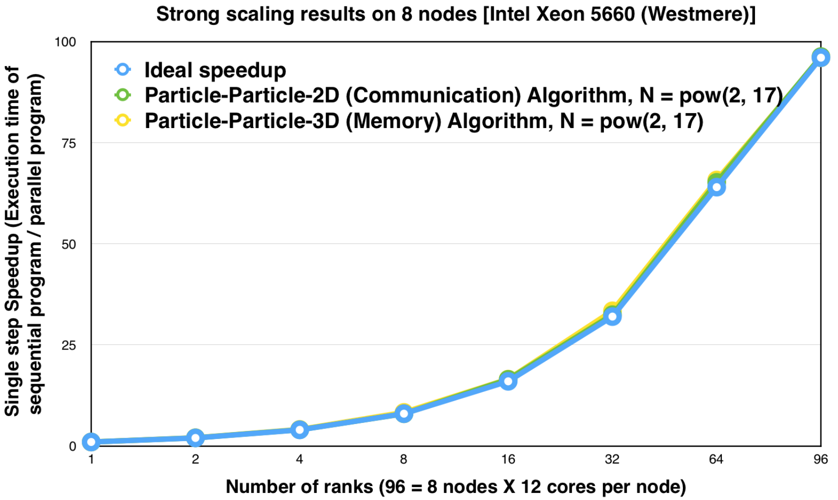
Experiments on Intel Xeon Phi for weak scaling - Single step



Observations on Intel Xeon Phi

- Barnes-Hut's implementation suffers from performance improvement relative to particle-particle based approach
  - Data is distributed across different nodes in the tree, hence resulting in spatial locality loss for vectorization
  - No loop tiling resulting in temporal locality loss
  - Interesting ideas on efficient tree traversals [Milind et.al PLDI 2016]
- Even, particle-particle based approach on Xeon-Phi suffers in case of strong scaling from 57 to 228 threads.
  - Each SMT thread requires use of vector processor unit to perform operations. Huge bottleneck on VPU!
  - Intel Knight's corner announced 2 VPU's per core

Experiments on a cluster (MPI) for strong scaling - Single step



Preliminary experiments with GPU

- Tesla K20 with 13 SMs and 2496 CUDA cores
  - Enabled most of optimization's done in the context of Multi-core
  - Used constant memory for broadcasting small constant values to all the SMs
  - Achieved an occupancy of 61% over $N = 32768$ particles

Learning's and Challenges

- Better acquainted with Intel compilers and Intel Advisor tool for vectorization and multi-threading.
- Fun in working as team in exploring different architectures (Xeon, Xeon-Phi, GPU), algorithms (Particle-Particle, tree based), different programming models (OpenMP, MPI, CUDA), and different parallelism styles (task-based, loop-based, SIMT-based, SPMD-based).

- Hard to efficiently vectorize and optimize for locality in case of tree traversals.