Scalable Molecular Dynamics with NAMD on the Summit System

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Changes for Summit

- Data layout for GPU and CPU vectorization
- Move integration to GPU
- Improvements to PAMI layer
- Intra-node load balancing
- Algorithmic improvements to NAMD

Data layout for Vectorization

- Vectorization critical for high performance on GPUs and modern CPUs
- Originally, NAMD used array-of-structures layout
  - Eased development, customization
- For performance, switched to structure-of-arrays
  - Data fields now contiguous across objects
  - Allows for SIMD execution

GPU Integrator

NAMD Phase	Time Spent
Non-bonded forces	90%
Long-range forces	5%
Bonded forces	2%
Exclusions	2%
Integration	1%

GPU Integrator

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GPU Work, CPU Work

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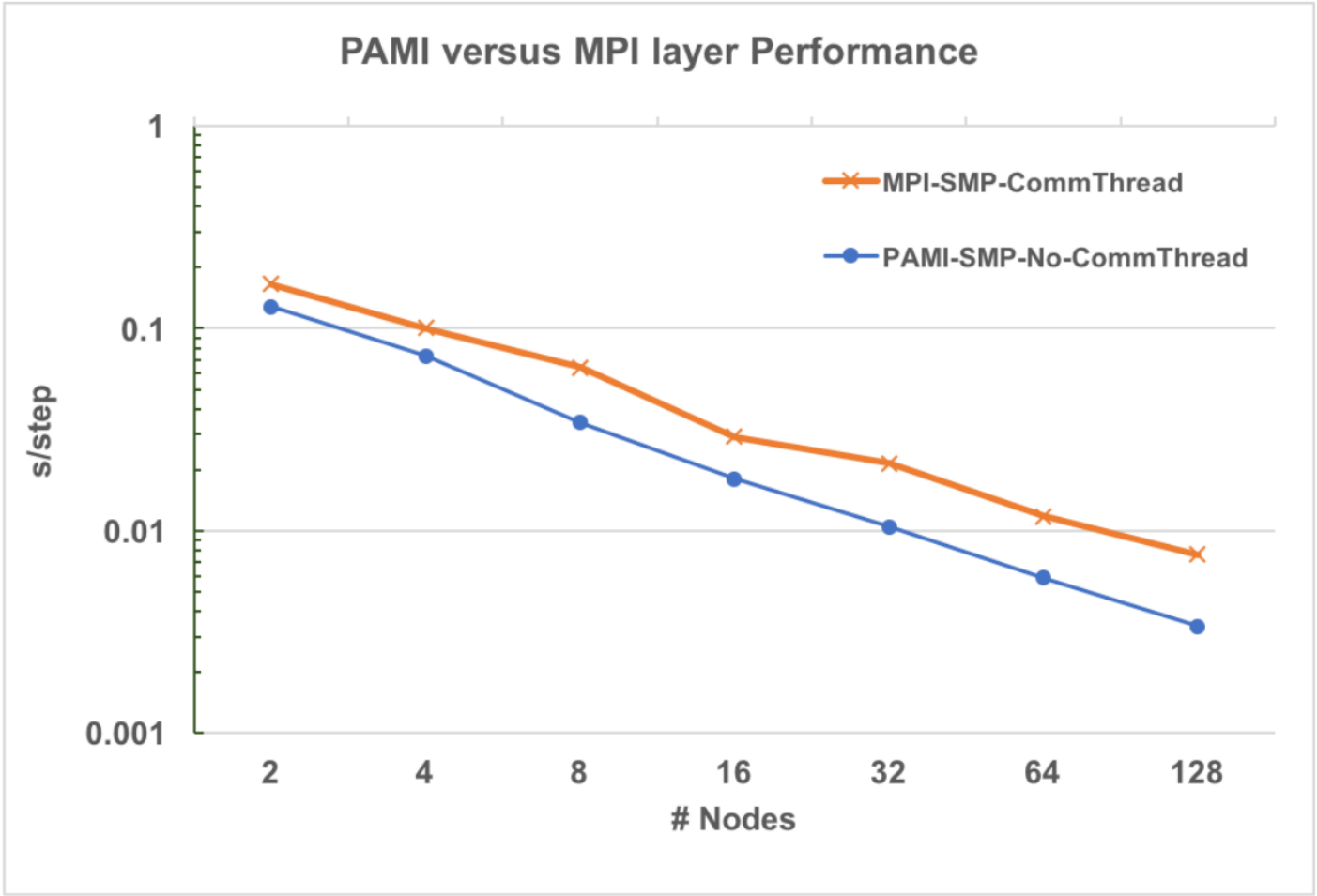
GPU Work, CPU Work

Voltas are so fast that what was once 1% of work now takes majority of time

$\Rightarrow$ Move integration step to GPU

PAMI Layer



Modified existing Charm++ PAMI layer for Blue Gene to support Summit network

Intra-Node Load Balancing

- To prepare for GPU transfer, CPU copies bonded force data to contiguous memory
  - In some cases, was done serially
- Became bottleneck for certain workloads
- Parallelized using CkLoop
- Improved total runtime by up to 1%

Summit Performance