Scaling NAno Molecular Dynamics(NAMD) on Petascale machines using Charm++

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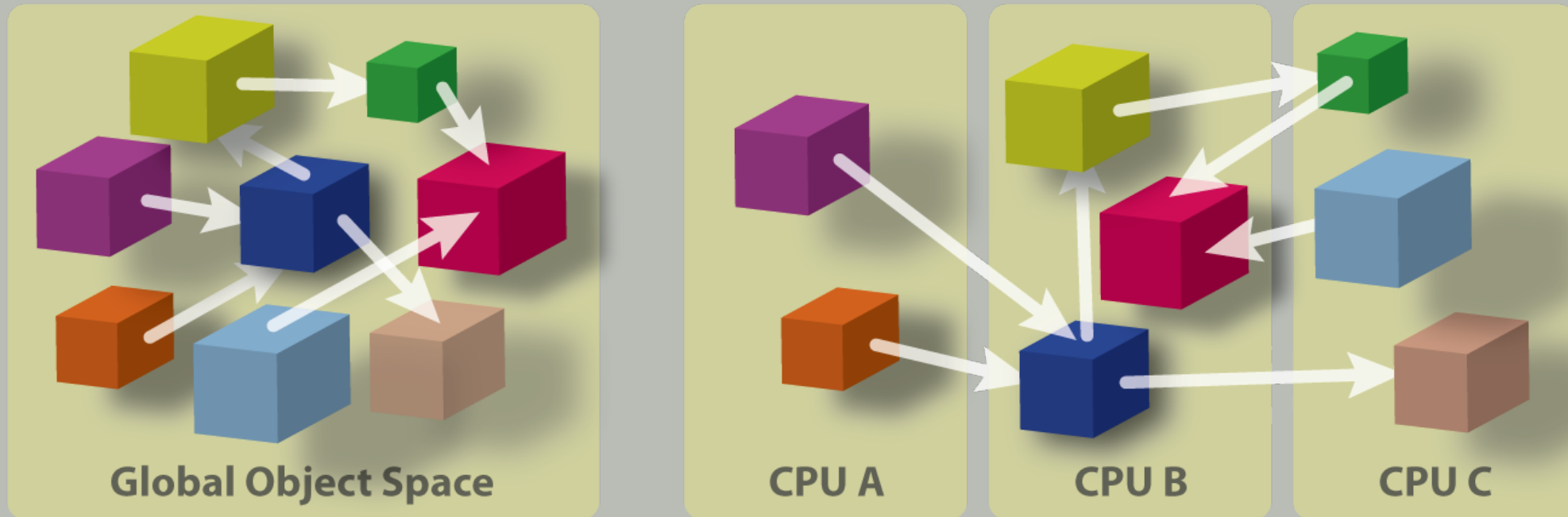
What is Charm++?

Charm++ is an asynchronous and message-driven paradigm developed by Parallel Programming Lab (PPL). Features in Charm++ include:

- Fine-grain decomposition and virtualization
- Asynchronous
- Adaptive run-time system support
- Automatic dynamic Load balancing
- Fault tolerance

Global Object Space   CPU A   CPU B   CPU C

What is NAMD?

NAMD is a parallel, object-oriented molecular dynamics code designed for high-performance simulation of large biomolecular systems. It is the result of an interdisciplinary collaboration between Prof. Kale, computer science Prof. Robert D. Skeel, and physics Prof. Klaus J. Schulten at the Theoretical and Computational Biophysics Group (TCBG) of Beckman Institute.


- An MD simulation models the motion of atoms within a molecular system.
- Simulation of process of milli-second time scale is important and challenging.
- Large system simulation

(http://www.ks.uiuc.edu/)
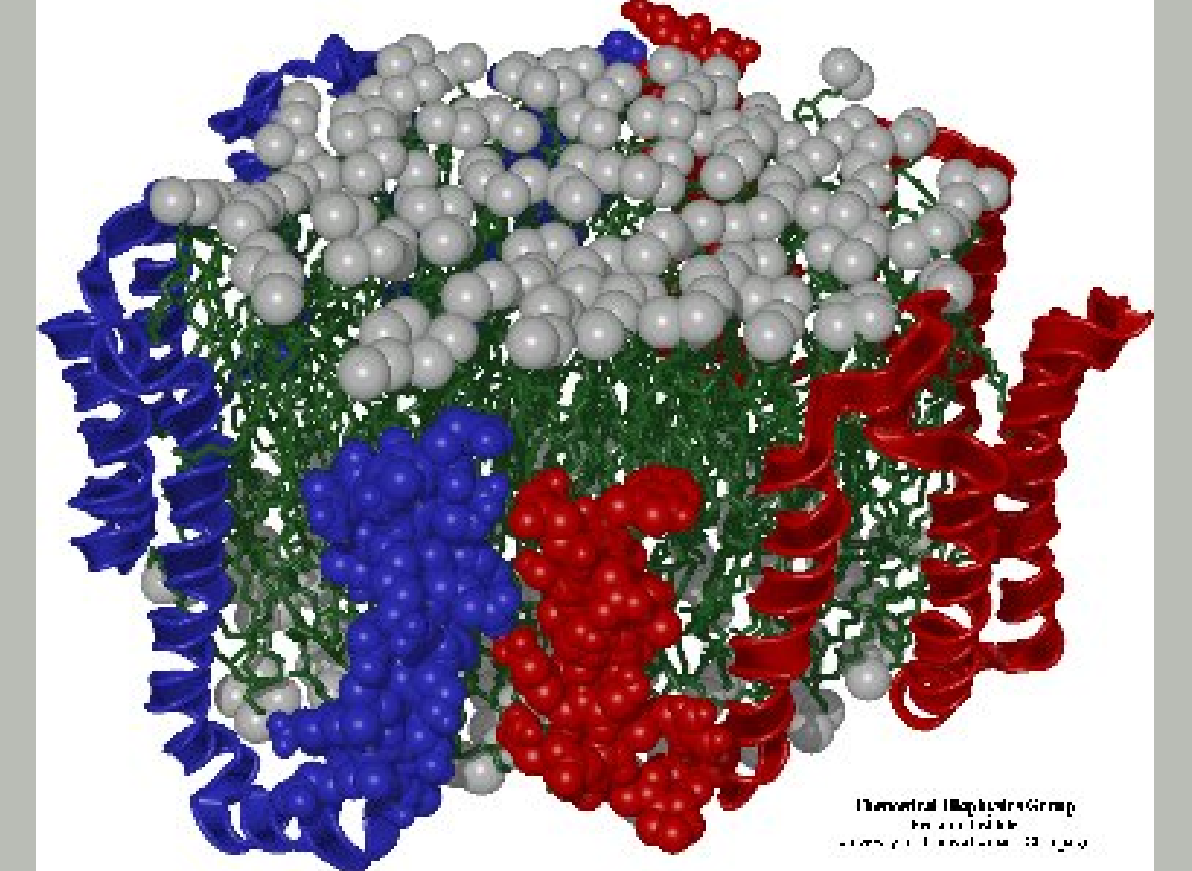
Parallelizing NAMD Using Charm++

- Reduce computation using short-range and long-range forces
- Non-bonded computation is intensive
- Spatial and force decomposition
- Overlap computation and communication
- Parallel I/O for large systems
- Load balancing
- Fine grain decomposition to increase parallelism
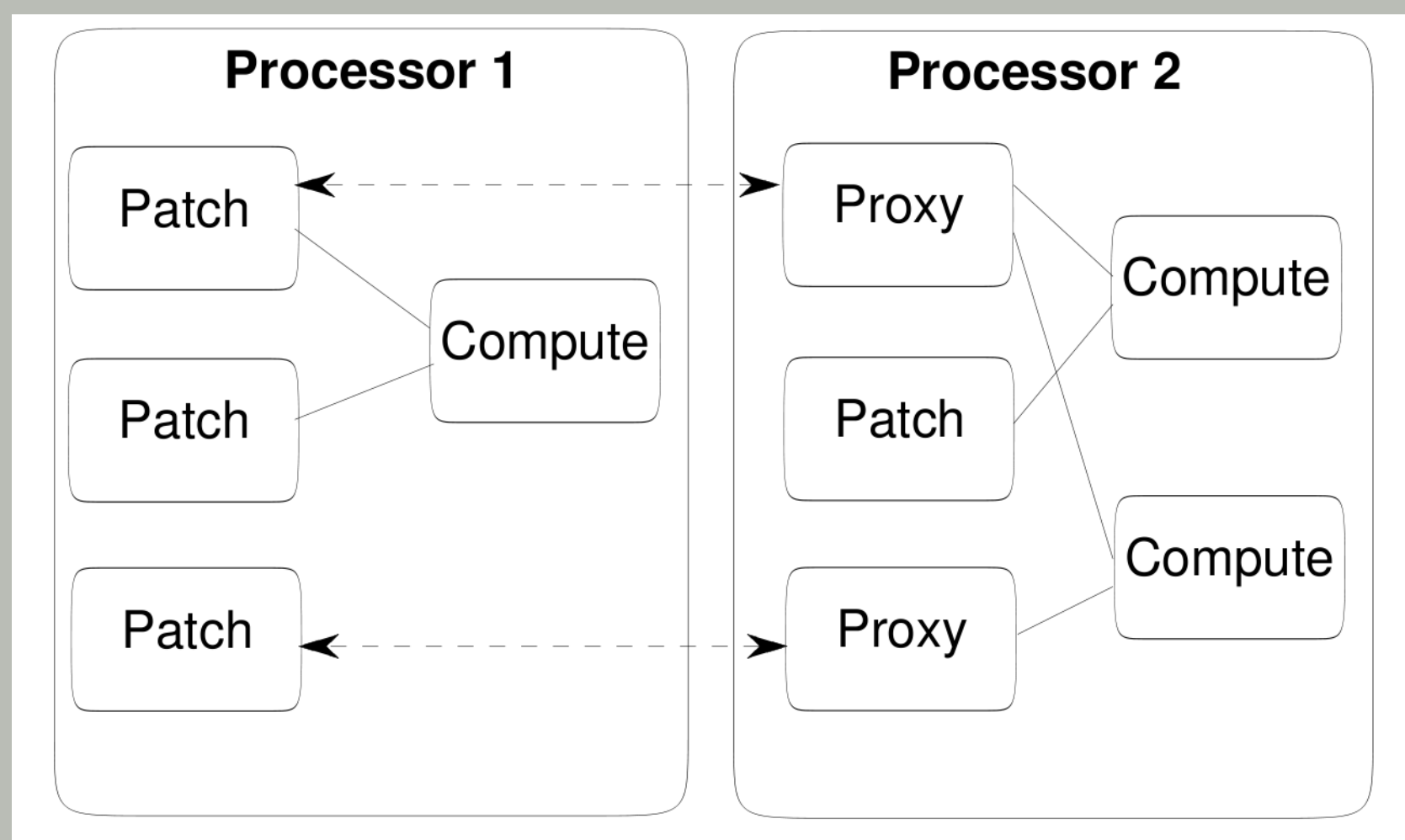
## Performance Visualization and Analysis
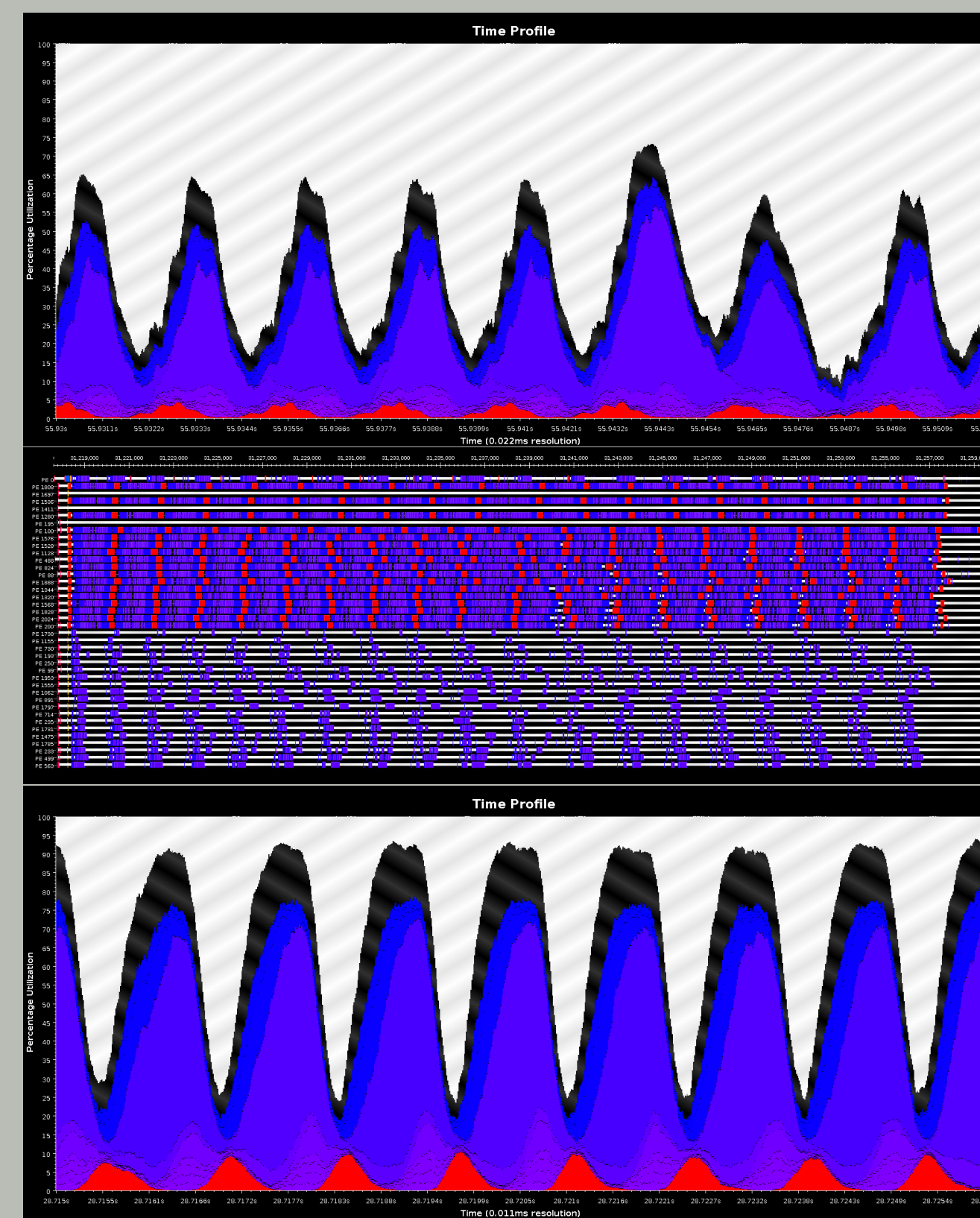
Projections framework

- Projections for performance tuning
- Instrument data during run-time
- Detect load balancing problem
- Communication problems
- Using Projections to find load balancing problem and fix it

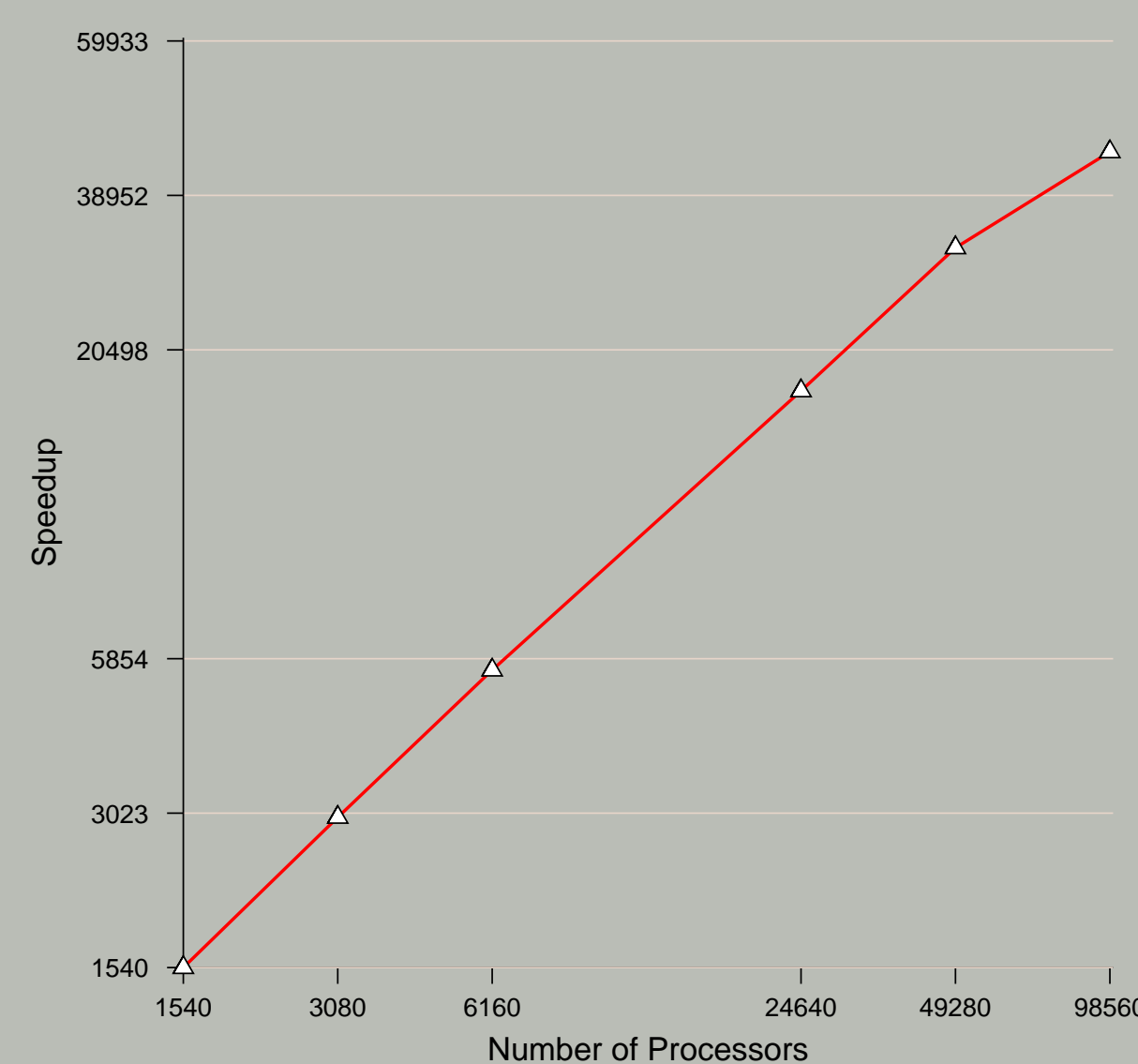## Strong Scaling for Small System

- DHFR - 23,558 atoms system
- Blue Gene/P at Argonne National Lab
  - 40,960 quad-core processors
  - Peak performance: 557 teraflops
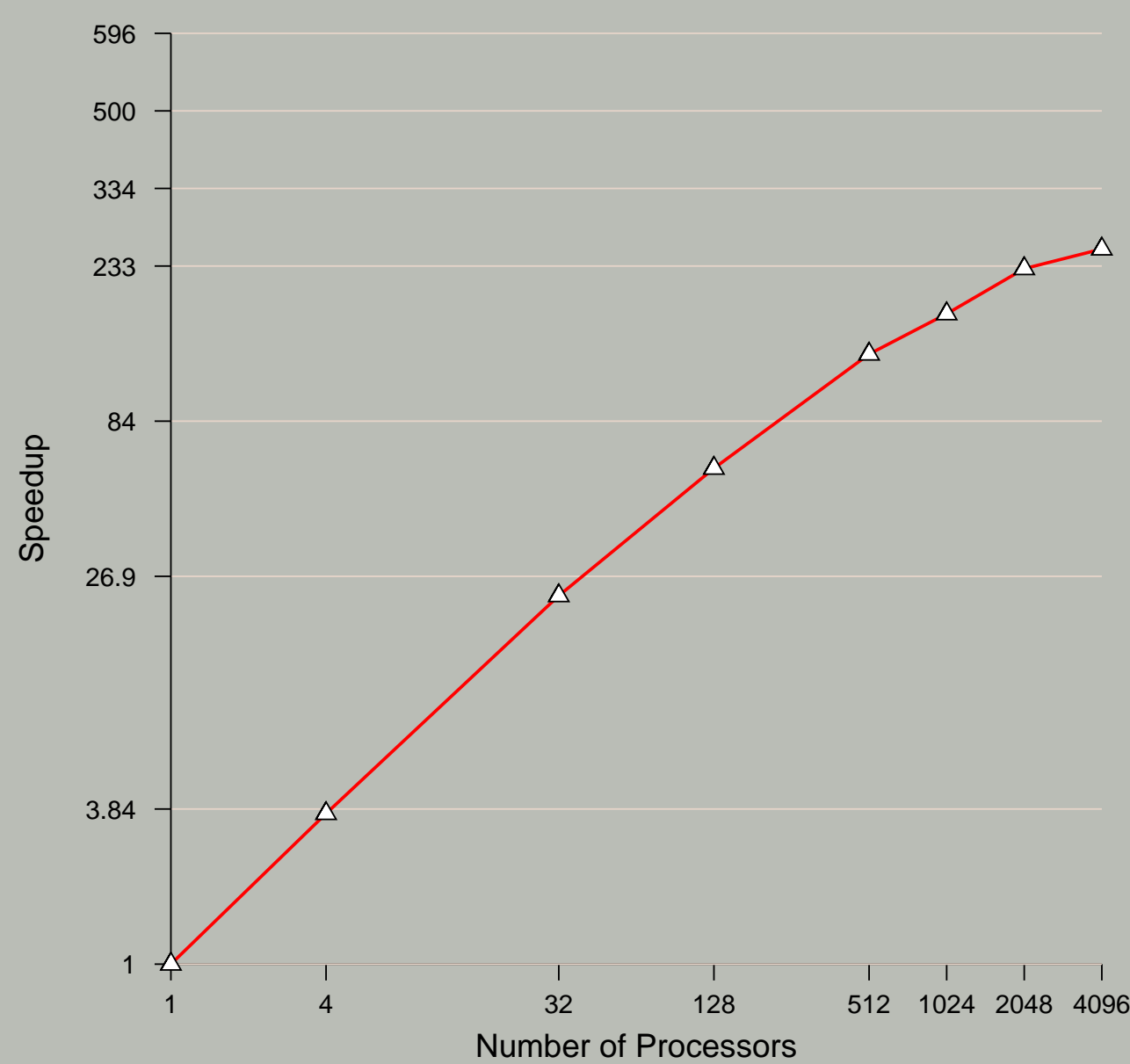
100M-atoms Simulation

- 100M atoms
- Jaguar at Oak Ridge
  - 224,256 AMD Opteron cores
  - Peak 2.3Petaflops
- 28ms/step on 100K cores

Future

- 1 ms/step using fine-grain decomposition
- Blue Waters @ Illinois
  - Power 7 processors
  - 300000 cores
  - Charm++ infrastructure is supported
  - Simulation of 100M-atom system benchmark on Blue Waters achieves 4ms/step

(http://www.ncsa.illinois.edu/)