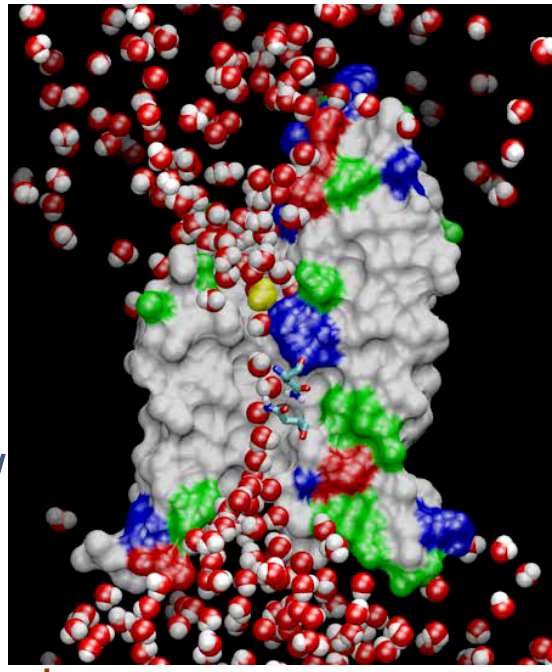
Molecular Dynamics in NAMD

- Collection of [charged] atoms, with bonds
  - Newtonian mechanics
  - Relatively small #of atoms (100K – 10M)
- At each time-step
  - Calculate forces on each atom
    - Bonds:
    - Non-bonded: electrostatic and van der W
      - Short-distance: every timestep
      - Long-distance: using PME (3D FFT)
      - Multiple Time Stepping : PME every 4 timesteps
  - Calculate velocities and advance positions
- Challenge: femtosecond time-step, millions needed!



Collaboration with K. Schulten, R. Skeel, and coworkers

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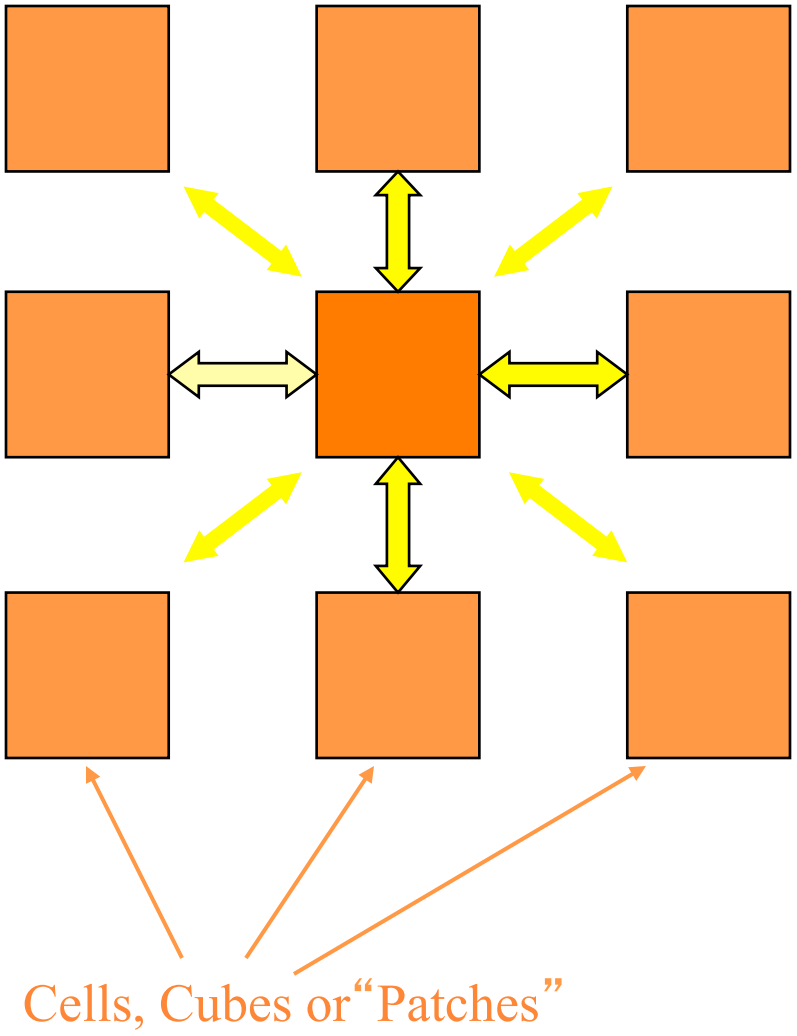
Spatial Decomposition Via Charm

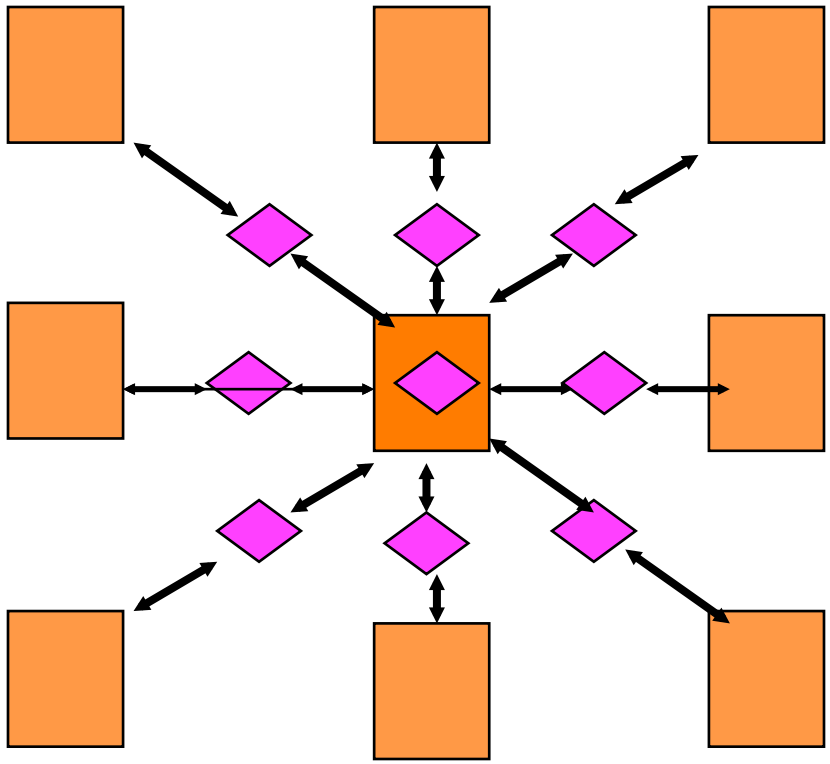


- Atoms distributed to cubes based on their location
- Size of each cube :
  - Just a bit larger than cut-off radius
  - Communicate only with neighbors
  - Work: for each pair of nbr objects
- C/C ratio: O(1)
- ***However:***
  - ***Load Imbalance***
  - ***Limited Parallelism***

Charm++ is useful to handle this

Object Based Parallelization for MD:

Force Decomposition + Spatial Decomposition



- Now, we have many objects to load balance:
  - Each diamond can be assigned to any proc.
  - Number of diamonds (3D):
    - 14·Number of Patches
  - 2-away variation:
    - Half-size cubes
    - 5x5x5 interactions
  - 3-away interactions: 7x7x7

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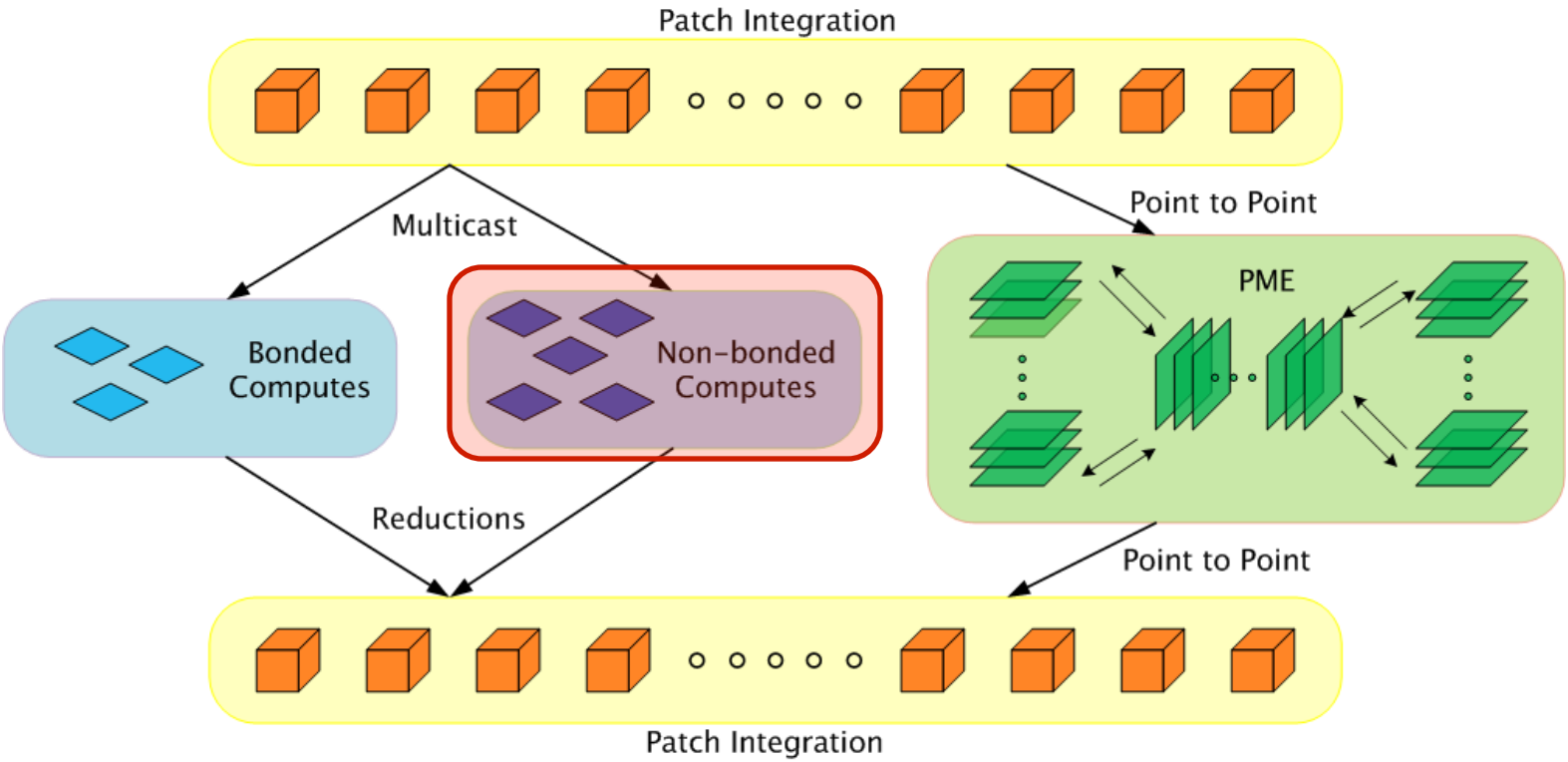
Parallelization Using Charm++

The computation is decomposed into "natural" objects of the application, which are assigned to processors by Charm++ RTS



Bhatele, A., Kumar, S., Mei, C., Phillips, J. C., Zheng, G. & Kale, L. V. 2008 **Overcoming Scaling Challenges in Biomolecular Simulations across Multiple Platforms**. In *Proceedings of IEEE International Parallel and Distributed Processing Symposium*, Miami, FL, USA, April 2008.

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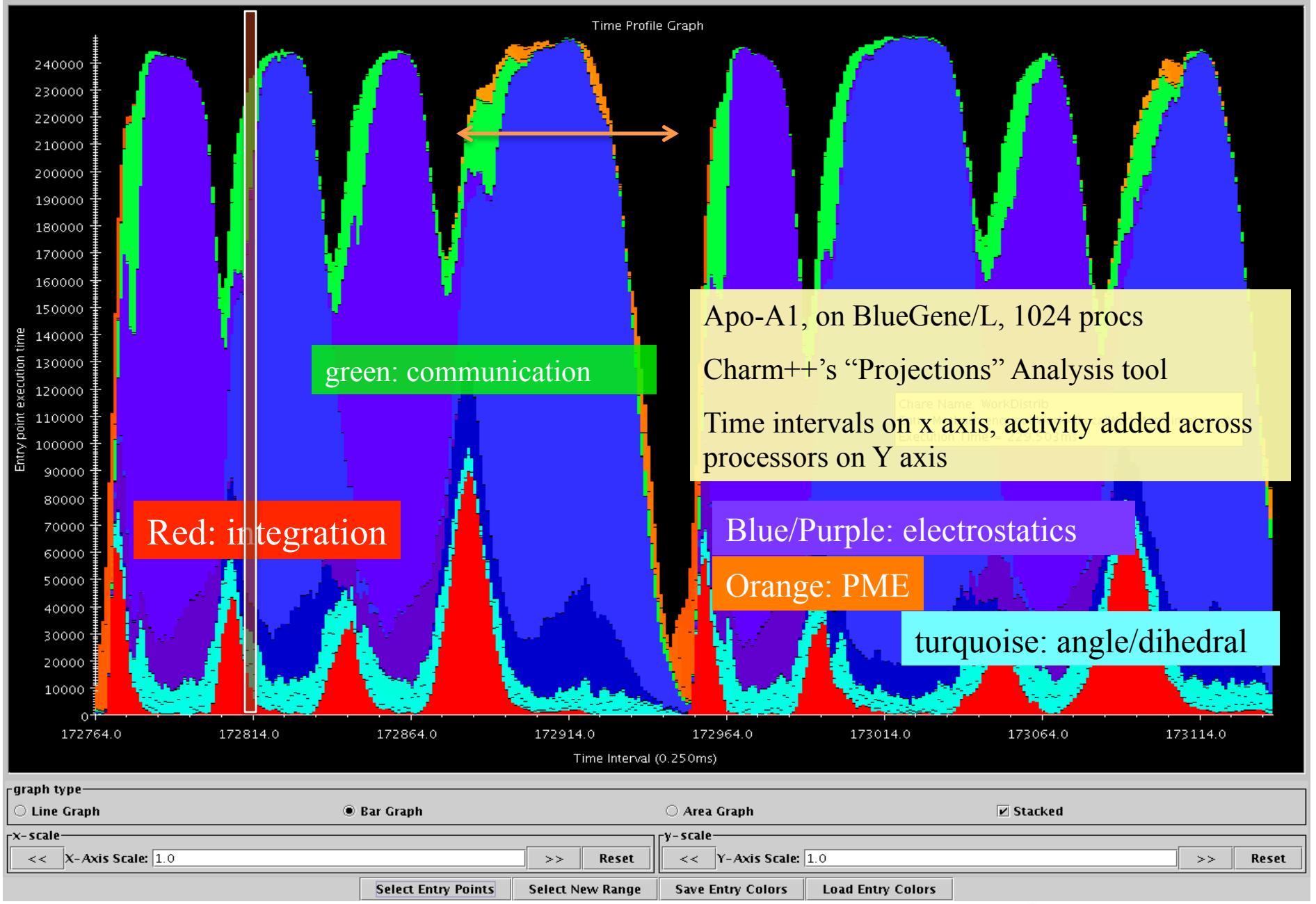

Time

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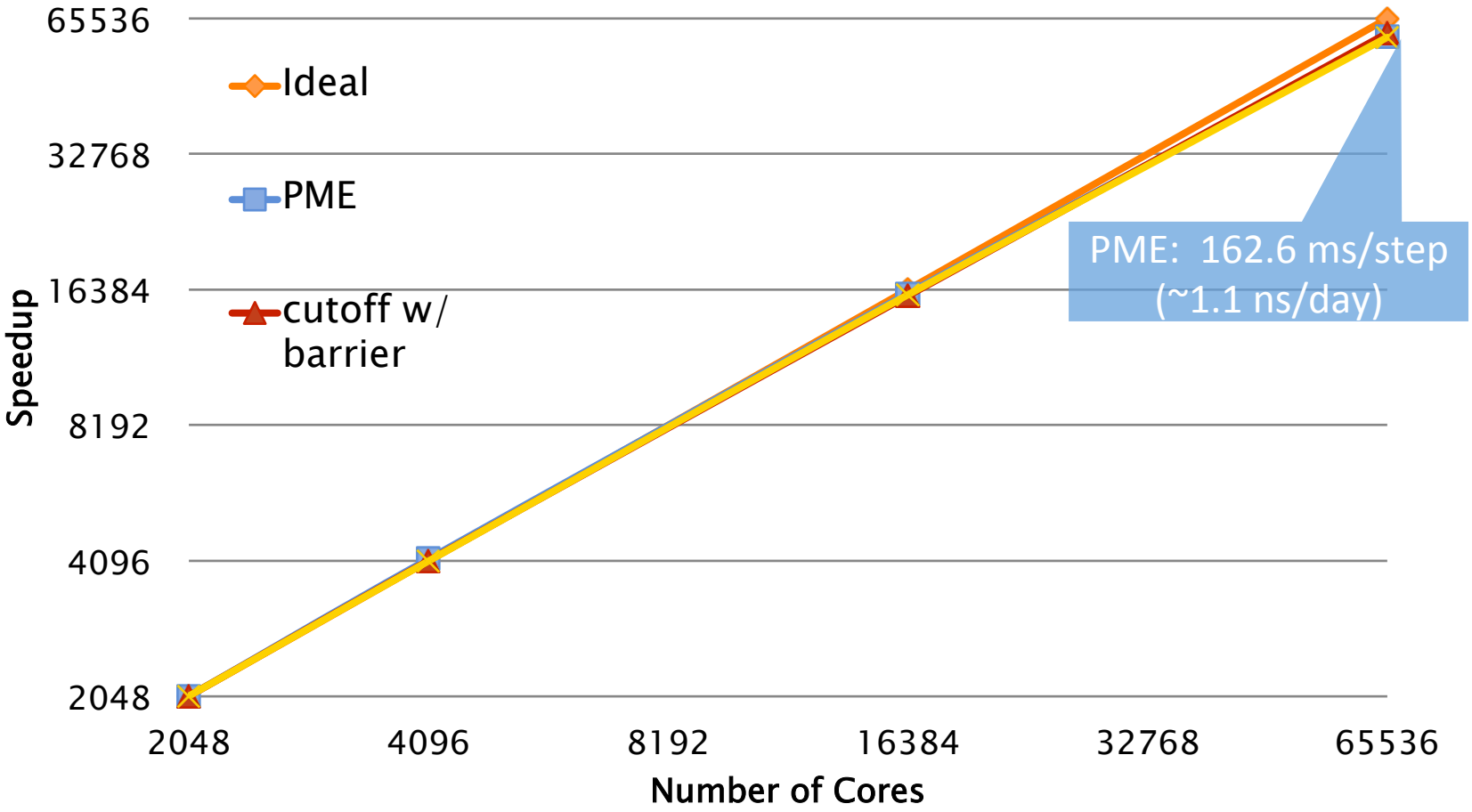
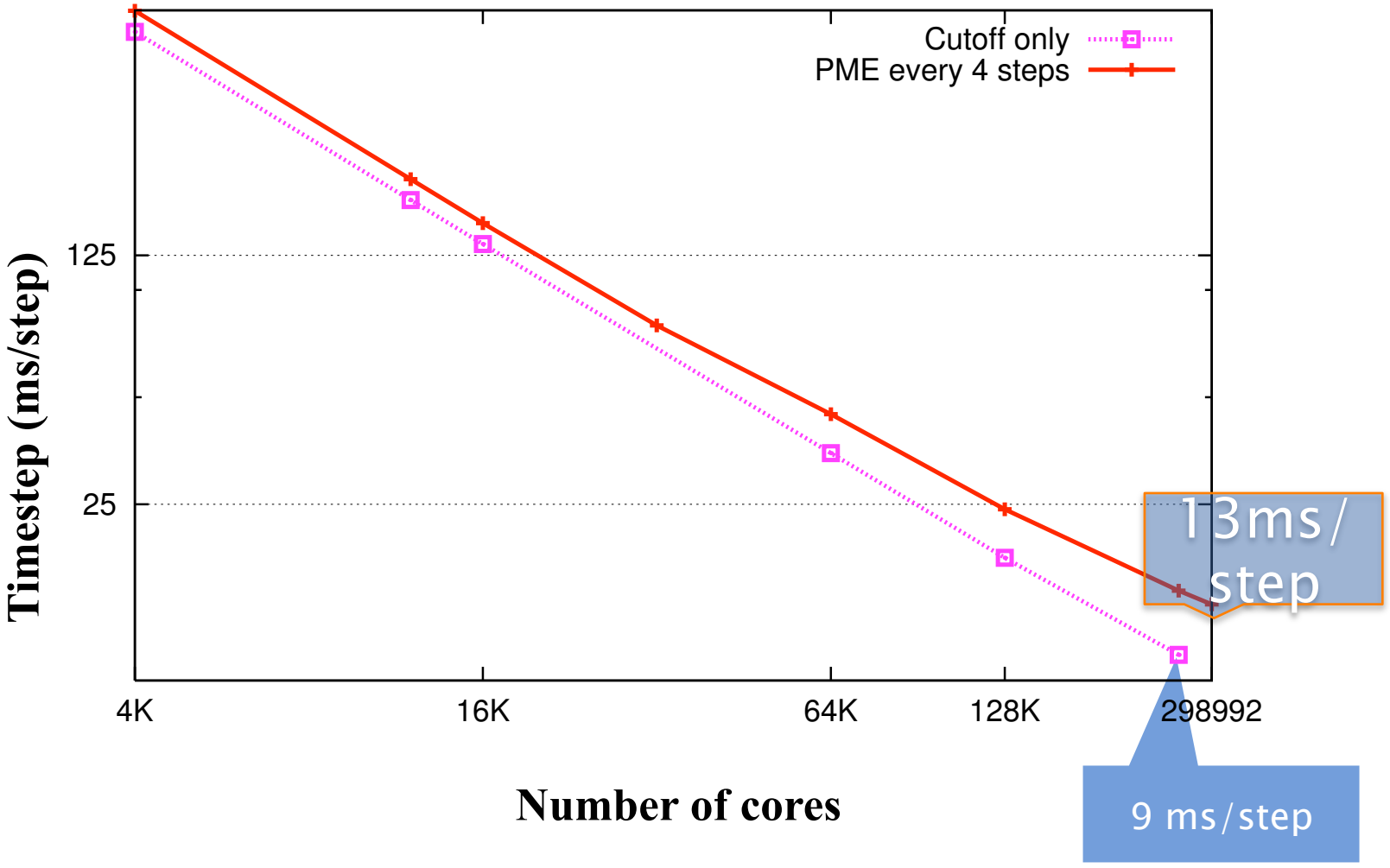
Performance on Intrepid (BG/P)



SMP Performance on Titan(Dev)



ChaNGa: Parallel Gravity

- Collaborative project (NSF)
  - with Tom Quinn, Univ. of Washington
- Gravity, gas dynamics
- Barnes-Hut tree codes
  - Oct tree is natural decomp
  - Geometry has better aspect ratios, so you "open" up fewer nodes
  - But is not used because it leads to bad load balance
  - Assumption: one-to-one map between sub-trees and PEs
  - Binary trees are considered better load balanced

Evolution of Universe and Galaxy Formation

With Charm++: Use Oct-Tree, and let Charm++ map subtrees to processors

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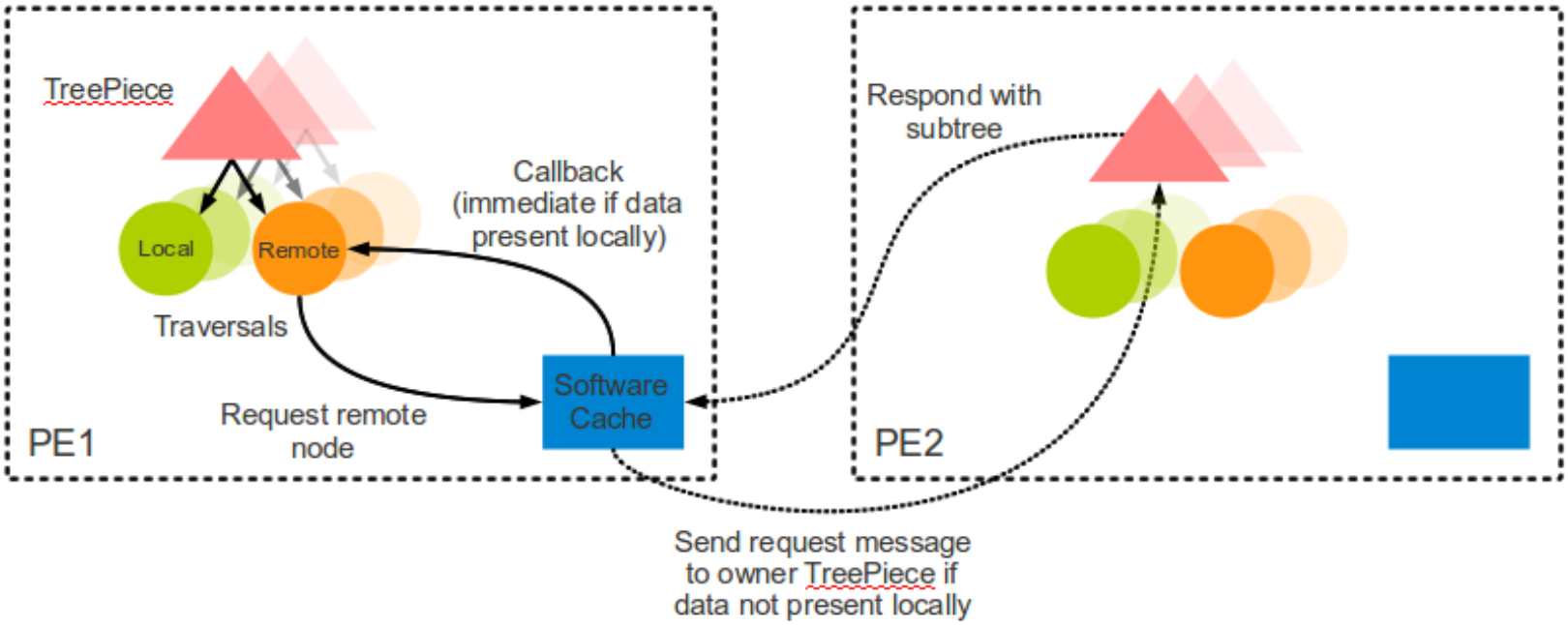
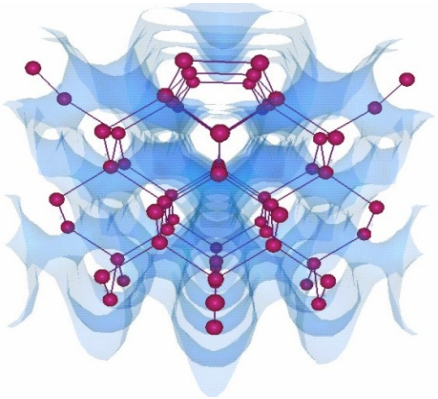
Control flow



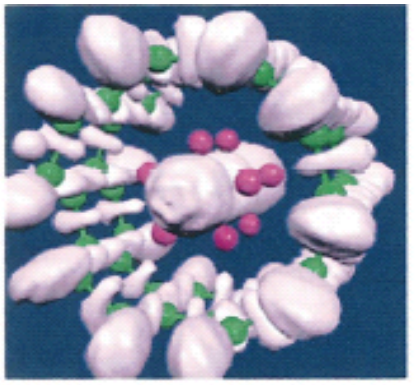
OpenAtom: MD with quantum effects

- Much more fine-grained:
  - Each electronic state is modeled with a large array

Semiconductor Surfaces:



Nanowires:



Collaboration with:
G. Martyna (IBM)
M. Tuckerman (NYU)
L. Kale (UIUC)

Using Charm++ virtualization, we can efficiently scale small (32 molecule) systems to thousands of processors

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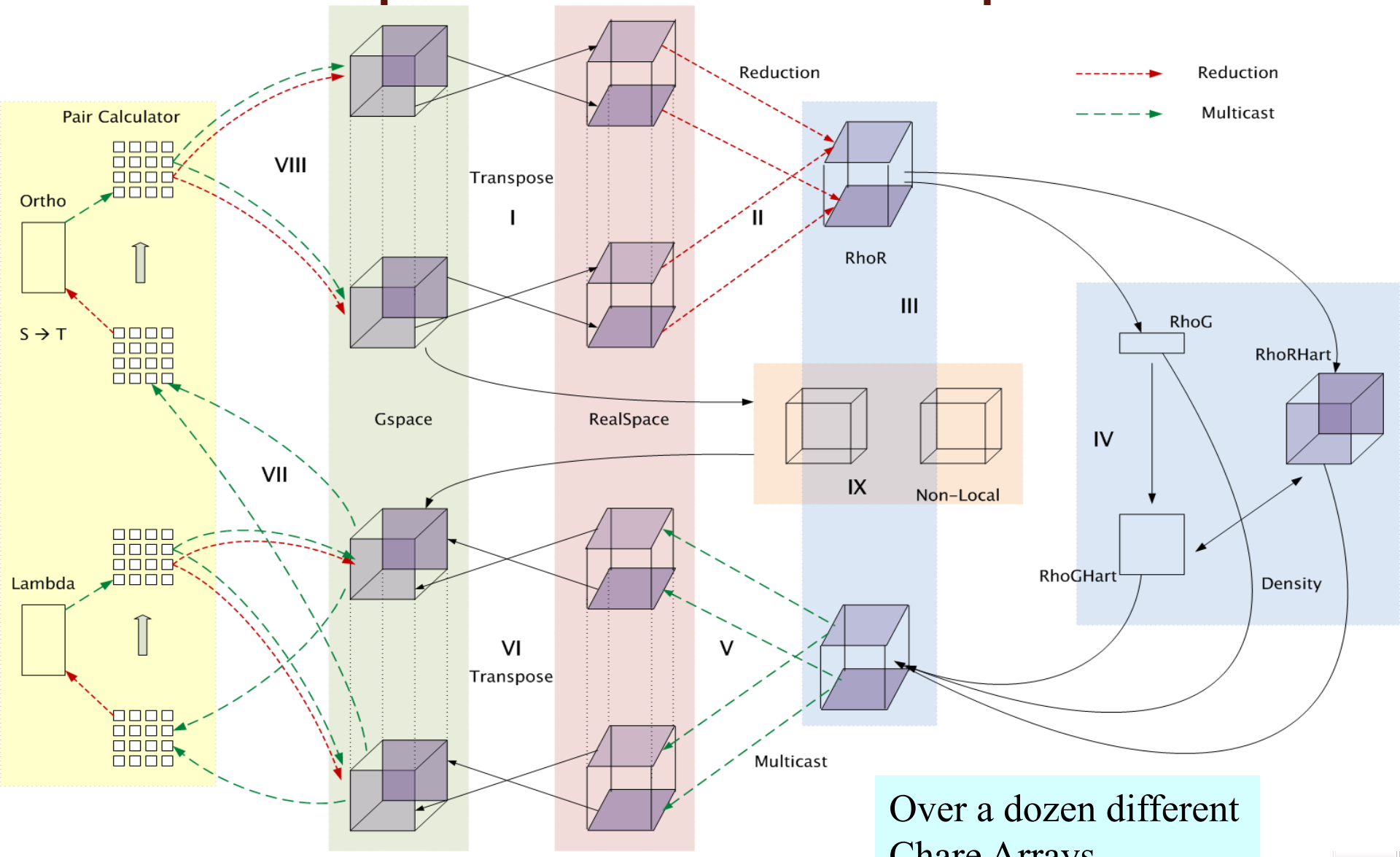
Decomposition and Computation



Over a dozen different Chare Arrays

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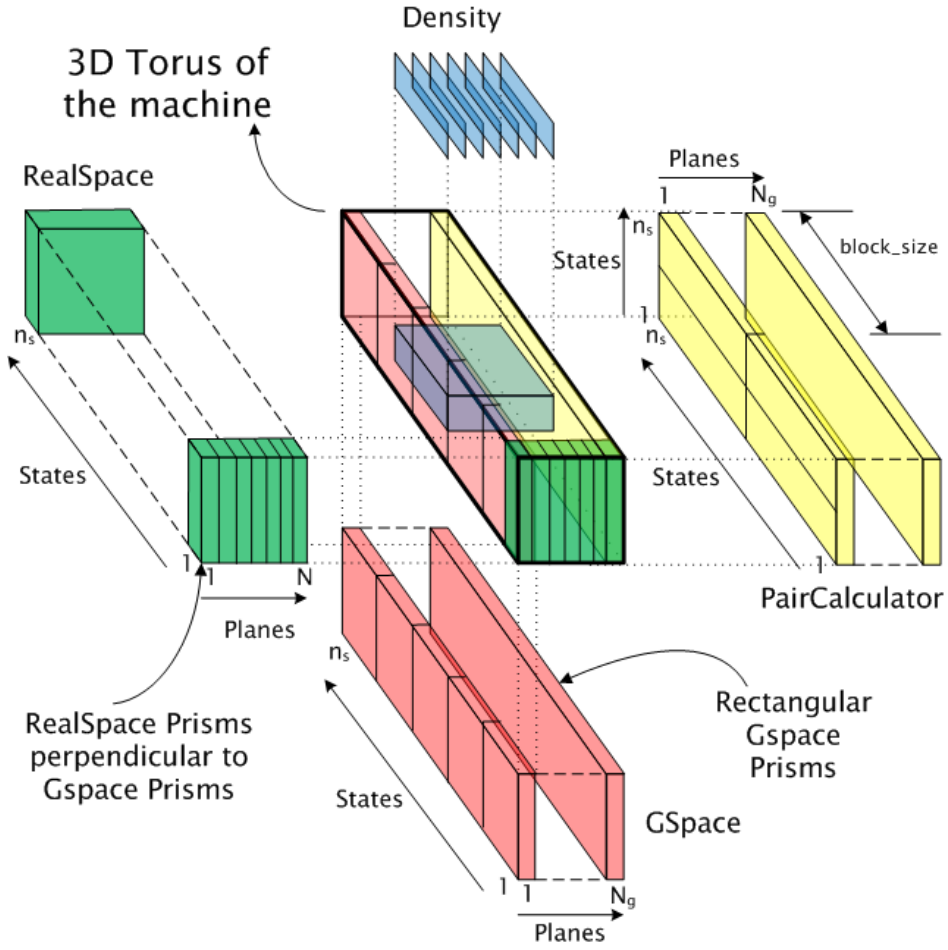
Topology Aware Mapping of Objects



- Object based decomposition provides new degrees of freeedom to easily try different mappings of objects to processors, to help minimize contention