

Towards Message-driven Mixed-Quantum/Classical dynamics in Atomic Simulation

Chris Harrison

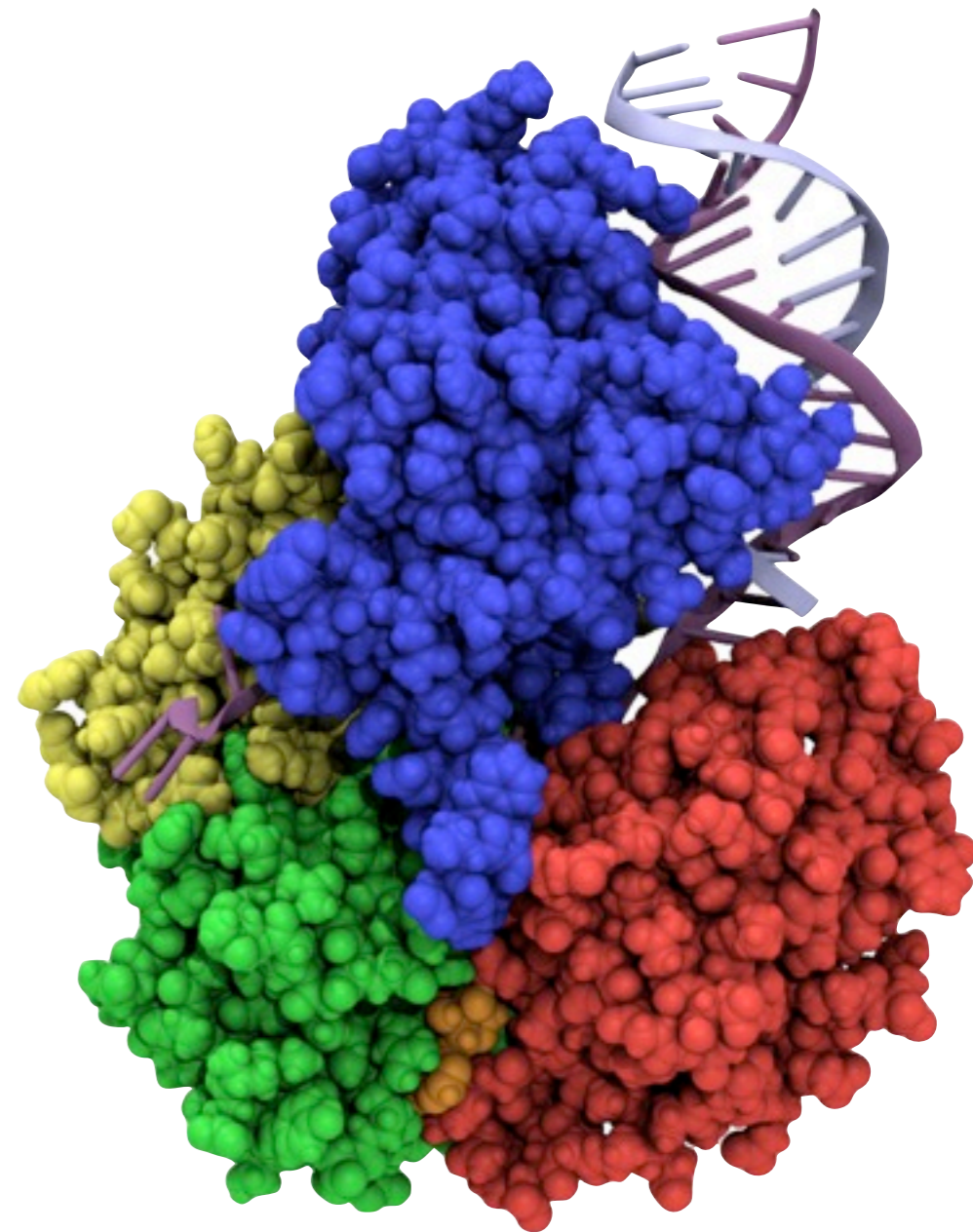
Beckman Institute, University of Illinois

<http://www.ks.uiuc.edu>

Eric Bohm, Phil Miller, Ramprasad Venkaterman

Jim Phillips

Glenn Martyna, Mark Tuckerman, Laxmikant Kale, Klaus Schulten



NIH Resource for Macromolecular Modeling and Bioinformatics
<http://www.ks.uiuc.edu>

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University of Illinois

Who and Where

Theoretical and Computational Biophysics Group



Beckman Institute



Parallel Programming Laboratory

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University of Illinois**



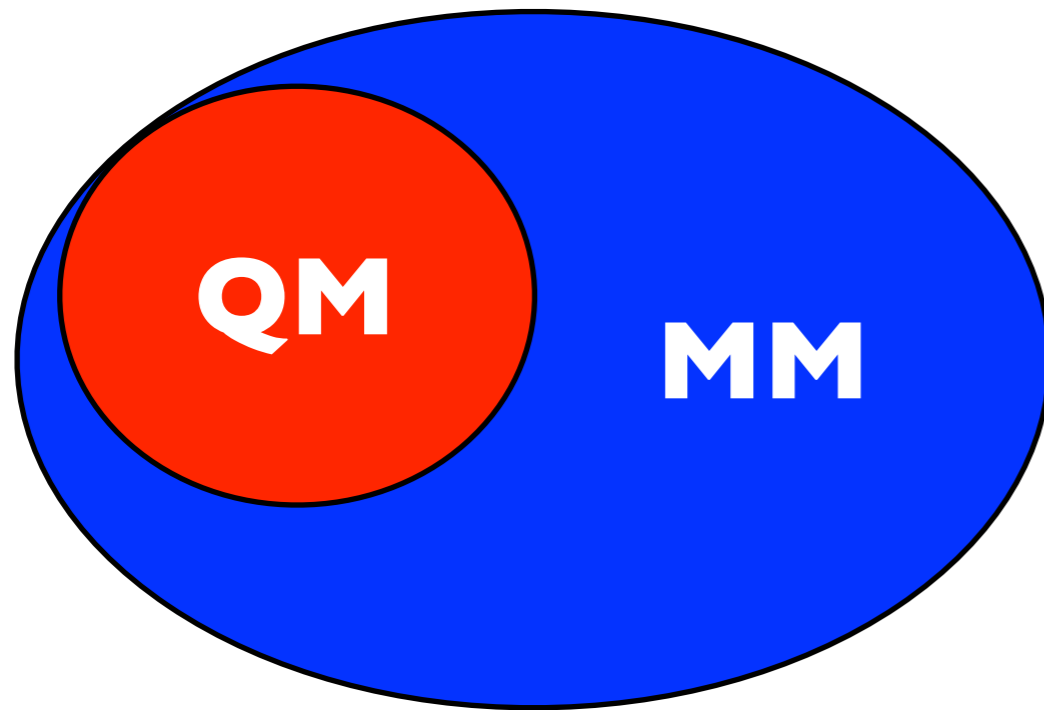
National Center for
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Outline

- QM/MM: Why
- QM Types
- The MM: NAMD
- The QM: OpenAtom
- QM/MM Design & Implementation
- Preliminary Results

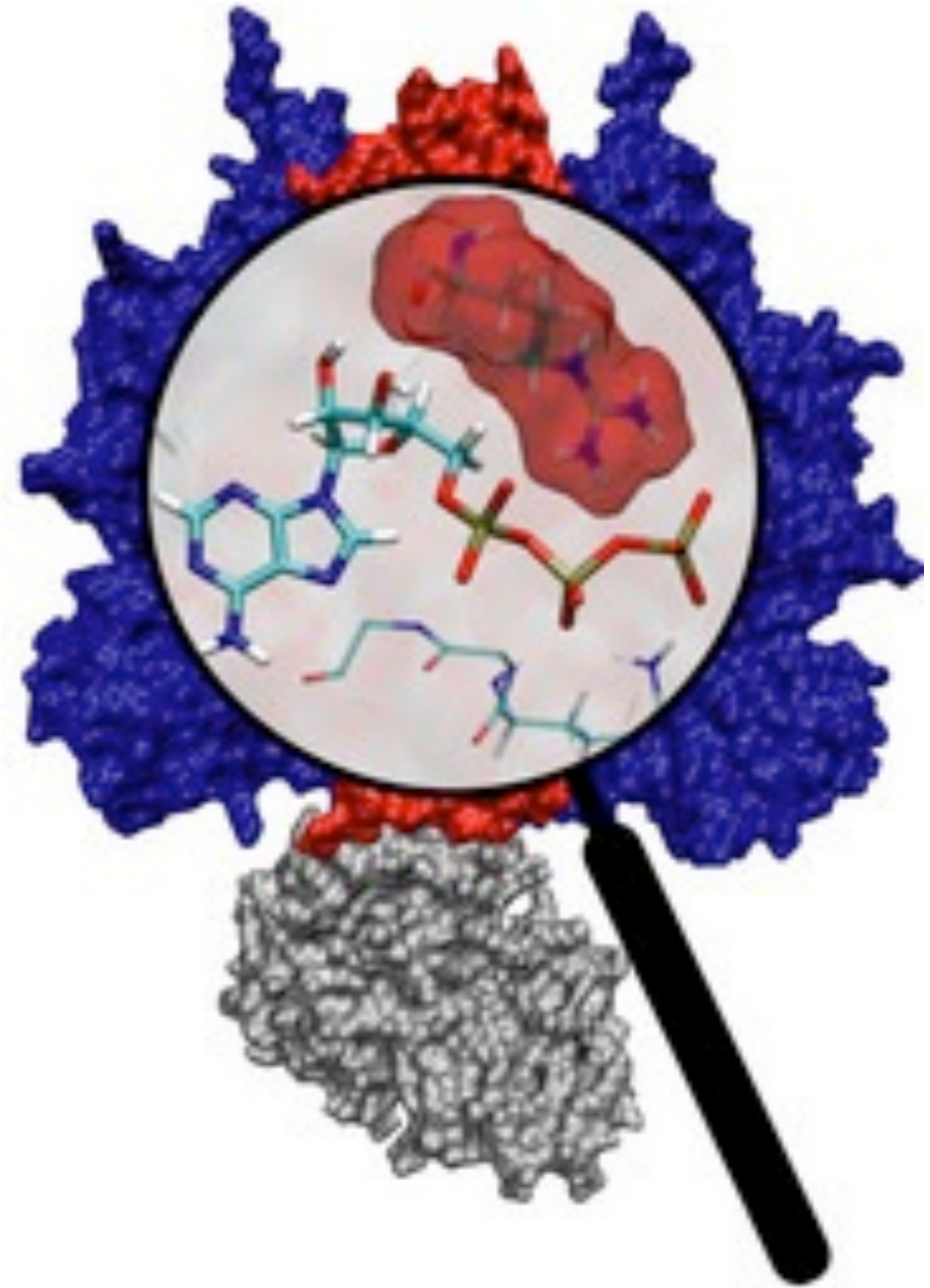


Why QM/MM?



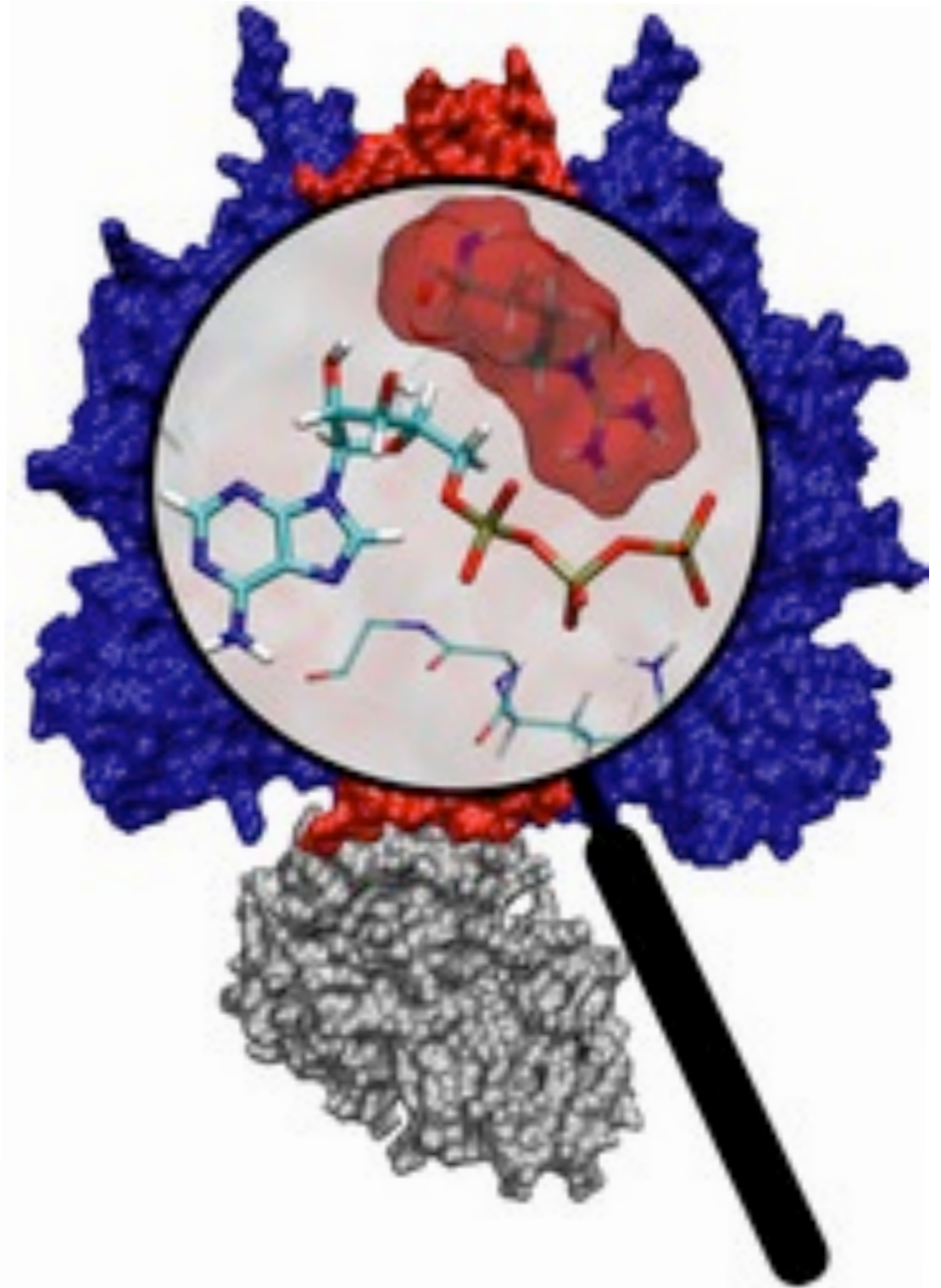
Why QM/MM?

- Chemical reactions coupled to environment
- Excited state dynamics
- Electron & Energy Transfer
- Vibrational spectroscopy
- Accurate potentials



Types of QM: Which to use?

- GCAO (Gaussian Centered Atomic Orbital)
- Plane wave (aka Car-Parinello)
- Semiempirical
- Electron Valence Bond



Yarne, Tuckerman, Martyna, *J. Chem. Phys.* | **115:3531**, 2001



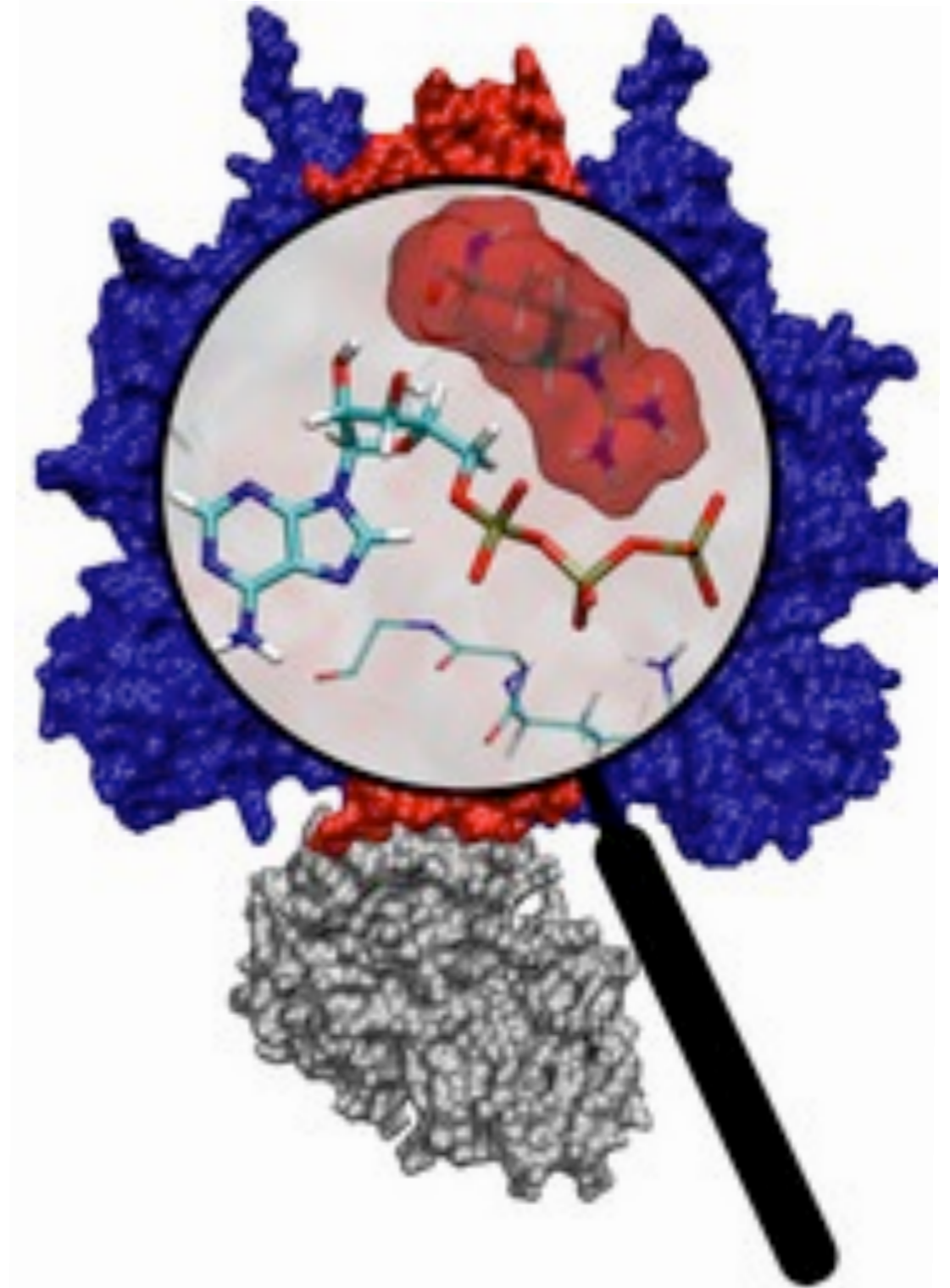
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QM/MM:

A Shotgun Wedding of **NAMD** and **OpenAtom** by an **MSA** Minister



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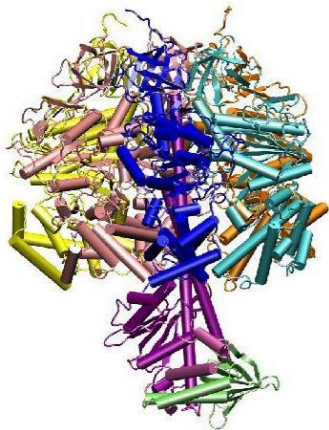


National Center for
Research Resources

Thursday, April 21, 2011

NAMD: Scalable Molecular Dynamics

2002 Gordon Bell Award



ATP Synthase



PSC Lemieux

37,000 Users, 1700 Citations



Computational Biophysics Summer School

Blue Waters Target Application



Illinois Petascale Computing Facility

GPU Acceleration

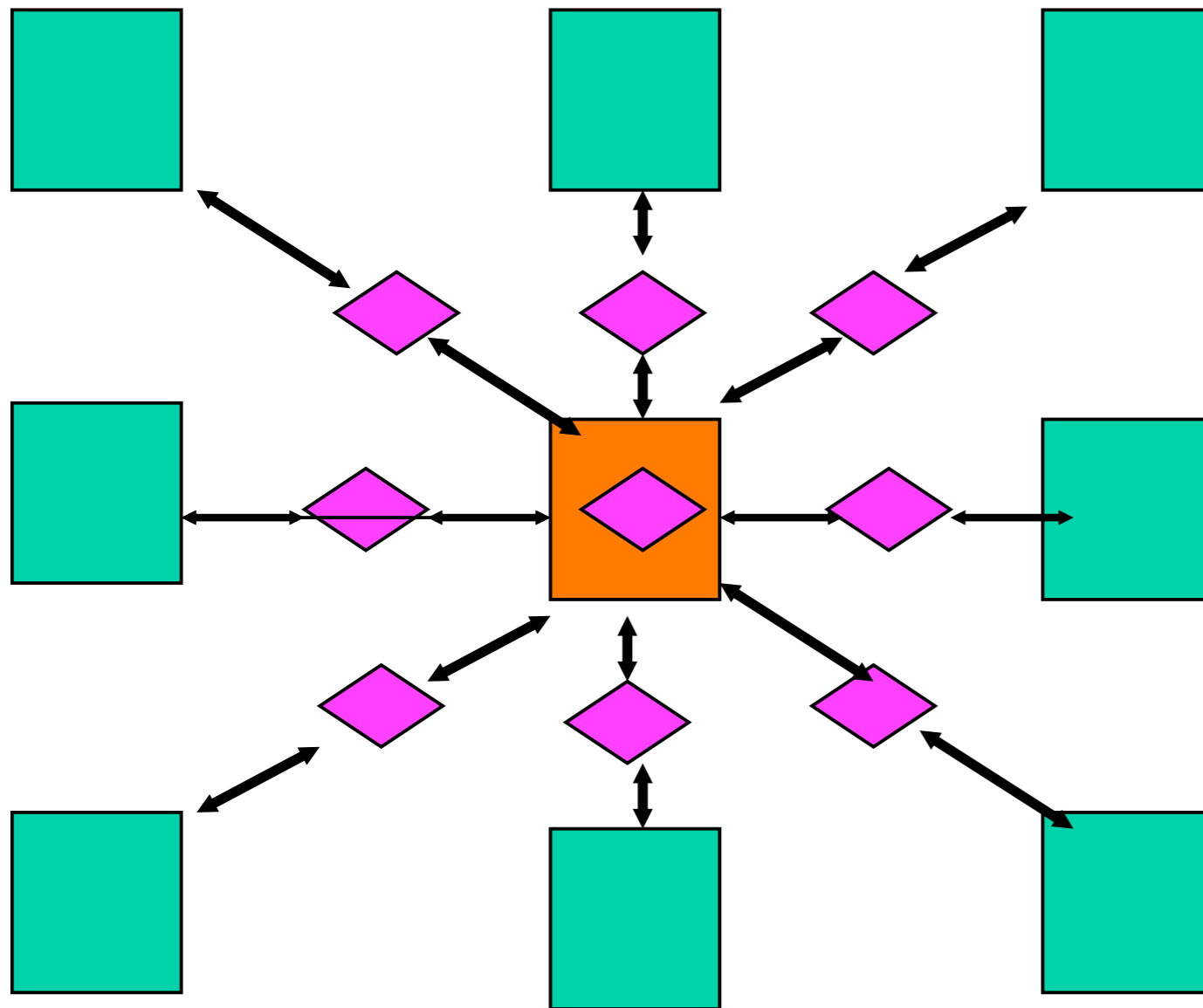


Nvidia Tesla

NCSA Lincoln

NAMD Decomposition

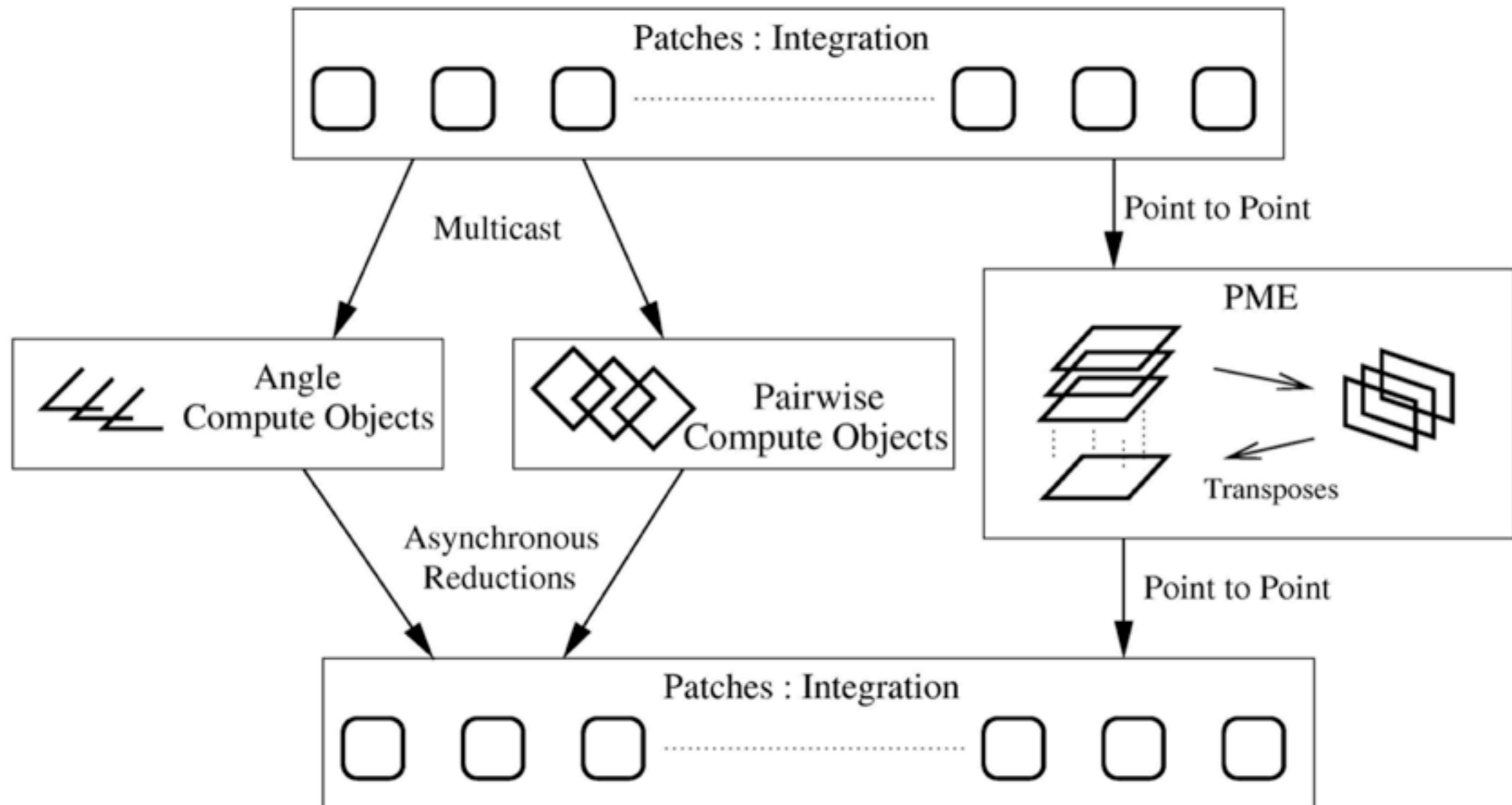
Kale et al., *J. Comp. Phys.* **151**:2833-2, 1999



- Spatially decompose data and communication
- Separate but related work decomposition
- “Compute objects” facilitate iterative, measurement-based load balancing system

How NAMMD works, sorta.

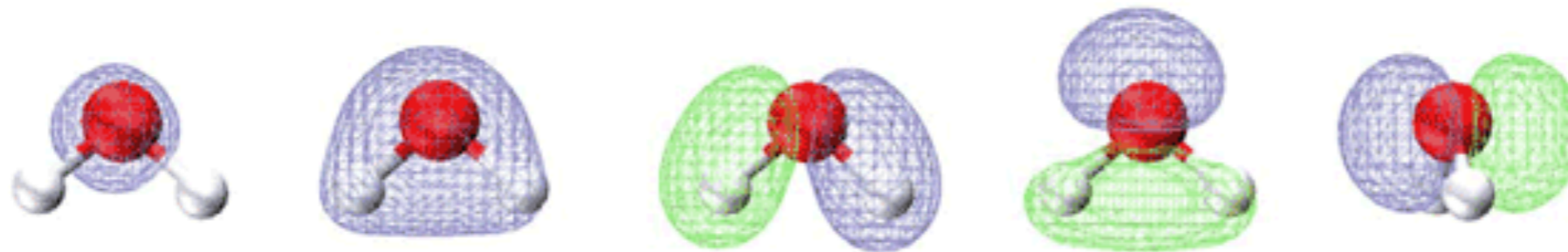
Phillips *et al.*, SC2002



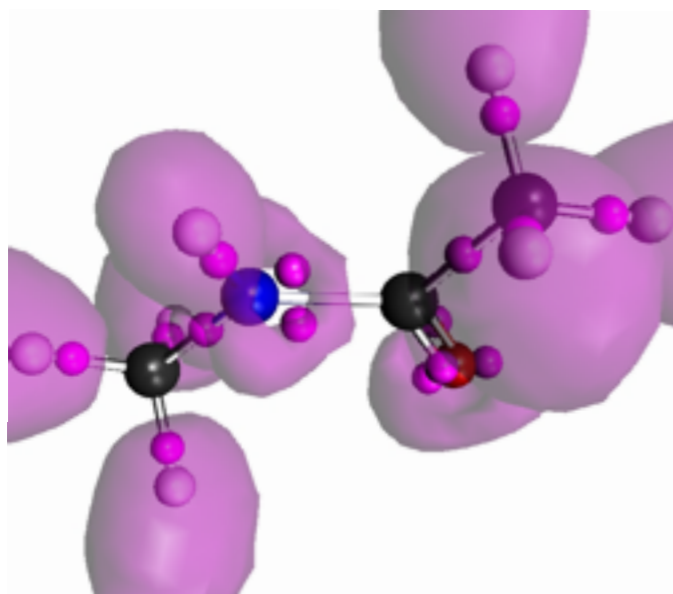
Objects are assigned to processors and queued as data arrives



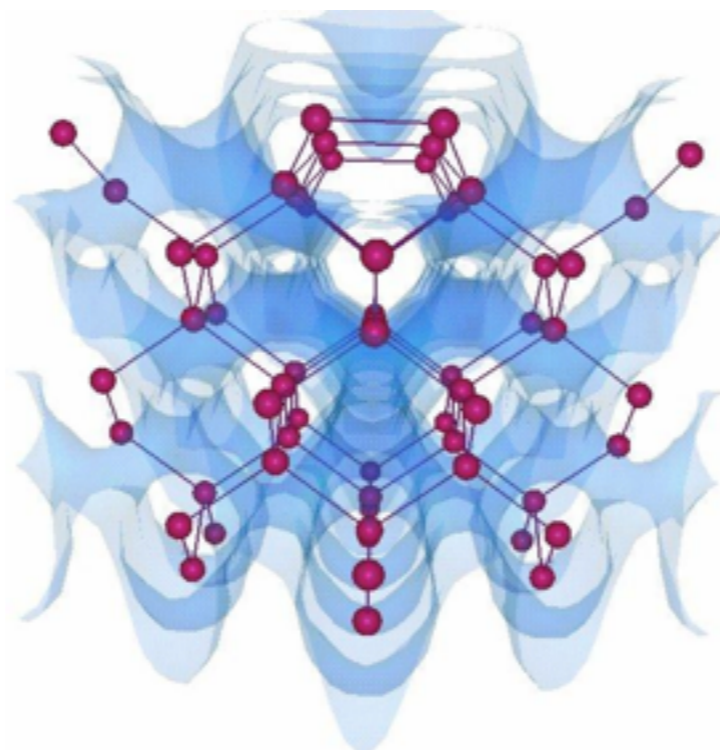
OpenAtom



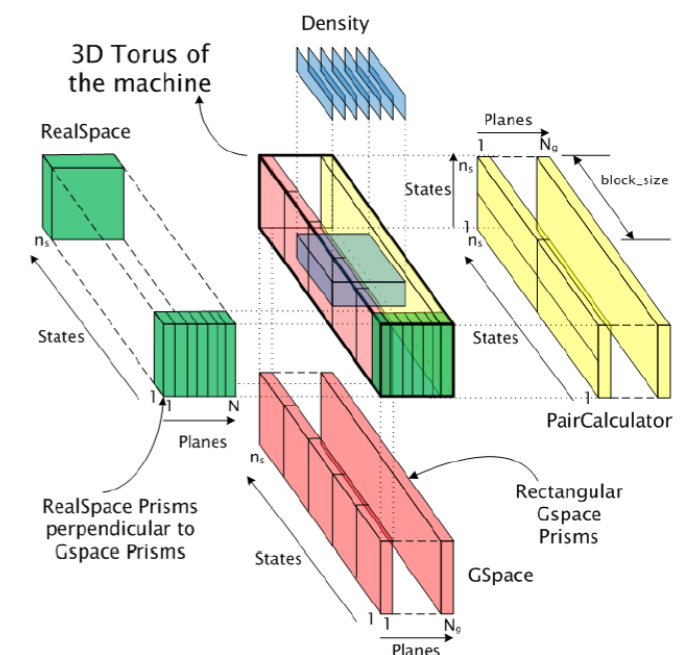
Electronic states/orbitals



Car-Parinello Dynamics



Plane Wave Basis

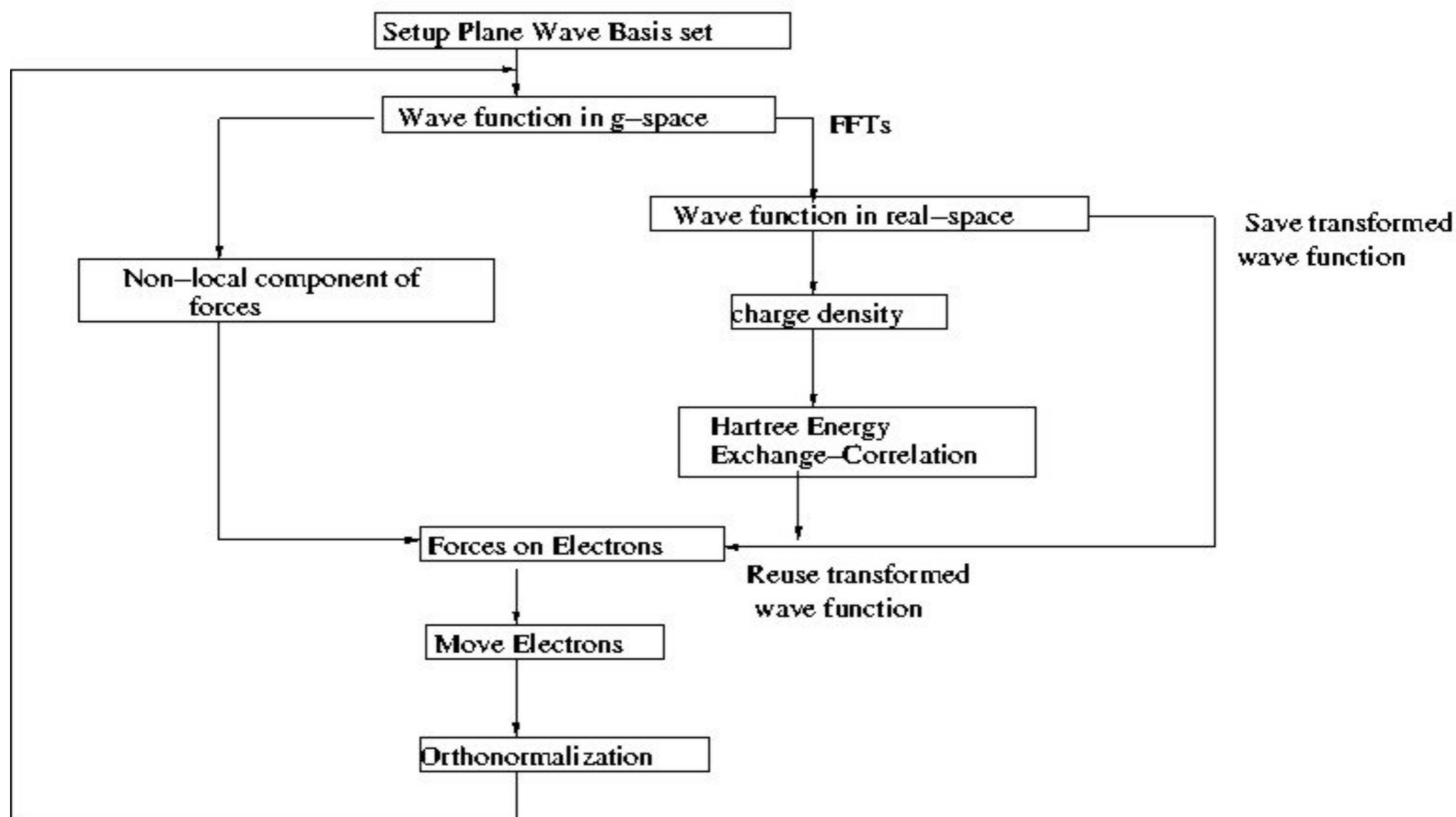


Topology Aware Mapping

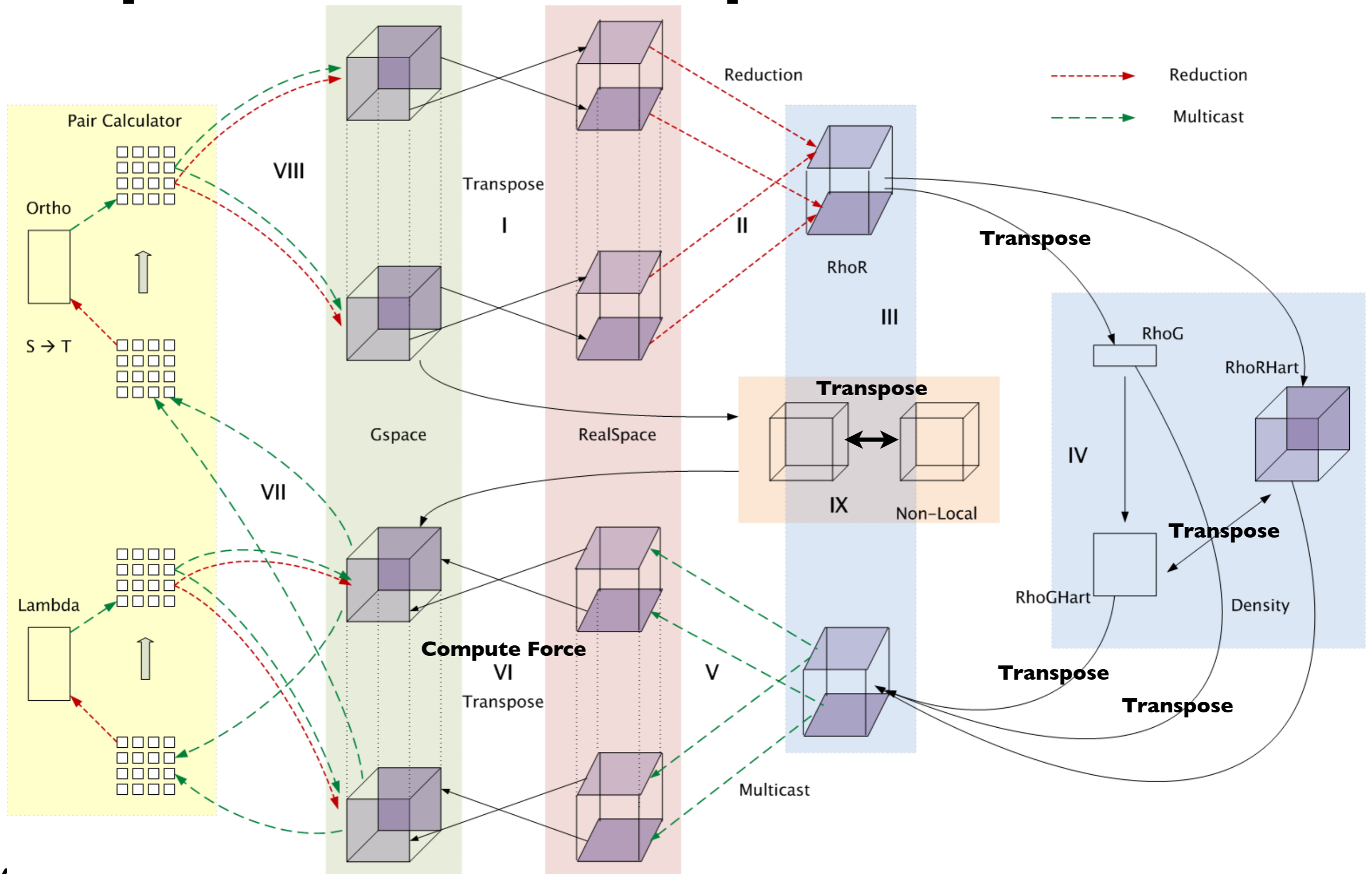
Euro-par
distinguished paper
award 2009



OpenAtom: Serial Algorithm



OpenAtom Implementation



QM/MM: Steps

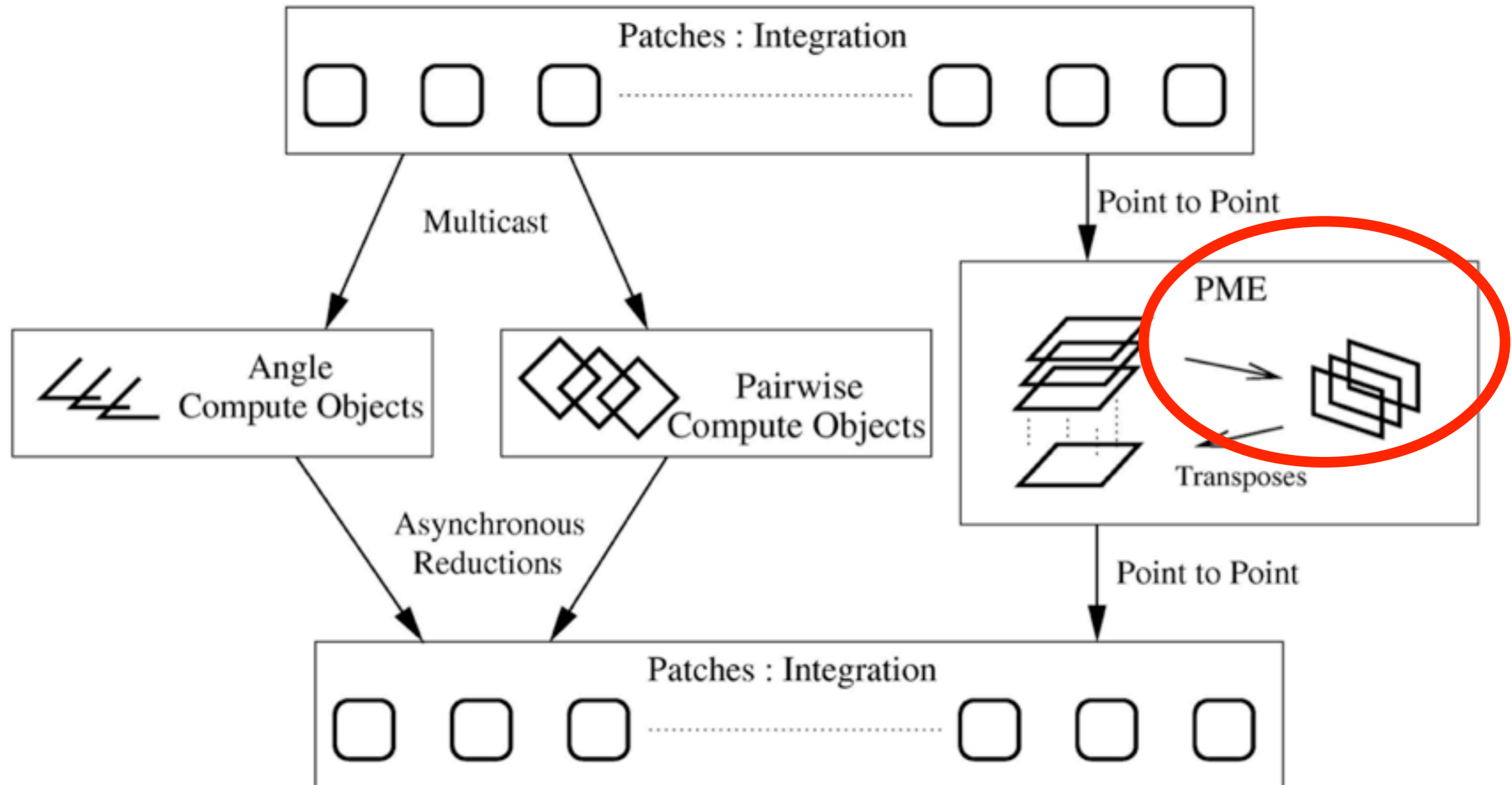
Yarne, Tuckerman, Martyna, *J. Chem. Phys.* **115**:3531, 2001

- Exchange Euler Grid Mappings [QM & MM]
- Collect/Accumulate Q & b grids [MM]
- Calculate S grid [MM]
- ReMap MM S grid as QM S grid [MM]
- Combine S grid & RhoG [QM]
- ReMap & Distribute forces [QM & MM]



QM/MM: Implementation

NAMD



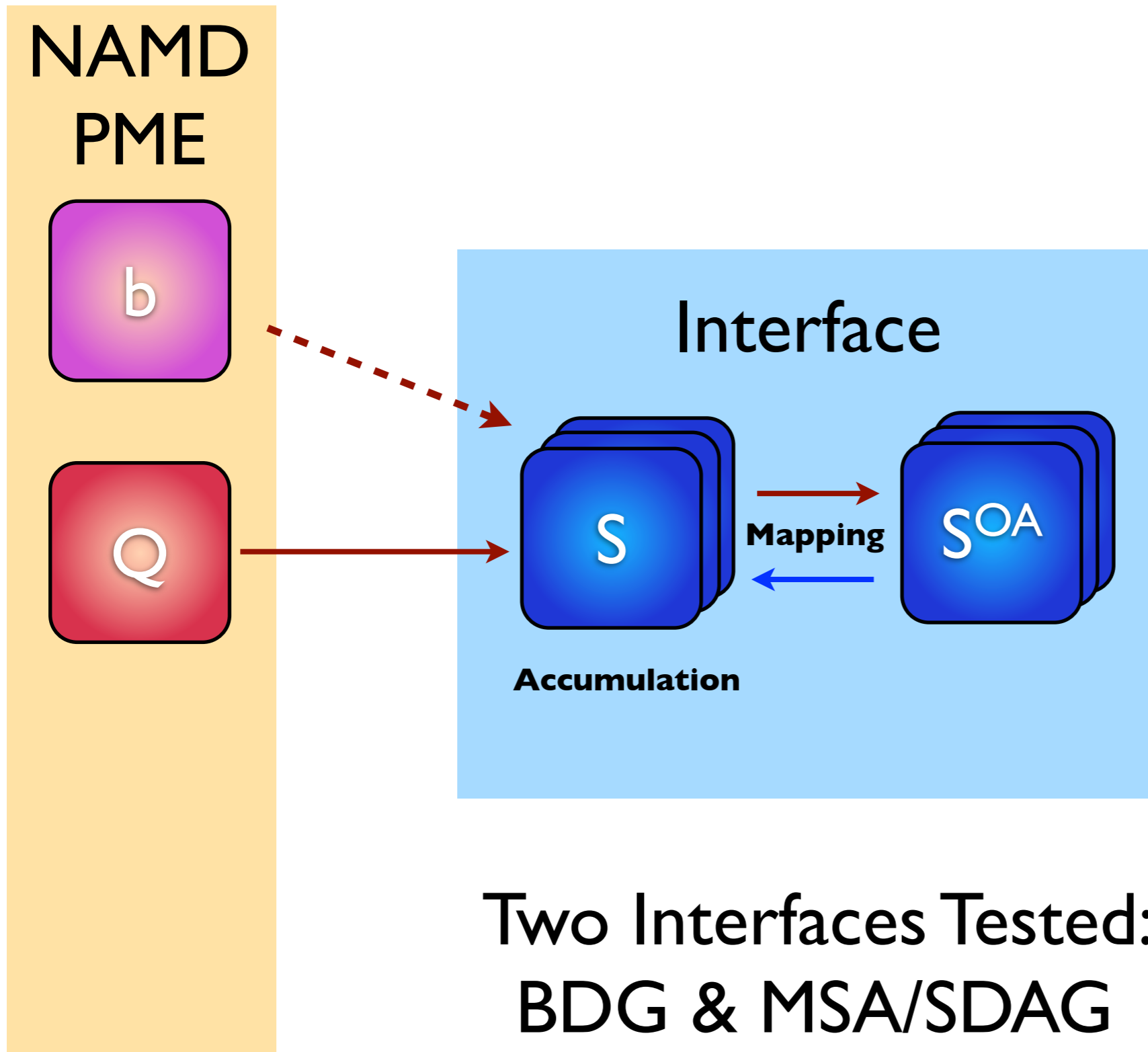
QM/MM: Implementation

NAMD

PME



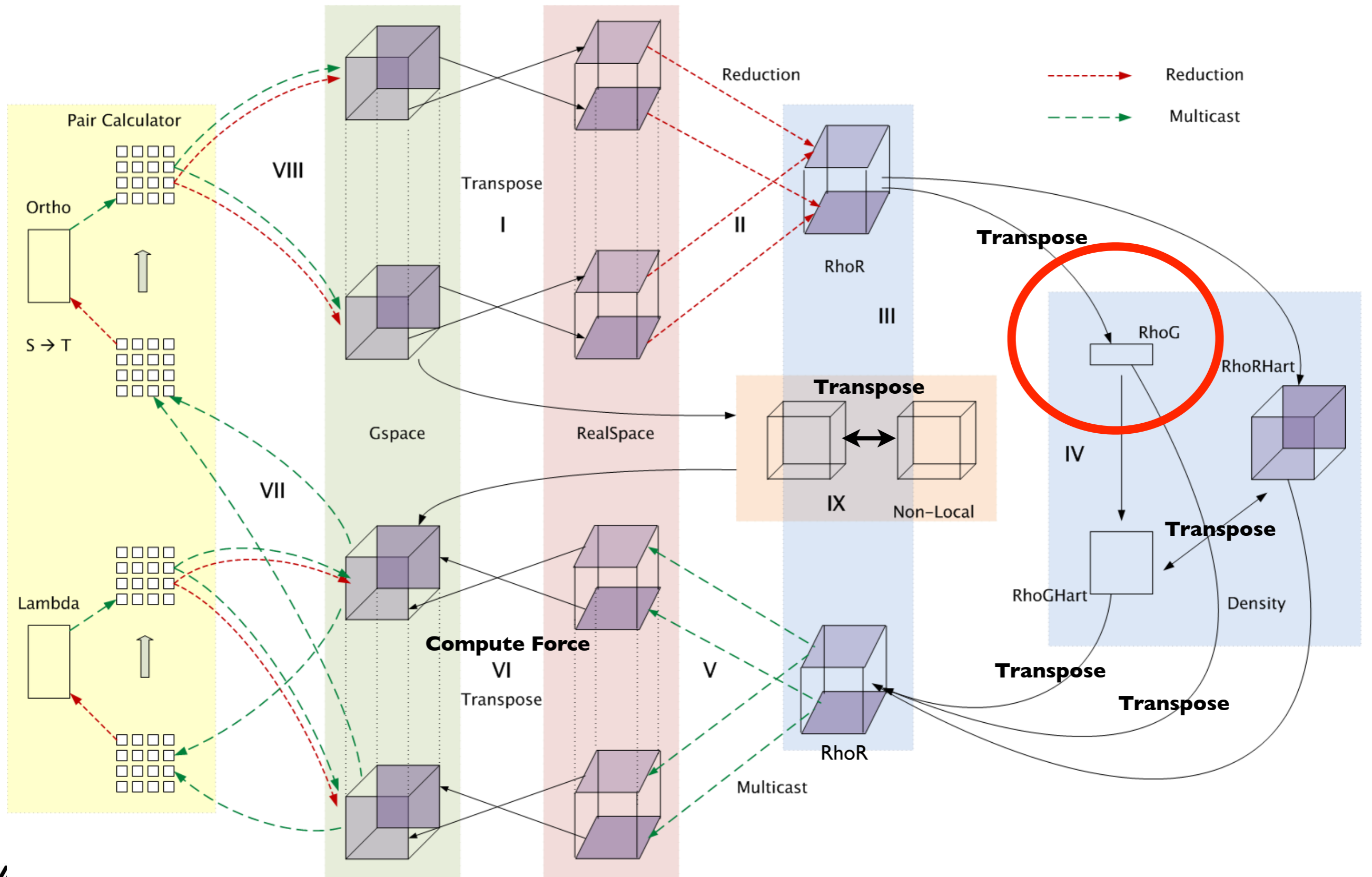
QM/MM: Implementation



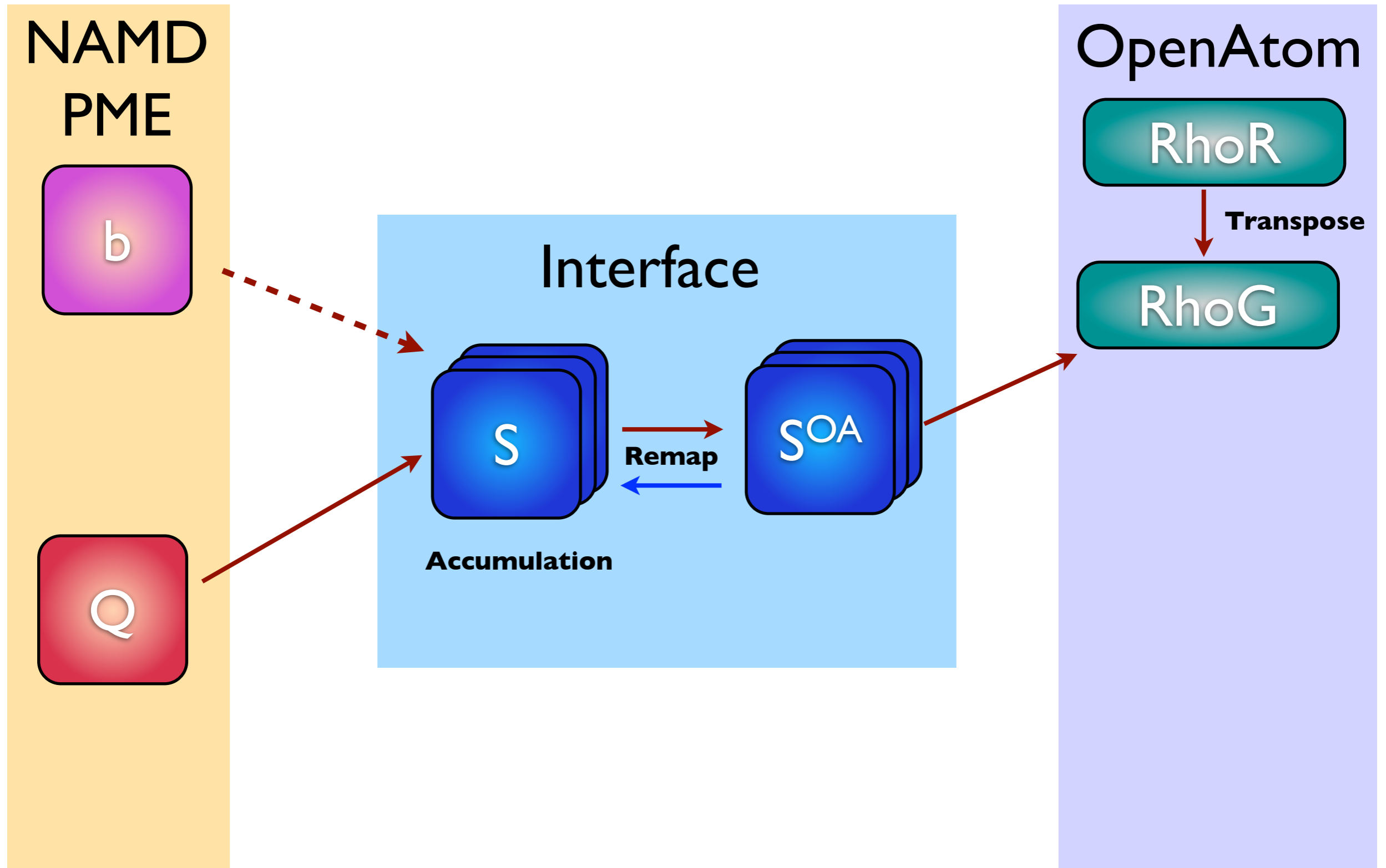
Two Interfaces Tested:
BDG & MSA/SDAG



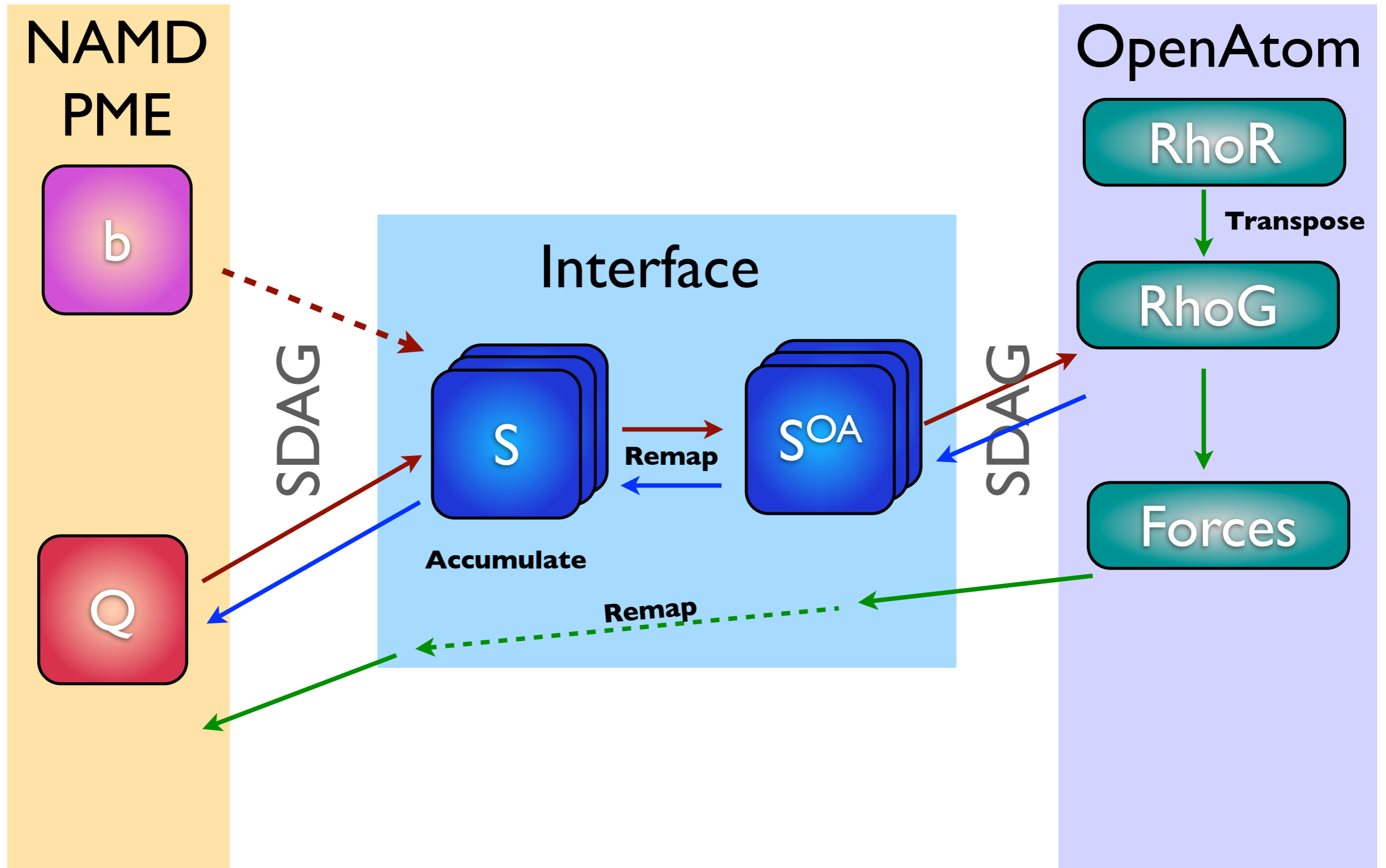
QM/MM: QM Insertion Pt



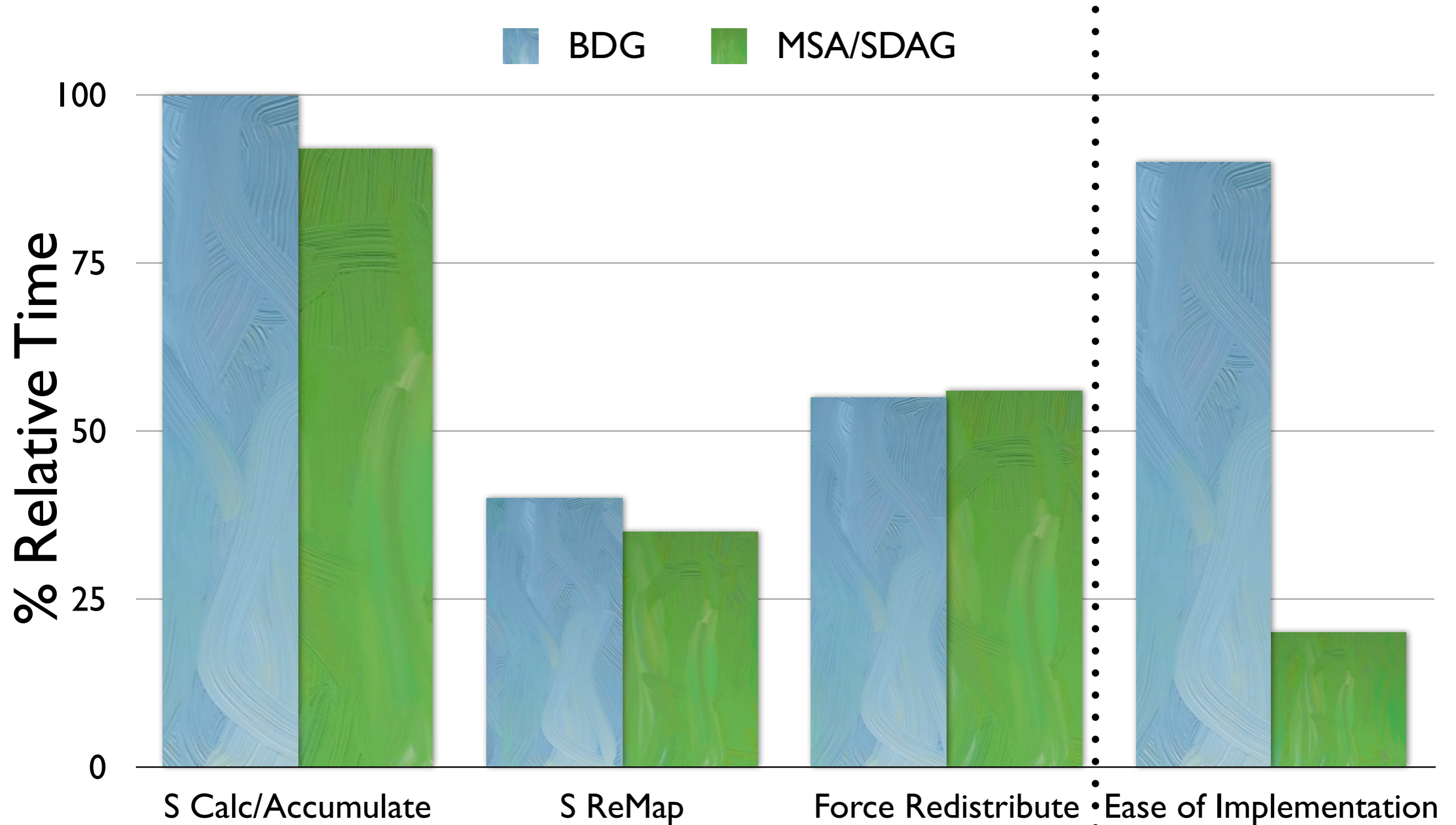
QM/MM: Implementation



QM/MM: Implementation



QM/MM: Results



QM/MM: Summary

- **Electrostatically embedded CPAIMD QM/MM**
- **MSA/SDAG preferable to ‘BDG’ Implementation**
- **MSA implicitly handles “shared data grids”, significantly simplified implementation**
- **Memory load of MSA implementation higher**



Thanks!

And the last quote:

Hans-Joachim Werner: With NAMD's MD and OpenAtom CPAIMD, you'll be able to consume all the SUs in the world!

Chris Harrison: Yeah

Hans-Joachim Werner: How do I use Charm++?

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