# Load Balancing in Parallel Molecular Dynamics

**Laxmikant V. Kalé,**

**Milind Bhandarkar, and Robert Brunner**

**Department of Computer Science**

**University of Illinois**

kale@cs.uiuc.edu

http://charm.cs.uiuc.edu

# Molecular Dynamics

- Simulate the motions of collections of atoms
- Forces due to bonds and non-bonded (Coulomb and Lennard-Jones) interactions
- Cutoff radius for non-bonded forces
- Sparse, but not very sparse, force matrix
- Configuration changes due to atom movement

## Existing Methods

- Computation cost is O($N/P$) for cutoff simulations
- Replicated Data: non scalable
- Atom decomposition:
  - Communication: O($N$)
- Force decomposition
  - Communication: O($N/\sqrt{P}$)
- "Irregular" force decomposition

## Spatial Decomposition

- Fixed size boxes vs. one box per processor
- Scalability of spatial decomposition
  - Computation: O($N/P$)
  - Communication: O($N/P$)

# Difficulties with Spatial Decomposition

- Load imbalance, especially for non-periodic configurations
- Parallelism limited to the number of Boxes

## Hybrid Decomposition

- Combines advantages of spatial and force decomposition
- Retains spatial decomposition in boxes
- One force-object for each pair of neighboring boxes
- Load balancer may map each force object to any processor!
- Flexible tradeoff between communication overhead and load imbalance

## Specifics of Load Balancing Strategy

Top level structure:

- Initial Balancer
- Learn from previous timesteps: explot temporal locality of performance characteristics
- Measurement based mapping
- Migratable and non-migratable objects

## Greedy Algorithm Variant

- Use “Greedy” heuristic, modified to take communication into account

## Multi-Paradigm Parallel Programming

- Irregular applications often need Multiparadigm parallel programming

Advantages of multi-paradigm programming

- One can use appropriate language for each module, separately
- Reuse existing libraries, irrespective of the language

## Multilingual Parallel Programming

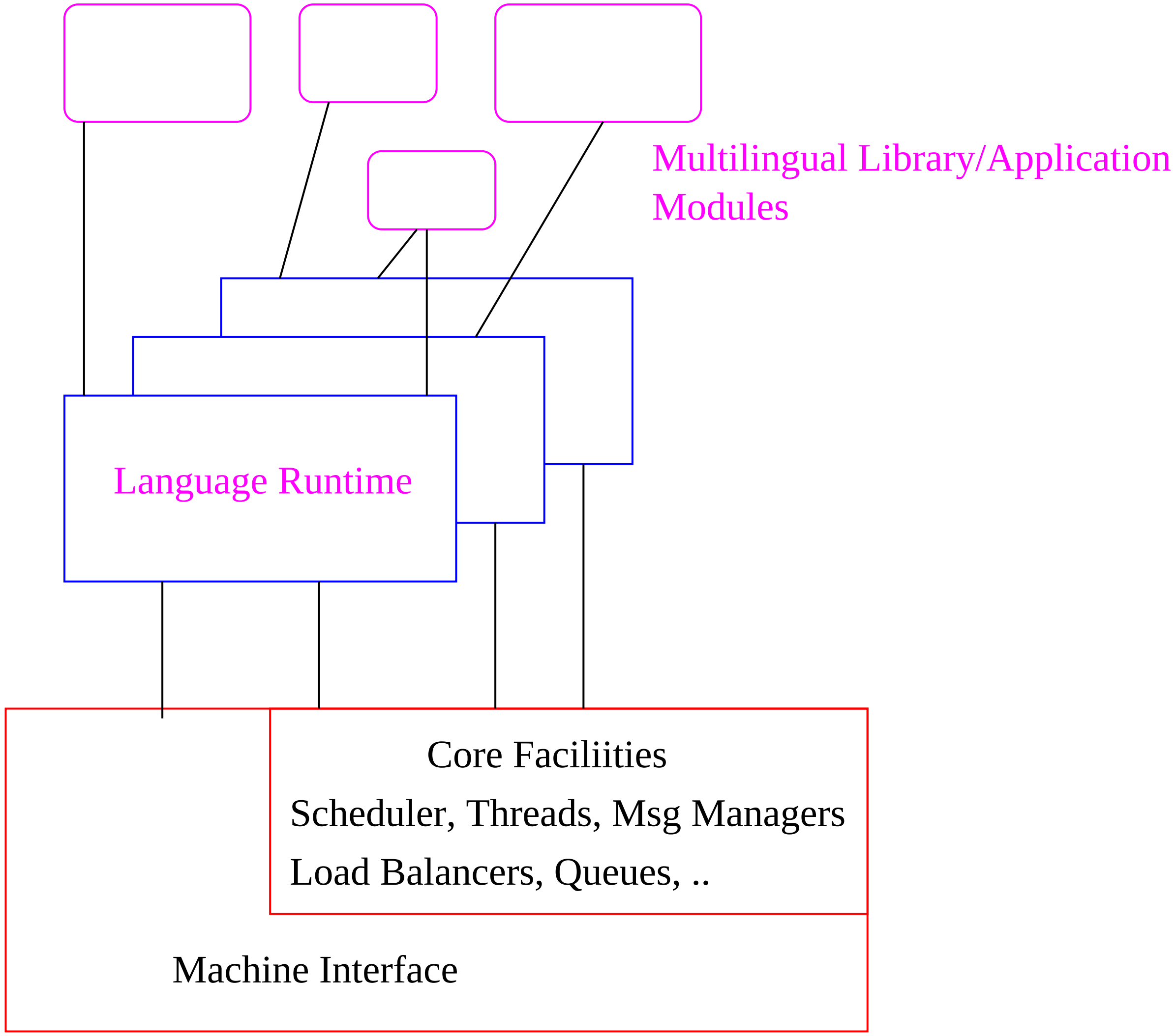
Challenges:

- Interoperating is difficult in face of concurrent languages (such as multi-threaded and object-based languages)
- Languages impose a processor scheduling policy
- Implicit vs. Explicit transfer of control
- Solution: exposed common scheduler (across languages)

## The Parallel Programming Framework

- Converse: multilingual interoperability
- Languages: Charm++, Charm, PC++, tSM, tPVM, MPI, threaded MPI, DP (HPF) Import (Simulation language), Agents
- Libraries:
- Applications: NAMD

# Using Converse



## Charm++ Overview

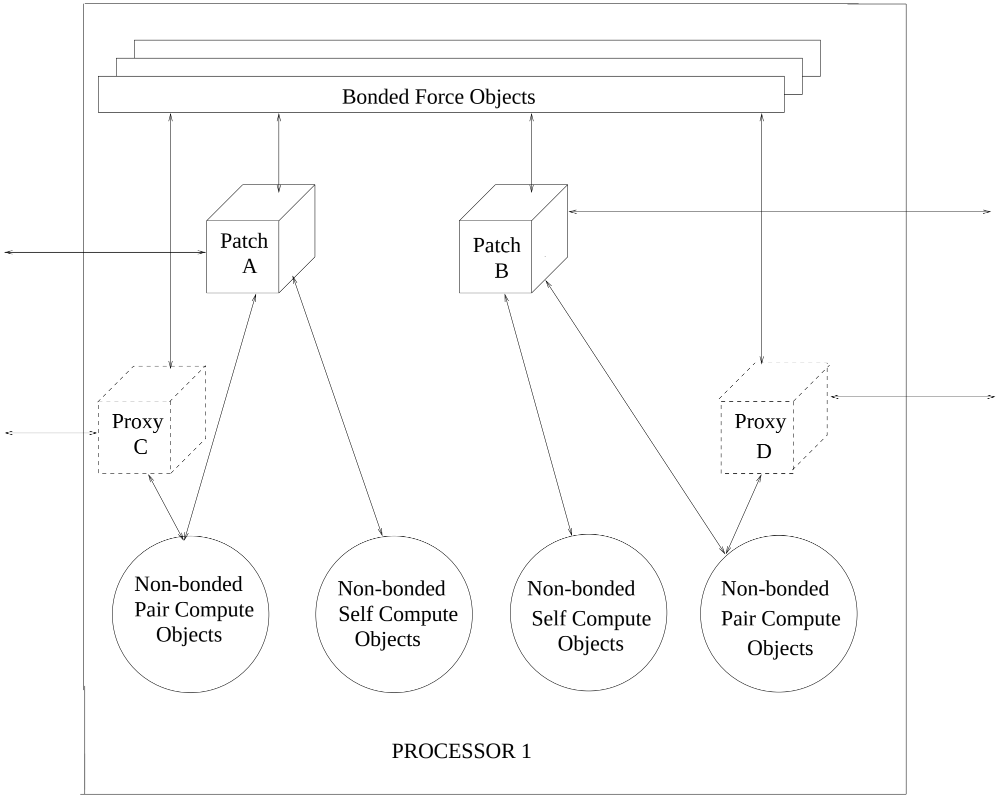
- Separation of sequential and parallel objects
- *Message driven objects*: dynamically load balanced
- *Asynchronous method invocation*: Message driven execution
- *Object groups*: distributed object with a branch on every processor
- *Object Arrays*: remappable
- No globally shared memory, but *globally shared object space.*

More info: http://charm.cs.uiuc.edu

# Object Groups

- When an object group is created, one object instance is created on each processor.
- You may invoke a method on any member of the group
- *Broadcast* invocation: when processor number is omitted
- Invoking a method in the local branch may be a synchronous function call

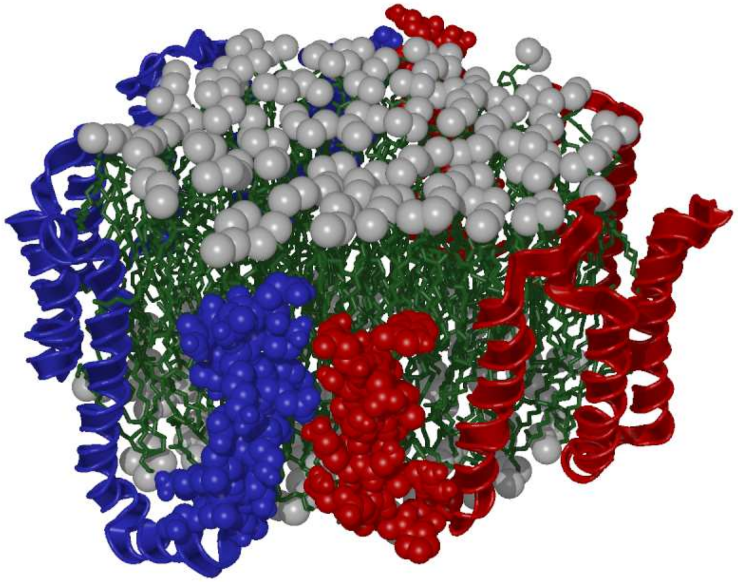
# NAMD Multilingual Modules



## NAMD Information

- NAMD is a production-quality program.
  - NAMD 2 contains over 23,000 lines of code
  - DPMTA is an additional 8,000 lines
  - SM is used in modules containing 4,900 lines
- Supports features required by application scientists

# Simulations using NAMD



A simulation of Apolipoprotein A-I is currently being done with NAMD. The ApoA-I simulation contains over 90,000 atoms.

# Load Balancing

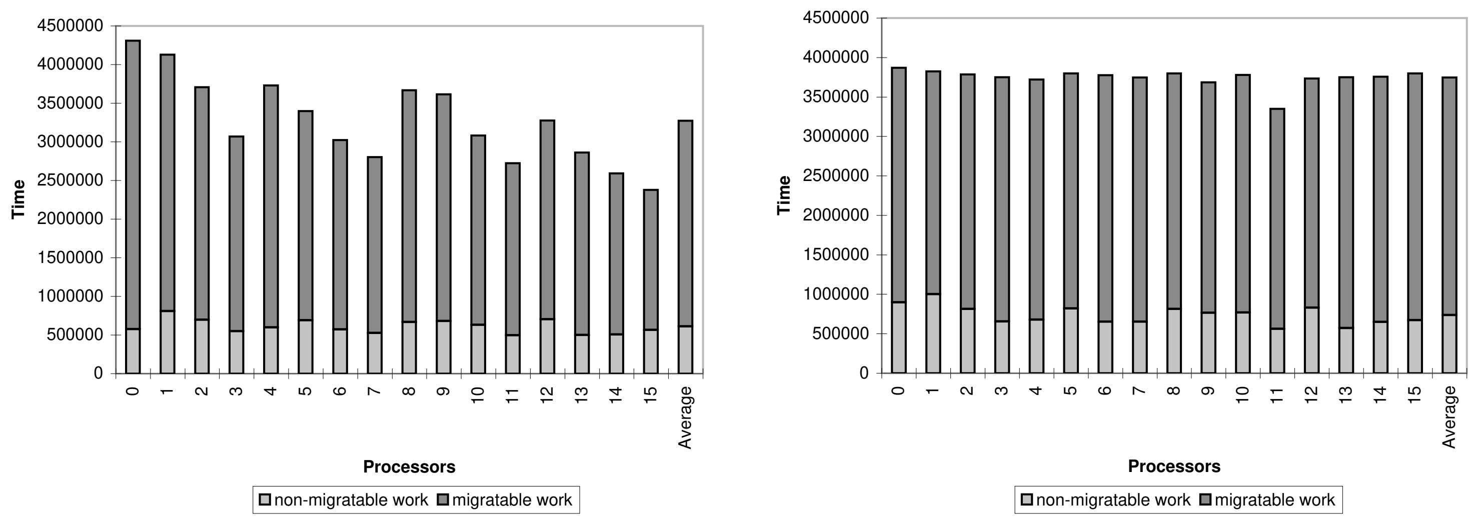



Figure 1: Load distribution for a 16 processor simulation, showing the load before (left) and after (right) running the load balancer.

# Performance

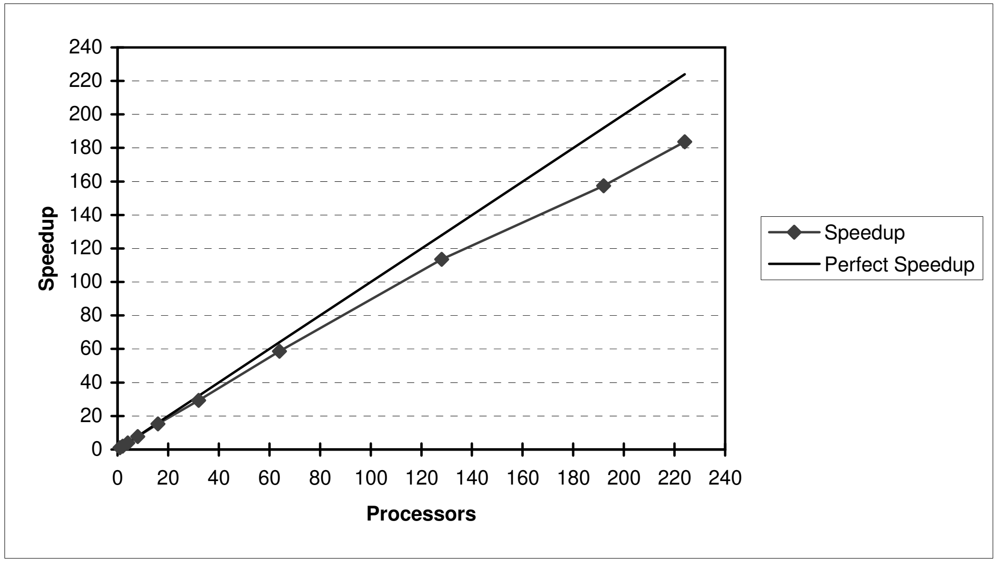



Figure 2: The speed-up for ApoA-I (92,224 atoms, 12Å cutoff) on the ASCI-RED.

# Performance

| Simulation<br># of atoms | Processors 1 | 2 | 4 | 8 | 16 | 32 | 64 | 128 | 160 |
|---|---|---|---|---|---|---|---|---|---|
| bR | 1.138 | 0.578 | 0.315 | 0.158 | 0.086 | 0.048 | | | |
| (3,762) | 1.0 | 1.97 | 3.61 | 7.20 | 13.2 | 23.7 | | | |
| ER-ERE | | 6.115 | 3.099 | 1.598 | 0.810 | 0.397 | 0.212 | 0.123 | 0.098 |
| (36,573) | | (1.97) | 3.89 | 7.54 | 14.9 | 30.3 | 56.8 | 97.9 | 123 |
| ApoA-I | | | 10.760 | 5.464 | 2.850 | 1.470 | 0.729 | 0.382 | 0.321 |
| (92,224) | | | (3.88) | 7.64 | 14.7 | 28.4 | 57.3 | 109 | 130 |

Table 1: Execution time (seconds) per timestep and speedups for several simulations on the CRAY T3E. All the simulations were run using a 12Å cutoff. Some simulations could not run on small numbers of processors due to lack of memory, so speed-up numbers in parantheses are estimates.

# Performance

| | Processors | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | 1 | 2 | 8 | 16 | 32 | 64 | 128 | 160 | 192 |
| T3E | | 6.12 | 1.60 | 0.810 | 0.397 | 0.212 | 0.123 | 0.098 | |
| | | (1.97) | 7.54 | 14.9 | 30.3 | 56.8 | 97.9 | 123 | |
| Origin2000 | 10.7 | 5.43 | 1.37 | 0.723 | 0.514 | 0.987 | | | |
| | 1.0 | 1.96 | 7.75 | 14.7 | 20.7 | 10.8 | | | |
| ASCI-RED | 28.0 | 13.9 | 3.76 | 1.91 | 1.01 | 0.500 | 0.279 | 0.227 | 0.196 |
| | 1.0 | 2.01 | 7.45 | 14.7 | 27.9 | 56.0 | 100 | 123 | 143 |
| NOWs | 24.1 | 12.4 | 3.69 | | | | | | |
| HP735/125 | 1.0 | 1.94 | 6.54 | | | | | | |

Table 2: Execution time (seconds) per timestep and speedups for ER-ERE (36,573 atoms, 12Å cutoff) on several parallel machines.