

# 6.189 IAP 2007

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## Student Project Presentation

### Molecular Dynamics

# Molecular Dynamics on the Playstation 3

Greg Pıntilie

# Overview

- Molecular Dynamics
- Algorithm
- Parallelization Approaches

# Molecular Dynamics


- Potential Energy:

$$E_p(\vec{x}) = E_{bonded} + E_{non-bonded}$$

# Molecular Dynamics

- Potential Energy:

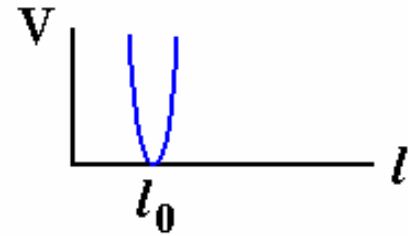
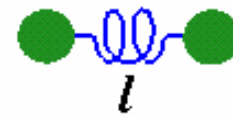
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$$E_{bonded} = E_{bonds} + E_{angles} + E_{dih,imp}$$

# Molecular Dynamics

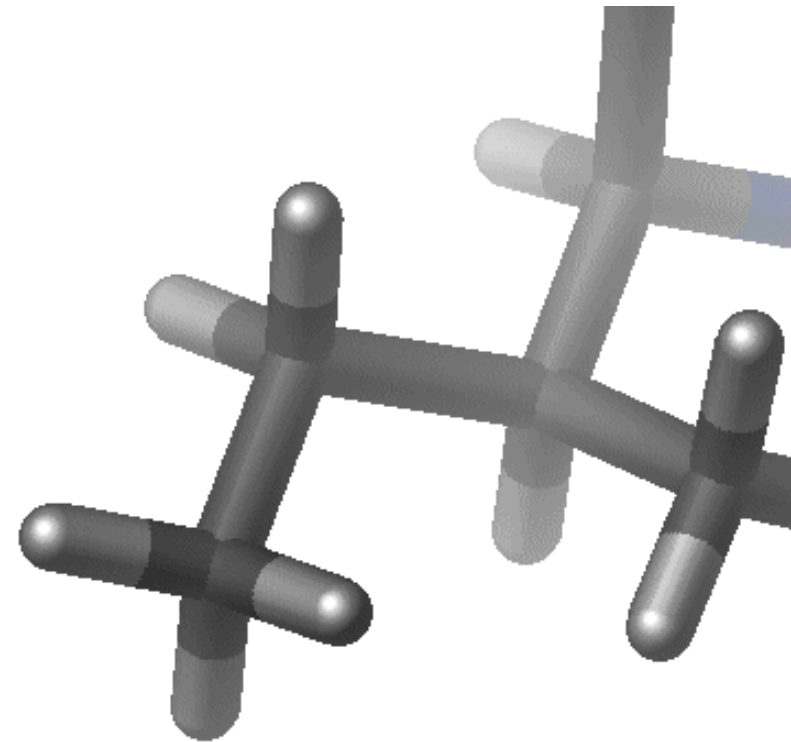
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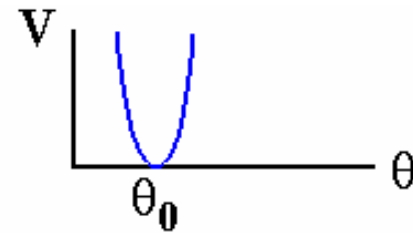
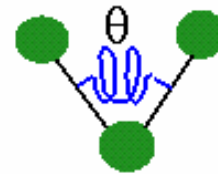
$$E_{bonds} = \sum_{bonds} k_b (l - l_0)^2$$



# Molecular Dynamics

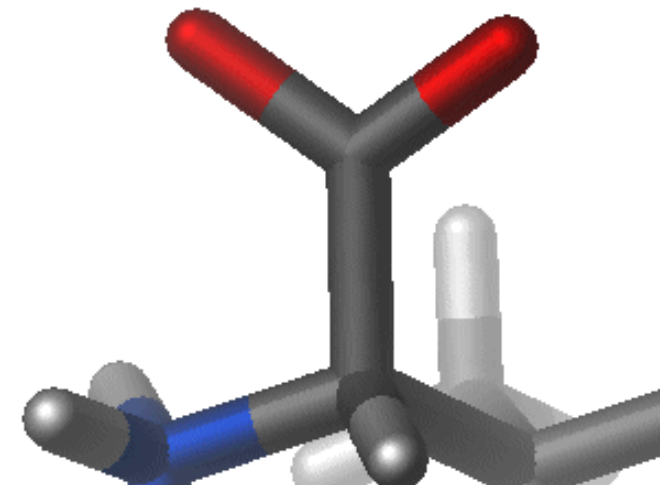
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$$E_p(\bar{x}) = E_{bonded} + E_{non-bonded}$$



$$E_{bonded} = E_{bonds} + E_{angles} + E_{dih,imp}$$

$$E_{angles} = \sum_{angles} k_{\theta} (\theta - \theta_0)^2$$

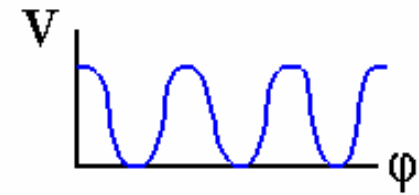
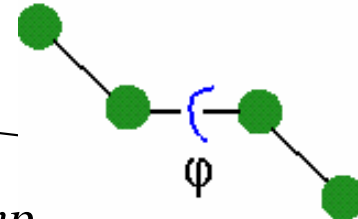
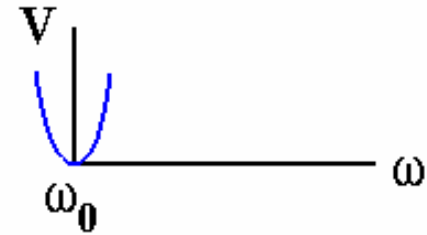
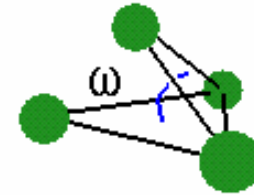


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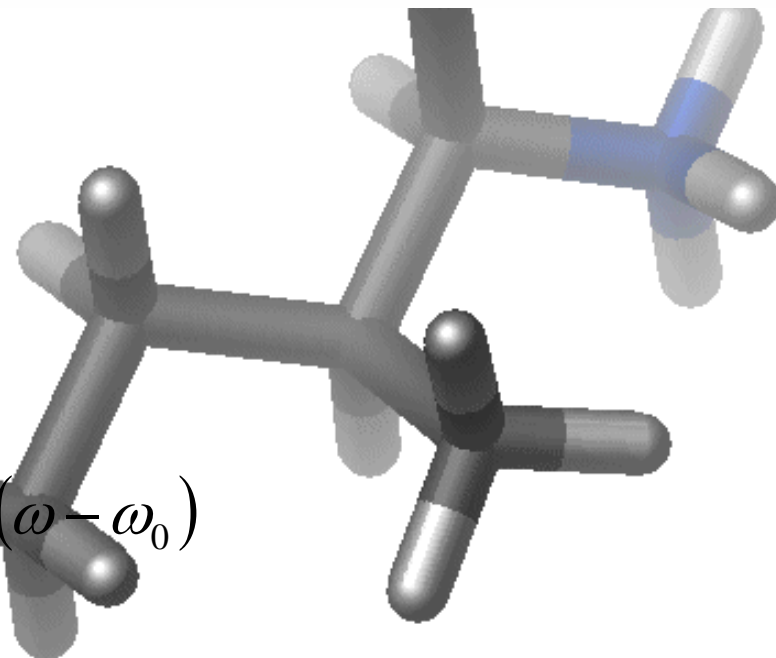
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$$F_{dih,imp} = \sum_{dihedrals} k_{\phi} (1 - \cos(n\phi)) + k_{\theta} (\theta - \theta_0) + \sum_{impropers} k_{\omega} (\omega - \omega_0)$$





# Molecular Dynamics

- Potential Energy:

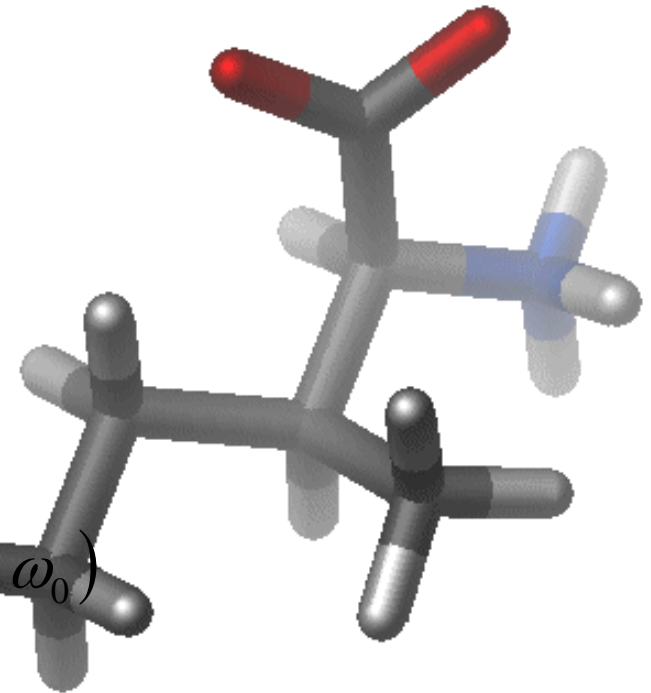
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# Molecular Dynamics

- Potential Energy:

$$E_p(\bar{x}) = E_{\text{bonded}} + E_{\text{non-bonded}}$$


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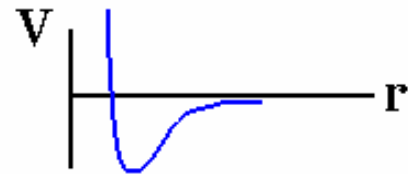
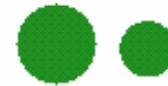
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# Molecular Dynamics

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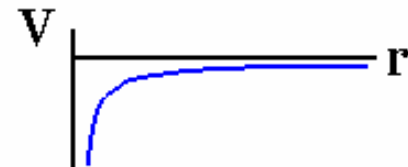
$$E_{\text{non-bonded}} = E_{\text{van-der-Waals}} + E_{\text{electrostatic}}$$

$$E_{\text{van-der-Waals}} = \sum_{\text{atoms}_{i,k}} \left( \frac{A_{ik}}{r_{ik}^{12}} - \frac{C_{ik}}{r_{ik}^6} \right)$$

$$E_{\text{electrostatic}} = \sum_{\text{atoms}_{i,k}} \frac{q_i q_k}{Dr_{ik}}$$

+

-



# Molecular Dynamics

- Compute forces :

$$\vec{f}(t) = M\vec{a}(t) = -\frac{\partial}{\partial \vec{x}} E_p(\vec{x})$$

- Integrate to obtain velocity, position:

$$\vec{v}\left(t + \frac{1}{2}\Delta t\right) = v\left(t - \frac{1}{2}\Delta t\right) + \Delta t \frac{\vec{f}(t)}{m}$$

$$\vec{x}(t + \Delta t) = \vec{x}(t) + \Delta t \cdot \vec{v}\left(t + \frac{1}{2}\Delta t\right)$$

# Kinetic Energy

- Kinetic Energy/Temperature:
  - from classical equipartition theory, each degree of freedom has, at thermal equilibrium, this much energy:

$$\frac{1}{2} k_B T$$

$$\langle E_k \rangle = \frac{1}{2} \sum_{i=1}^{3N} m_i v_i^2 = \frac{1}{2} N_F k_B T$$

# Langevin Dynamics

- Account for collisions with imaginary molecules (heat bath)
- e.g. in solvent such as water

$$F = M\bar{a} = -\nabla E_p(\bar{x}) - \gamma Mv + R(t)$$

$$\langle R(t) \rangle = 0 \quad \langle R(t), R(t')^T \rangle = 2\gamma k_B T M \delta(t - t')$$

# Solvation in Dielectric Material

- Molecules that are polar/ionic ‘shield’ electrostatic forces
- Water:
  - distance-dependent dielectric:

$$E_{electrostatic} = \sum_{atoms\_i,k} \frac{q_i q_k}{D r_{ik}}$$

↓

$$D = r$$

↓

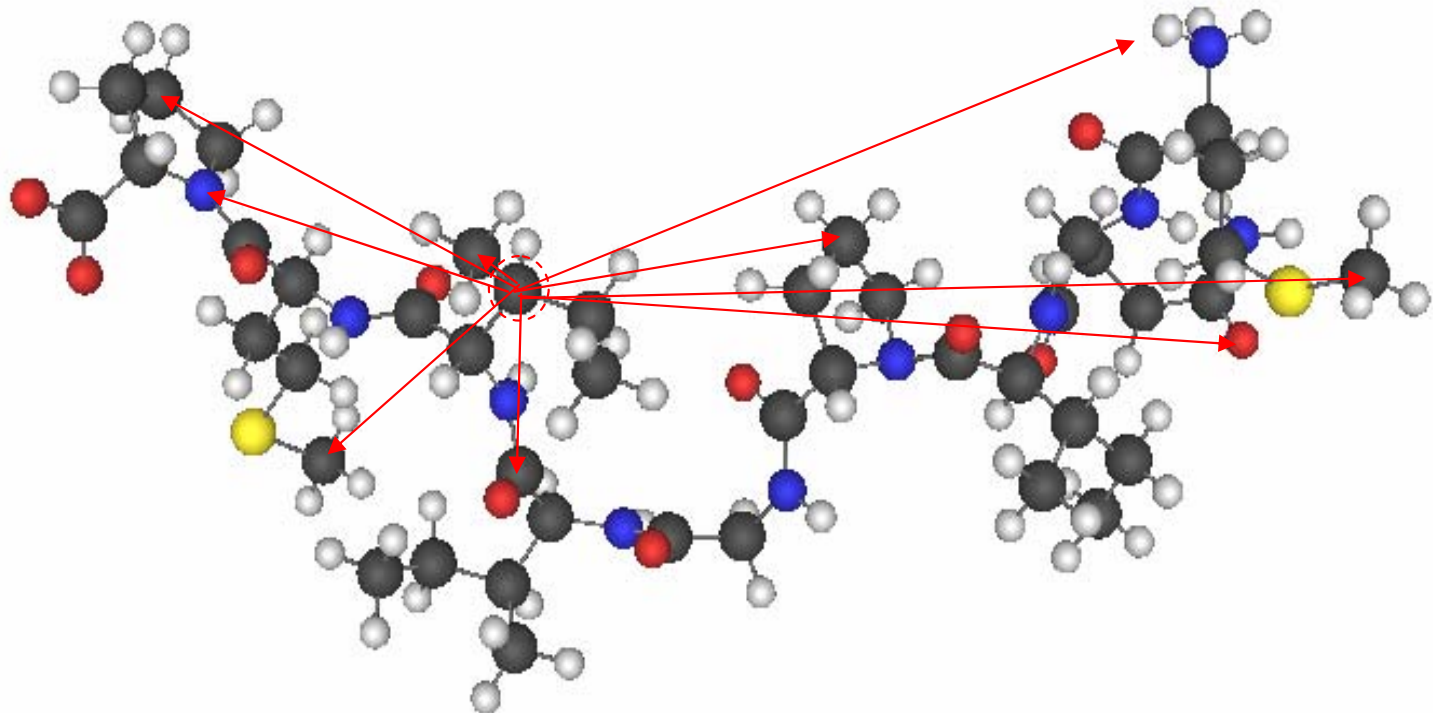
$$E_{electrostatic} = \sum_{atoms\_i,k} \frac{q_i q_k}{r_{ik}^2}$$



# Non-bonded Cut-offs

$$E_{non-bonded} = \sum_{atoms\_i,k} \left\{ \left( \frac{A_{ik}}{r_{ik}^{12}} - \frac{C_{ik}}{r_{ik}^6} \right) + \frac{q_i q_k}{D r_{ik}} \right\}$$

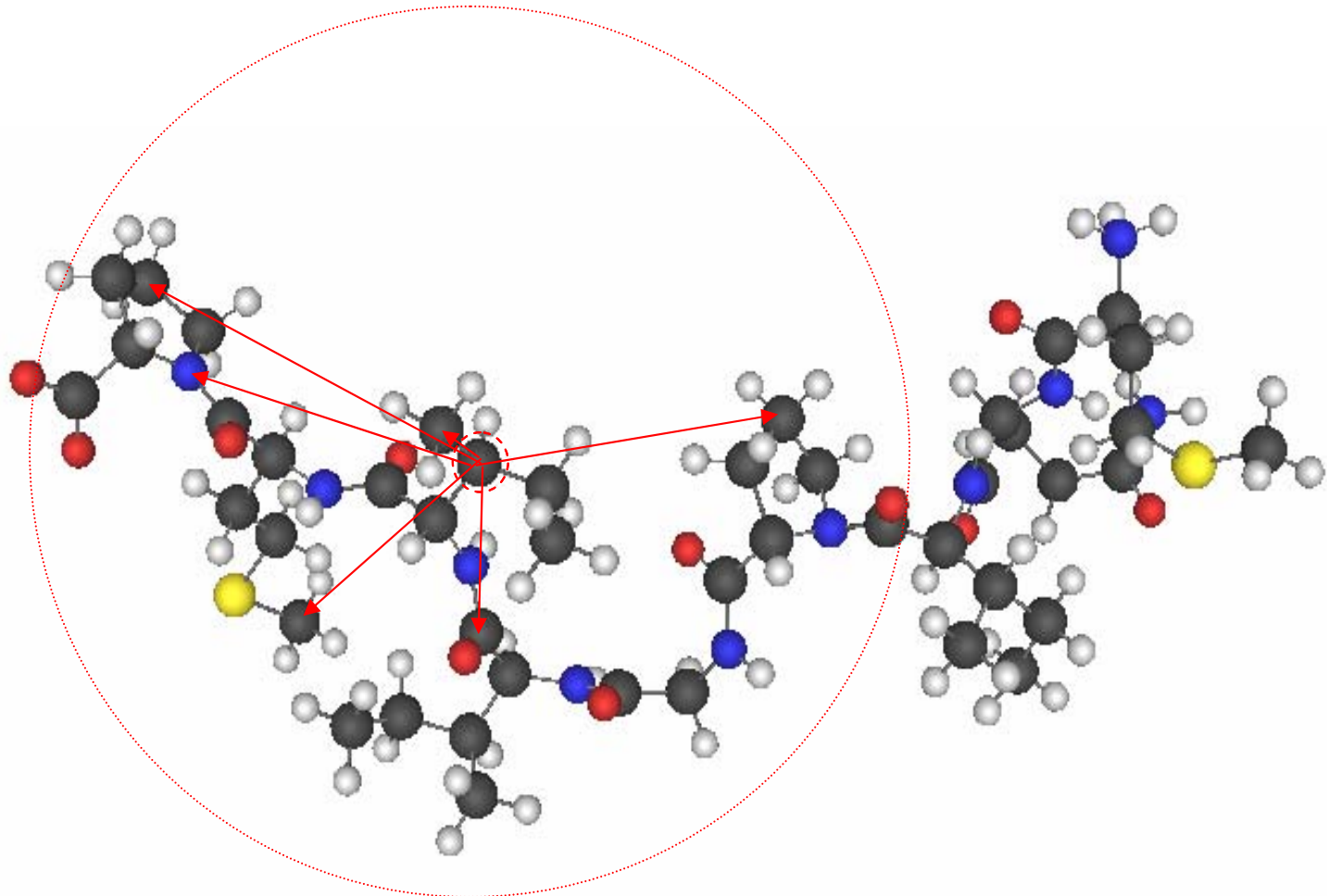
- Cut-off ~12Å



# Non-bonded Cut-offs

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- Cut-off ~12Å



# Basic MD Algorithm

```
For i=0 to numsteps
```

```
  if i % ap_freq == 0
```

```
    find atom pairs
```

```
  Compute 'bonded' forces
```

```
    bonds, angles, dihedrals,  
    impropers
```

```
  Compute 'non-bonded' forces
```

```
    atom pairs
```

```
  Integrate
```

# Data Structures

## Bonded Forces

## Non-Bonded Forces

### Vector

double x, y, z

### Atom

Vector pos, vel, force

double Mass

double Charge

double Rmin

double Eps

### Molecule

list Atom atoms

list Bond bonds

list Angle angles

list Improper impropers

list Dihedrals dihedrals

list AtomPair atompairs

### Bond

Atom \*a1, \*a2

double k, b0

### Angle

Atom \*a1, \*a2, \*a3

double k, t0

### Improper

Atom \*a1, \*a2, \*a3, \*a4

double k, t0

### Dihedral

Atom \*a1, \*a2, \*a3, \*a4

list DihedralValue vals

### DihedralValue

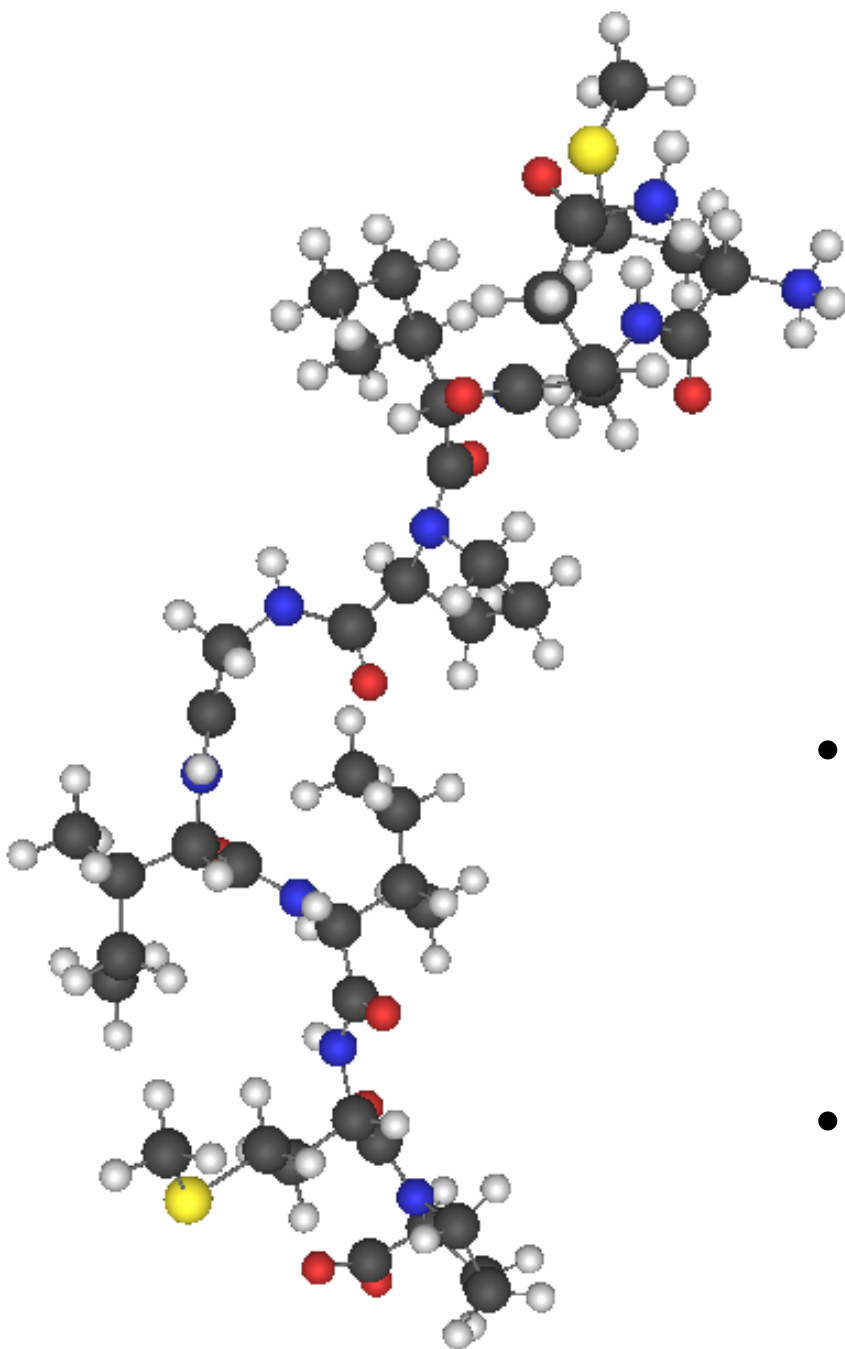
double k, phase

int n

### Atom Pair

Atom \*a1, \*a2

double eij



- A8m

- ‘Bonded’ - total **41,652**
  - 146 atoms x 104 bytes = **15,184**
  - 147 bonds x 24 bytes = **3,528**
  - 275 angles x 28 bytes = **7,700**
  - 393 dihedrals x 16 bytes +  
414 dihedral values x 20 bytes = **14,568**
  - 21 impropers 32 bytes = **672**
- ‘Non-bonded’ – total **176,000**
  - 11,000 Atom Pairs x 16 bytes
    - (1-3 bonded atoms excluded)

- 10 x A8m

- ‘Bonded’ – total **416,520**
- ‘Non-bonded’ – total **16,976,000**

- 20 x A8m

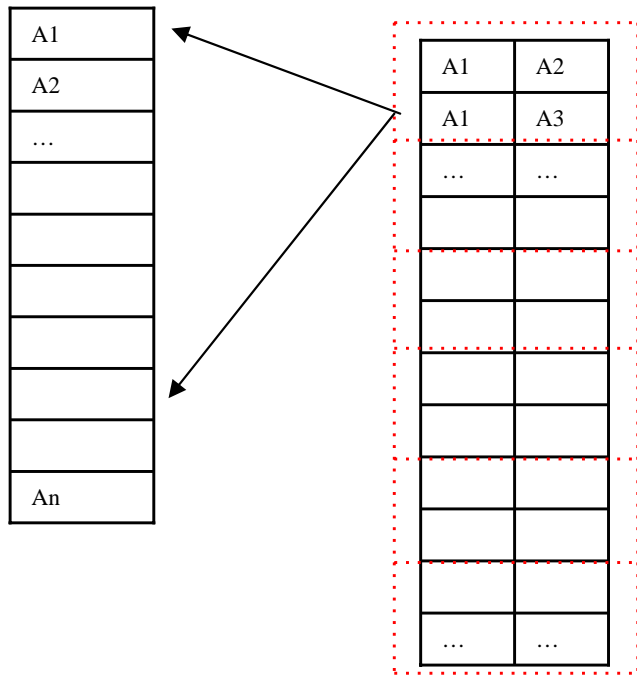
- ‘Bonded’ – total **833,040**
- ‘Non-bonded’ – total **68,064,000**

# Sequential Algorithm

	No cutoff	With cutoff
<code>For i=0 to numsteps</code>		
<code>  if i%ap_freq==0</code> <code>    find atom pairs</code>	0 ms	Bf / Kd 6,090 / 880 ms 24,440 / 1,750 ms
<code>  'bonded' forces</code> <code>    bonds, angles,</code> <code>    dihedrals, impropers</code>	50ms	50ms
<code>  'non-bonded' forces</code> <code>    atom pairs</code>	1,480ms 1,060,850 pairs	150ms 116,434 pairs
<code>  integrate</code>	10ms	10ms

# Parallelization Approaches

- Force Decomposition



- force operation includes both atom positions, returns the force on both atoms
- scales well with system size and #processors

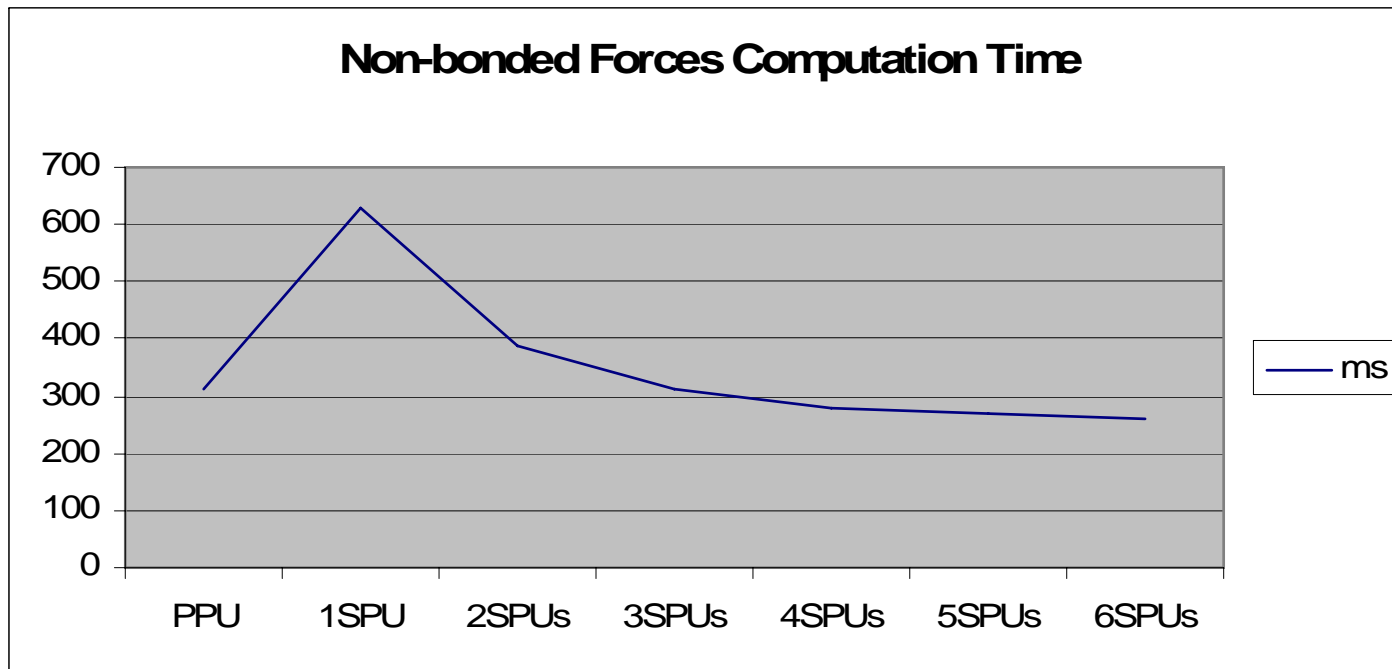




# Parallelization Approaches

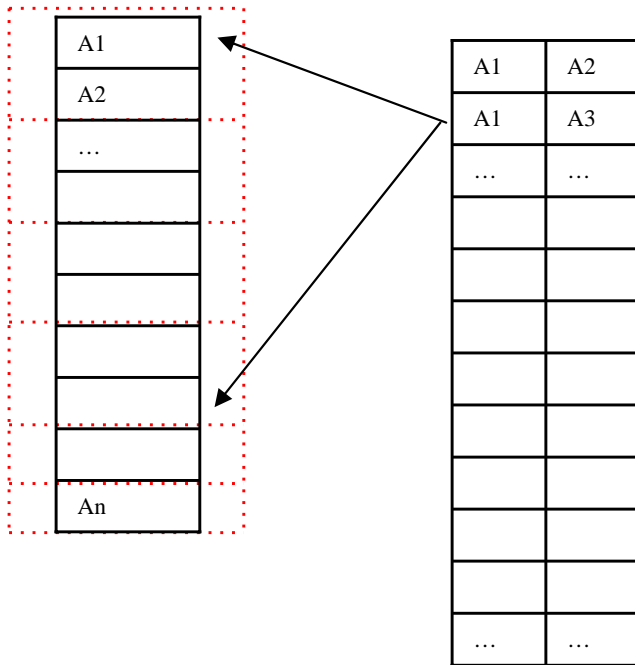
- Force Decomposition - performance

PPU	1SPU	2SPUs	3SPUs	4SPUs	5SPUs	6SPUs
310	630	390	310	280	270	260



# Parallelization Approaches

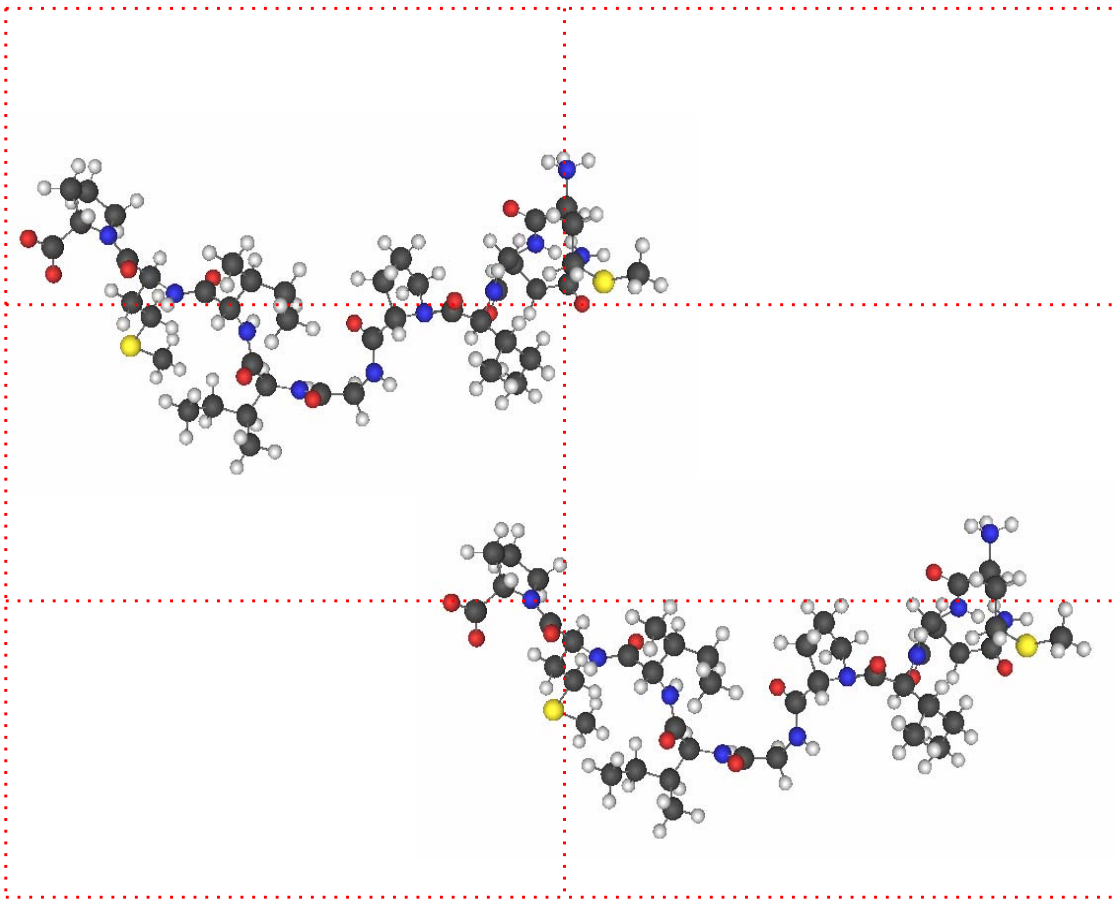
- Atomic Decomposition



- atoms and forces stored independently
- doesn't scale as easily with system size

# Parallelization Approaches

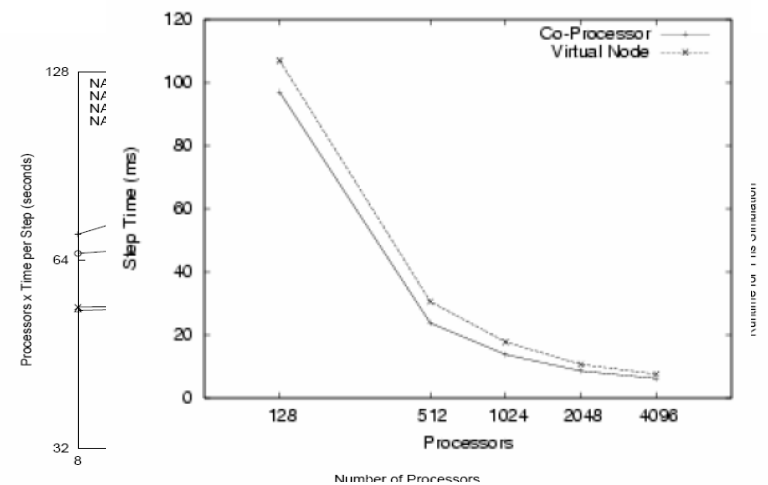
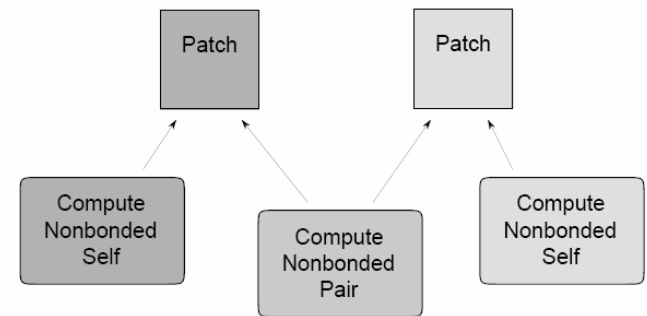
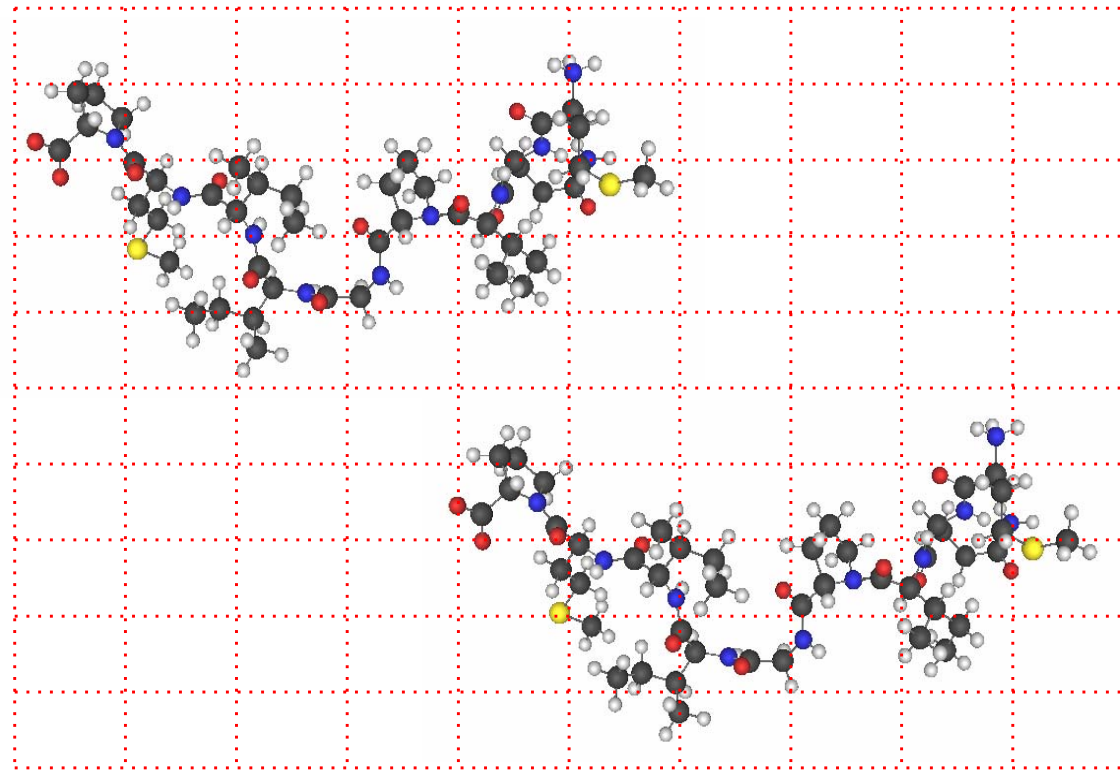
- Spatial Decomposition



- not load-balanced
- atom positions must be communicated between processors
- periodically re-assign atoms

# State of the Art - NAMD

- force-spatial decomposition



Achieving Strong Scaling with NAMD on Blue Gene/L

NA