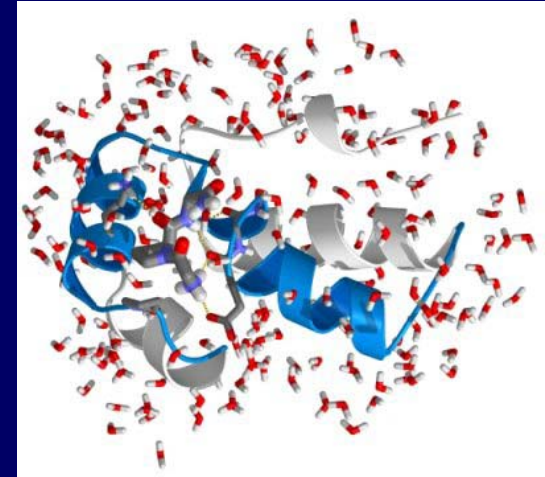


# Gromacs

## Molecular Dynamics Simulator

Eric Lindhal, Erik Darve, Vidya Rangasayee



### Nonbonded forces

Force Function (~90% compute time):

$$F_i(\mathbf{r}_{ij}) = \left( \frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{\epsilon_r r_{ij}^2} + 12 \frac{C_{12}}{r_{ij}^{12}} - 6 \frac{C_6}{r_{ij}^6} \right) \frac{\mathbf{r}_{ij}}{r_{ij}}$$

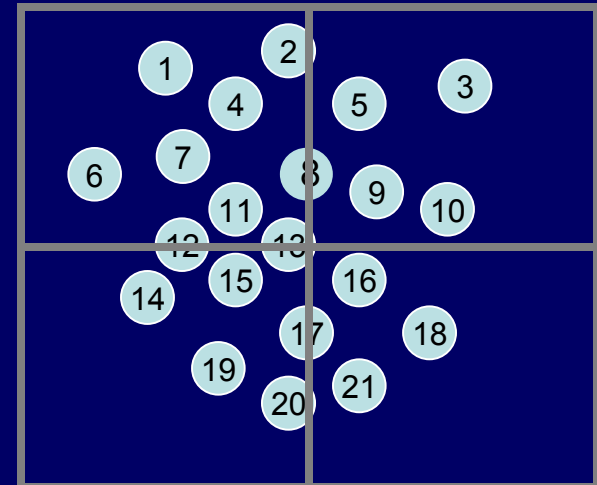


Electrostatics



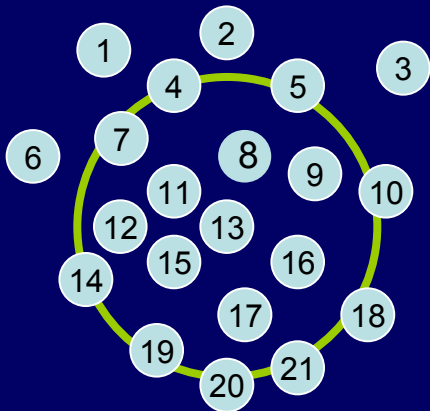
Lennard-Jones

### Acceleration Structure:



# Using cutoffs & neighbor lists

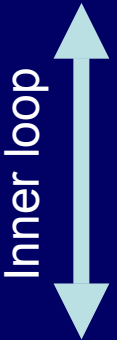
- Neighbor list constructed every 10 steps.
- List padded to 16 per atom
- Atoms repeated if more than 16 interactions



Neighbor list for atom 13 =  
{ 8, 9, 11, 12, 15, 16, 17 }

# What we do in the inner loop?

```
For each i atom {  
  fetch atom i data  
  i_force = 0;  
  For each j atom in our neighborlist {  
    fetch atom j data  
    calculate vectorial distance;  $\mathbf{dr} = \mathbf{r}_i - \mathbf{r}_j$   
    calculate  $r^2 = dx*dx + dy*dy + dz*dz$ , and  $1/r = 1/\text{sqrt}(r^2)$   
    Calculate potential and vectorial force  
    Subtract the force from the j atom force  
    i_force += force;  
  }  
  Store i_force;  
}
```



# What we do in the inner loop?

```
d1      = imolecule - jmolecule1;
d2      = imolecule - jmolecule2;
d3      = imolecule - jmolecule3;
d4      = imolecule - jmolecule4;
rinv.x  = 1.0/sqrt(dot (d1, d1));
rinv.y  = 1.0/sqrt(dot (d2, d2));
rinv.z  = 1.0/sqrt(dot (d3, d3));
rinv.w  = 1.0/sqrt(dot (d4, d4));
```

Compute 4 force interactions  
in parallel

```
/* Calculate interactions */
```

```
rinvsq   = rinv*rinv;
rinvsix  = rinvsq*rinvsq*rinvsq;
vnb6     = rinvsix*c6;
vnb12    = rinvsix*rinvsix*c12;
vcoul    = qq*rinv;
fs       = (twelve*vnb12-six*vnb6+vcoul)*rinvsq;
```

```
/* Calculate vectorial force and update local i atom force */
```

```
t1       = d1 * fs.x;
t2       = d2 * fs.y;
t3       = d3 * fs.z;
t4       = d3 * fs.w;
force    = prev + t1 + t2 + t3 + t4;
```

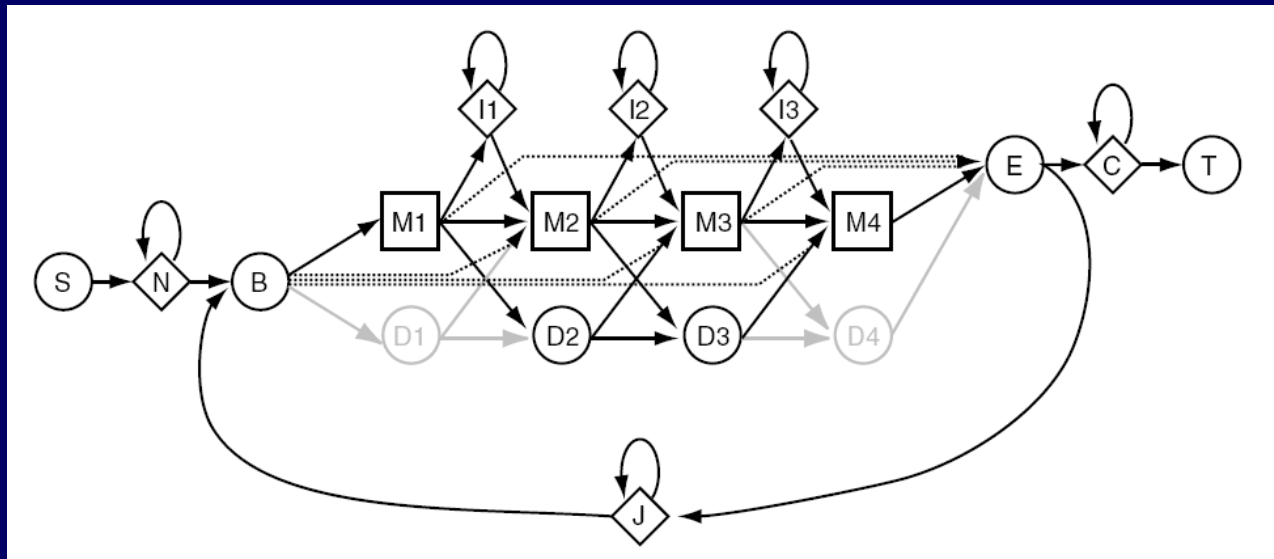
# Gromacs Status

- Running on Brook GPU
  - Still debugging...
  - ATI Radeon 5 times faster than 3GHZ P4
- Similar kernels will run on Merrimac

# HMMER

## Sequence analysis using profile hidden Markov models Sean Eddy, Washington Univeristy in St. Louis

Query: 1 MKRRSWLKILGICLGSSIVLGFILFLPQLLSTESRKYLVFSLIHKESGLSCSAEELKISW  
MKR W KI G L + L L LP+ S+ES KYL S ++KE+GL E+L +SW  
Sbjct: 1 MKRSPWYKIFGYLLVGVPLALLALLPKFFSSESGKYLFLSVLNKETGLQFEIEQLHLSW

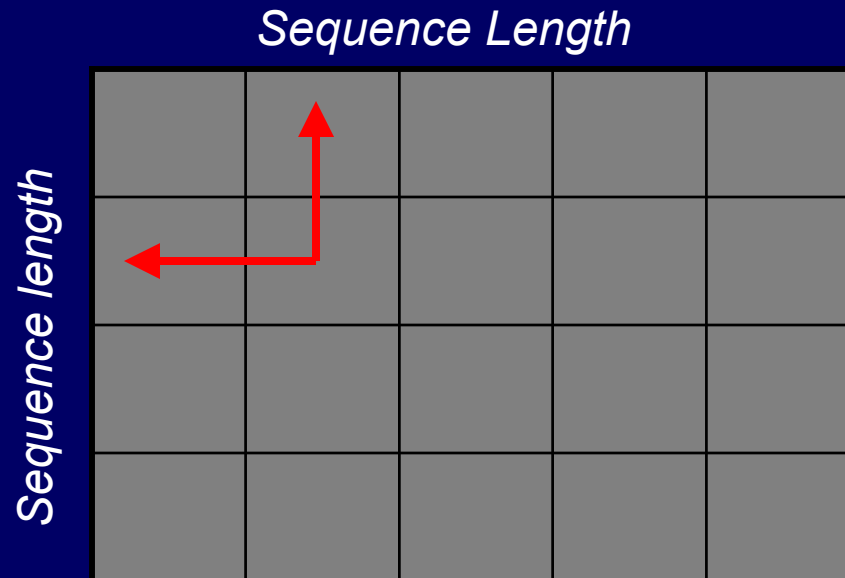


# HMMER

Sequence analysis using profile hidden Markov models

Sean Eddy, Washington Univeristy in St. Louis

- Compute probability of HMM generating a given sequence
- Dynamic programming
- Sweep algorithms



# Bioinformatics

- Protein Folding: Gromacs
- Protein Matching: HMMER
- Others ?
  - Protein Docking: GRAMM