Many-Body Forces for Molecular Dynamics

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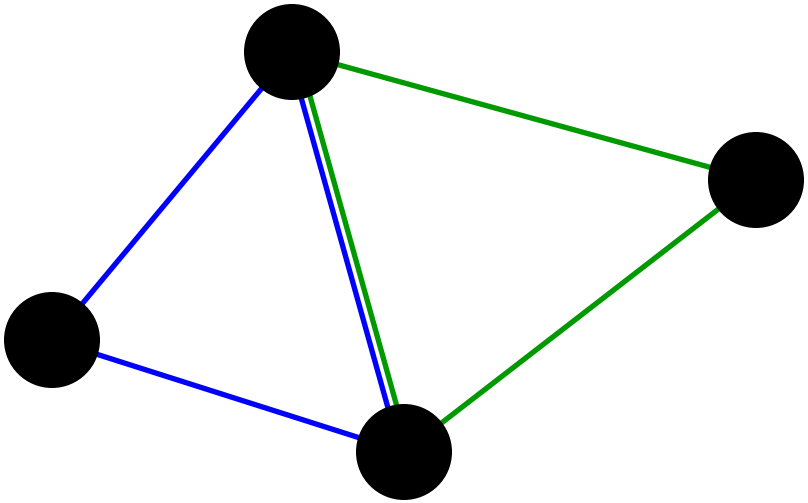
What Are Many-Body Forces?



Example: Axilrod-Teller

$$E = \frac{C\left(1 + 3\cos\theta_{123}\cos\theta_{231}\cos\theta_{312}\right)}{\left(r_{12}r_{13}r_{23}\right)^3}$$

Example: Stillinger-Weber

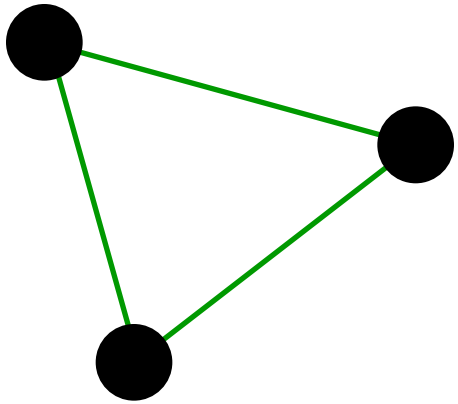
$$E_2 = A\varepsilon\left(B\left(\frac{\sigma}{r}\right)^p - \left(\frac{\sigma}{r}\right)^q\right)\exp\left(\frac{\sigma}{r - a\sigma}\right)$$

$$E_3 = L\varepsilon\left(\cos\theta_{312} + \frac{1}{3}\right)^2 \exp\left(\frac{\sigma\gamma}{r_{12} - a\sigma}\right)\exp\left(\frac{\sigma\gamma}{r_{13} - a\sigma}\right)$$

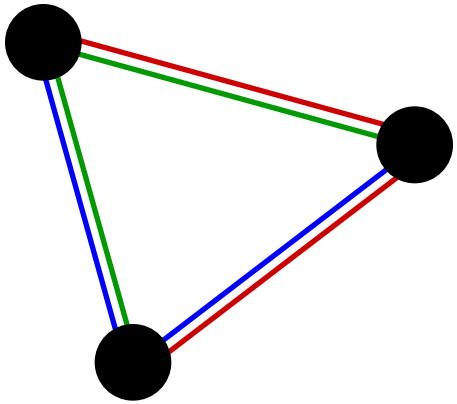
Axilrod-Teller in OpenMM

```
force = CustomManyParticleForce(3, """
    C*(1+3*cos(theta1)*cos(theta2)*cos(theta3))/(r12*r13*r23)^3;
    theta1=angle(p1,p2,p3); theta2=angle(p2,p3,p1); theta3=angle(p3,p1,p2);
    r12=distance(p1,p2); r13=distance(p1,p3); r23=distance(p2,p3)""")
```

Permutation Modes



Single Permutation

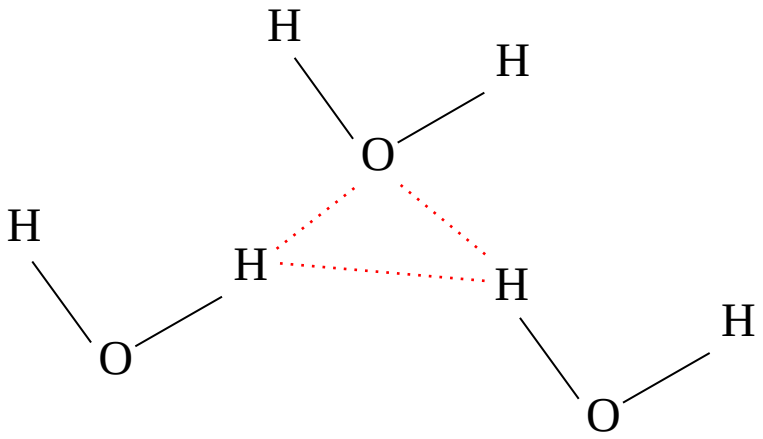


Unique Central Particle

Exclusions

- Specify *pairwise* exclusions
- Skip an interaction if any two atoms are excluded

Type Filters




```
force.setTypeFilter(0, [0])
force.setTypeFilter(1, [1])
force.setTypeFilter(2, [1])
```

Step 1: Build Neighbor List

- For atom i, find every atom j within cutoff
  - Omit excluded atoms
  - In single permutation mode, require i<j

Atom	Neighbors
0	1, 2, 4, 17, ...
1	0, 2, 3, 4, ...
2	0, 1, 4, 15, ...

Unique Central Particle

Atom	Neighbors
0	1, 2, 4, 17, ...
1	2, 3, 4, ...
2	4, 15, ...

Single Permutation

Step 2: Compute Interactions

- One thread block processes neighbors of one atom

Atom	Neighbors
0	1, 2, 4, 17

- One thread computes each interaction

Thread	Atoms
0	0, 1, 2
1	0, 1, 4
2	0, 1, 17

Thread	Atoms
3	0, 2, 4
4	0, 2, 17
5	0, 4, 17

How to Generate Combinations?

- We need all sets of N-1 neighbors
  - Easy to iterate over them:

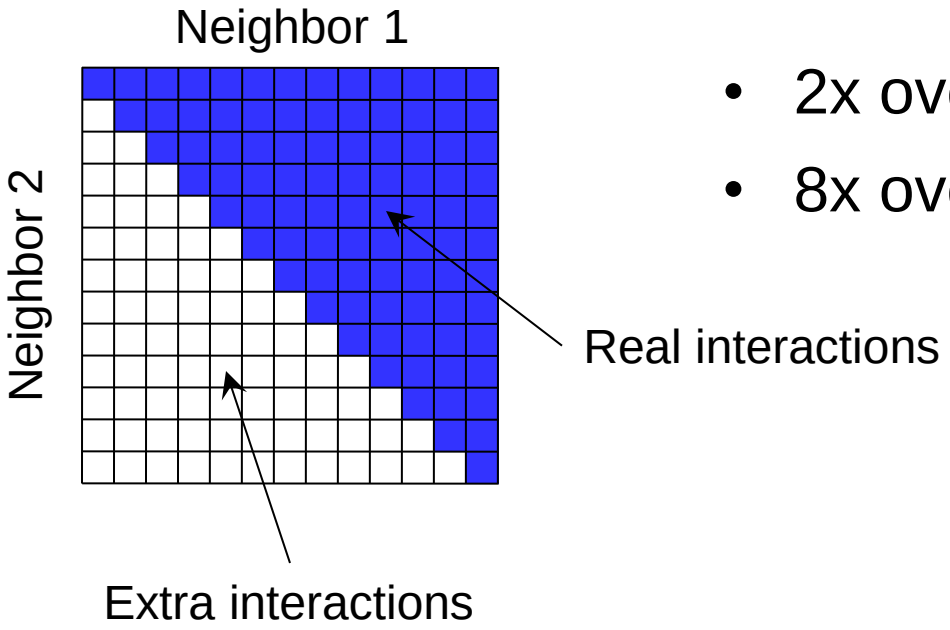
```
for i = 0 to M:
    for j = i+1 to M:
        for k = j+1 to M:
            ...
```

  - Hard to generate in parallel!

Solution

- Generate all permutations, skip redundant ones:

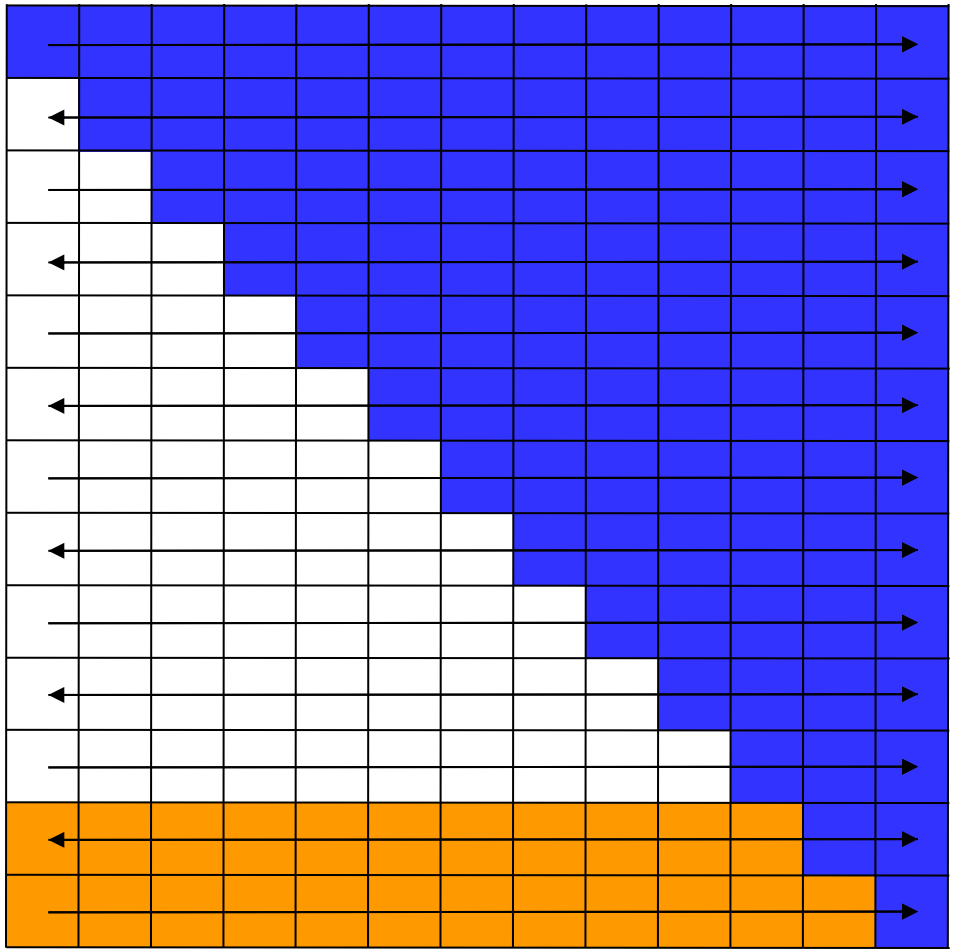
```
for index = 0 to M*M:
    i = index/M
    j = index%M
    if j > i:
        ...
```



- 2x overhead for 3-body
- 8x overhead for 4-body

- Actual overhead is less
  - Some warps have *all* extra interactions

A Simple Optimization



Type Filters

- Use a lookup table based on atom types

```
order = table[type1][type2][type3]
if order == -1:
   skip interaction
atoms = [atom1, atom2, atom3]
atom1 = atoms[first[order]]
atom2 = atoms[second[order]]
atom3 = atoms[third[order]]
```

Full Algorithm

```
For thread block i:
    Load the neighbors of atom i
    Loop over permutations:
        Is this an "extra" interaction?
            continue
        Are any atom pairs excluded?
            continue
        In single permutation mode:
            Are any atoms beyond the cutoff distance?
                continue
        If using type filters:
            If no valid permutation:
                continue
            Permute atoms
        Evaluate the interaction
```

Performance

- Simulated a box of 11,278 waters

Water Model	ns/day
mW (Stillinger-Weber)	469
TIP-3P	182

OpenMM 6.3 on a GTX Titan. mW uses 10 fs time step. TIP-3P uses PME with a 5 fs time step.

Acknowledgements

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http://openmm.org