A Simple LJ Many-Body Simulator Optimization and Parallelization

Dr. Axel Kohlmeyer

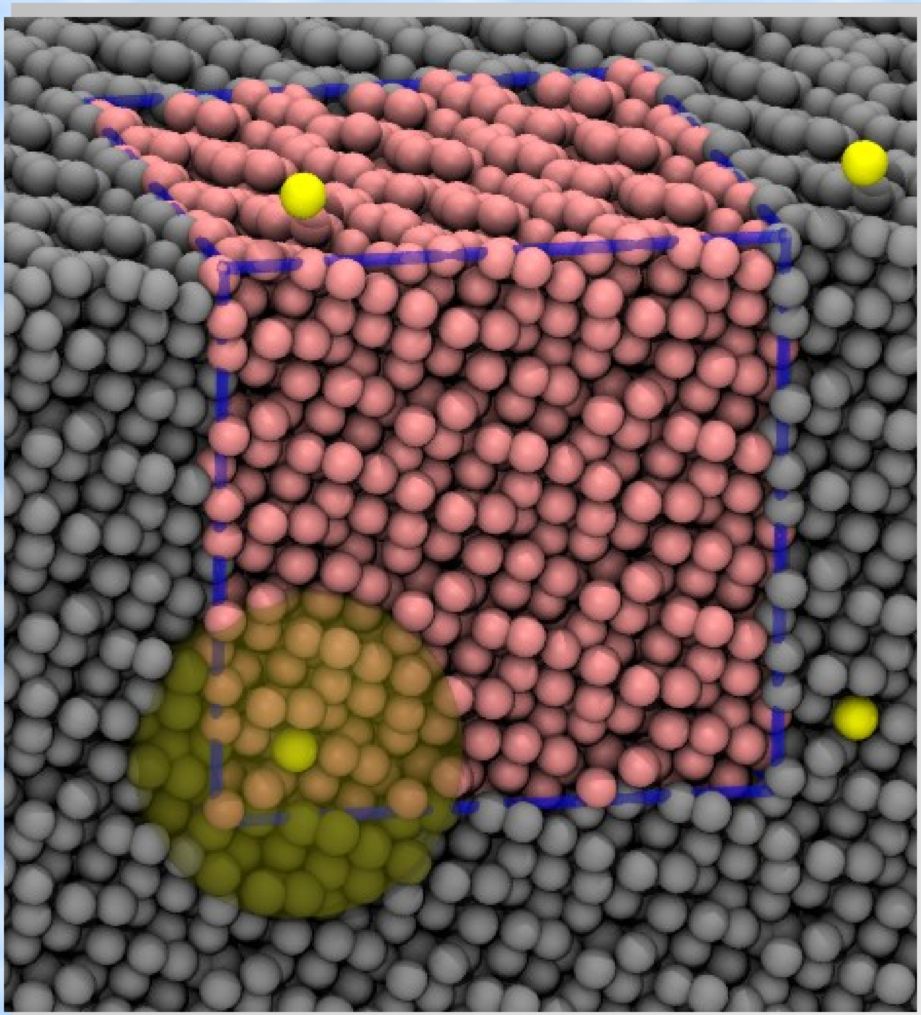
Research Professor, Dept. of Mathematics
Associate Director, ICMS
College of Science and Technology
Temple University, Philadelphia

http://sites.google.com/site/akohlmey/

a.kohlmeyer@temple.edu

MHPC
Master in High Performance Computing

The LJ Model for Liquid Argon



- Cubic box of particles with a Lennard-Jones type pairwise additive interaction potential

$$V=\sum_{i,j}\begin{cases}4\epsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12}-\left(\frac{\sigma}{r_{ij}}\right)^{6}\right], & r_{ij}<r_c\\ 0 \quad , & r_{ij}\geq r_c\end{cases}$$

- Periodic boundary conditions to avoid surface effects

Newton's Laws of Motion

- We consider our particles to be classical objects so Newton's laws of motion apply:
- 1. In absence of a force a body rests or moves in a straight line with constant velocity
- 2. A body experiencing a force **F** experiences an acceleration **a** related to **F** by **F** = m**a**, where m is the mass of the body.
- 3. Whenever a first body exerts a force **F** on a second body, the second body exerts a force **−F** on the first body

Velocity Verlet Algorithm

- The velocity Verlet algorithm is used to propagate the positions of the atoms

$$\vec{x}_i(t+\Delta t) = \vec{x}_i(t) + \vec{v}_i(t)\Delta t + \frac{1}{2}\vec{a}_i(t)(\Delta t)^2 \qquad \vec{v}_i\left(t+\frac{\Delta t}{2}\right) = \vec{v}_i(t) + \frac{1}{2}\vec{a}_i(t)\Delta t$$

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

$$\vec{a}_i(t+\Delta t) = -\frac{1}{m}\nabla V(\vec{x}_i(t+\Delta t)) \qquad \vec{a}_i(t+\Delta t) = -\frac{1}{m}\nabla V(\vec{x}_i(t+\Delta t))$$

$$\vec{v}_i(t+\Delta t) = \vec{v}_i\left(t+\frac{\Delta t}{2}\right) + \frac{1}{2}\vec{a}_i(t+\Delta t)\Delta t \qquad \vec{v}_i(t+\Delta t) = \vec{v}_i\left(t+\frac{\Delta t}{2}\right) + \frac{1}{2}\vec{a}_i(t)\Delta^2$$

Force calculation

$$\begin{cases} 4\epsilon\left[-12\left(\frac{\sigma}{r_{ij}}\right)^{13} + 6\left(\frac{\sigma}{r_{ij}}\right)^{7}\right], & r_{ij} < r_c \\ 0, & r_{ij} \geq r_c \end{cases}$$

L. Verlet, Phys. Rev. 159, 98 (1967); Phys. Rev. 165, 201 (1967).

What Do We Need to Program?

1. Read in parameters and initial status and compute what is missing (e.g. accelerations)
2. Integrate Equations of motion with Velocity Verlet for a given number of steps
   a) Propagate all velocities for half a step
   b) Propagate all positions for a full step
   c) Compute forces on all atoms to get accelerations
   d) Propagate all velocities for half a step
   e) Output intermediate results, if needed

Initial Serial Code: Velocity Verlet

```
void velverlet(mdsys_t *sys) {
    for (int i=0; i<sys->natoms; ++i) {
        sys->vx[i] += 0.5*sys->dt / mvsq2e * sys->fx[i] / sys->mass;
        sys->vy[i] += 0.5*sys->dt / mvsq2e * sys->fy[i] / sys->mass;
        sys->vz[i] += 0.5*sys->dt / mvsq2e * sys->fz[i] / sys->mass;
        sys->rx[i] += sys->dt*sys->vx[i];
        sys->ry[i] += sys->dt*sys->vy[i];
        sys->rz[i] += sys->dt*sys->vz[i];
    }

    force(sys);

    for (int i=0; i<sys->natoms; ++i) {
        sys->vx[i] += 0.5*sys->dt / mvsq2e * sys->fx[i] / sys->mass;
        sys->vy[i] += 0.5*sys->dt / mvsq2e * sys->fy[i] / sys->mass;
        sys->vz[i] += 0.5*sys->dt / mvsq2e * sys->fz[i] / sys->mass;
    }
}
```

Initial Code: Force Calculation

```
for(i=0; i < (sys->natoms); ++i) {
  for(j=0; j < (sys->natoms); ++j) {
    if (i==j) continue;

    rx=pbc(sys->rx[i] - sys->rx[j], 0.5*sys->box);
    ry=pbc(sys->ry[i] - sys->ry[j], 0.5*sys->box);
    rz=pbc(sys->rz[i] - sys->rz[j], 0.5*sys->box);
    r = sqrt(rx*rx + ry*ry + rz*rz);

    if (r < sys->rcut) {
      ffac = -4.0*sys->epsilon*(-12.0*pow(sys->sigma/r,12.0)/r
                         +6*pow(sys->sigma/r,6.0)/r);
      sys->epot += 0.5*4.0*sys->epsilon*(pow(sys->sigma/r,12.0)
                         -pow(sys->sigma/r,6.0));
      sys->fx[i] += rx/r*ffac;
      sys->fy[i] += ry/r*ffac;
      sys->fz[i] += rz/r*ffac;
    }}
```

Compute distance between atoms i & j

Compute energy and force

Add force contribution of atom j on atom i

How Well Does it Work?

- Compiled with:
  `gcc -o ljmd.x ljmd.c -lm`
  Test input: 108 atoms, 10000 steps: 49s
  Let us get a profile:

```
 %   cumulative   self              self     total
time   seconds   seconds    calls  ms/call  ms/call  name
73.70     13.87    13.87    10001     1.39     1.86  force
24.97     18.57     4.70 346714668     0.00     0.00  pbc
 0.96     18.75     0.18                             main
 0.37     18.82     0.07    10001     0.01     0.01  ekin
 0.00     18.82     0.00    30006     0.00     0.00  azzero
 0.00     18.82     0.00      101     0.00     0.00  output
 0.00     18.82     0.00       12     0.00     0.00  getline
```

Compiler Optimization

- Use of pbc() is convenient, but costs 25%
  => compiling with -O3 should inline it
- Loops should be unrolled for superscalar CPUs
  => compiling with -O2 or -O3 should do it for us

  Time now: 39s (1.3x faster) Only a bit faster
- Now try some more optimization options:
  -ffast-math -fexpensive-optimizations -msse3

  Time now: 10s (4.9x faster) Much better!
- Compare to LAMMPS: 3.6s => need to do more

Now Modify the Code

- Use physics! Newton's 3rd law: $F_{ij} = -F_{ji}$

```
for(i=0; i < (sys->natoms)-1; ++i) {
  for(j=i+1; j < (sys->natoms); ++j) {
    rx=pbc(sys->rx[i] - sys->rx[j], 0.5*sys->box);
    ry=pbc(sys->ry[i] - sys->ry[j], 0.5*sys->box);
    rz=pbc(sys->rz[i] - sys->rz[j], 0.5*sys->box);
    r = sqrt(rx*rx + ry*ry + rz*rz);
    if (r < sys->rcut) {
      ffac = -4.0*sys->epsilon*(-12.0*pow(sys->sigma/r,12.0)/r
                                +6*pow(sys->sigma/r,6.0)/r);
      sys->epot += 0.5*4.0*sys->epsilon*(pow(sys->sigma/r,12.0)
                                -pow(sys->sigma/r,6.0));
      sys->fx[i] += rx/r*ffac;      sys->fx[j] -= rx/r*ffac;
      sys->fy[i] += ry/r*ffac;      sys->fy[j] -= ry/r*ffac;
      sys->fz[i] += rz/r*ffac;      sys->fz[j] -= rz/r*ffac;
}}}
```

Time now: 5.4s (9.0x faster) Another big improvement

More Modifications

- Avoid expensive math: pow(), sqrt(), division

```
c12=4.0*sys->epsilon*pow(sys->sigma,12.0);
c6 =4.0*sys->epsilon*pow(sys->sigma, 6.0);
rcsq = sys->rcut * sys->rcut;
for(i=0; i < (sys->natoms)-1; ++i) {
  for(j=i+1; j < (sys->natoms); ++j) {
    rx=pbc(sys->rx[i] - sys->rx[j], 0.5*sys->box);
    ry=pbc(sys->ry[i] - sys->ry[j], 0.5*sys->box);
    rz=pbc(sys->rz[i] - sys->rz[j], 0.5*sys->box);
    rsq = rx*rx + ry*ry + rz*rz;
    if (rsq < rcsq) {
      double r6,rinv; rinv=1.0/rsq;  r6=rinv*rinv*rinv;
      ffac = (12.0*c12*r6 - 6.0*c6)*r6*rinv;
      sys->epot += r6*(c12*r6 - c6);
      sys->fx[i] += rx*ffac;  sys->fx[j] -= rx*ffac;
      sys->fy[i] += ry*ffac;  sys->fy[j] -= ry*ffac;
      sys->fz[i] += rz*ffac;  sys->fz[j] -= rz*ffac;
}}}
```

=> 108 atoms: 4.0s (12.2x faster) still worth it

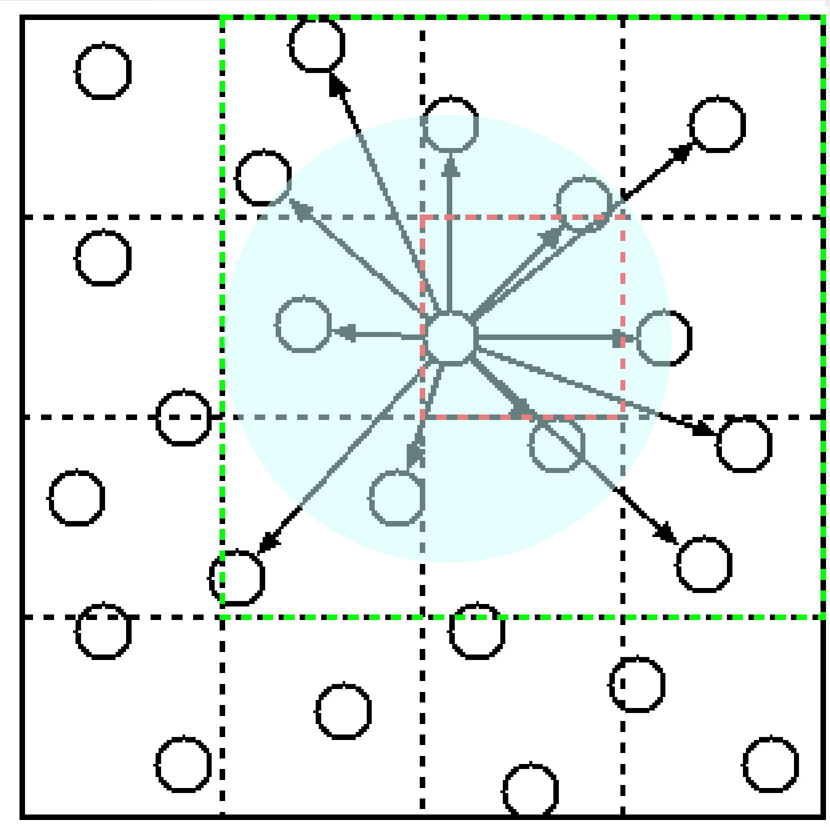
Improvements So Far

- Use the optimal compiler flags => ~5x faster but some of it: inlining, unrolling could be coded
- Use our knowledge of physics => ~2x faster since we need to compute only half the data.
- Use our knowledge of computer hardware => 1.35x faster. (there could be more: SSE)

  We are within 10% (4s vs. 3.6s) of LAMMPS.
- Try a bigger system: 2916 atoms, 100 steps
  Our code: 13.3s LAMMPS: 2.7s => Bad scaling with system size

Making it Scale with System Size

- We compute all distances between pairs
- But for larger systems not all pairs contribute yet our effort is $O(N^2)$
- Avoid distant pairs
  - Divide system in cells of size >= cutoff.
  - Sort atoms into cells
  - Look only at 26 cells around central cell



The Cell-List Variant

- At startup build a list of lists to store atom indices for atoms that “belong” to a cell
- Compute a list of pairs between cells which contain atoms within cutoff. Doesn't change!
- During MD sort atoms into cells
- Then loop over list of “close” pairs of cells *i* and *j*
- For pair of cells loop over pairs of atoms in them
- Now we have linear scaling with system size at the cost of using more memory and an O(N) sort

Cell List Loop

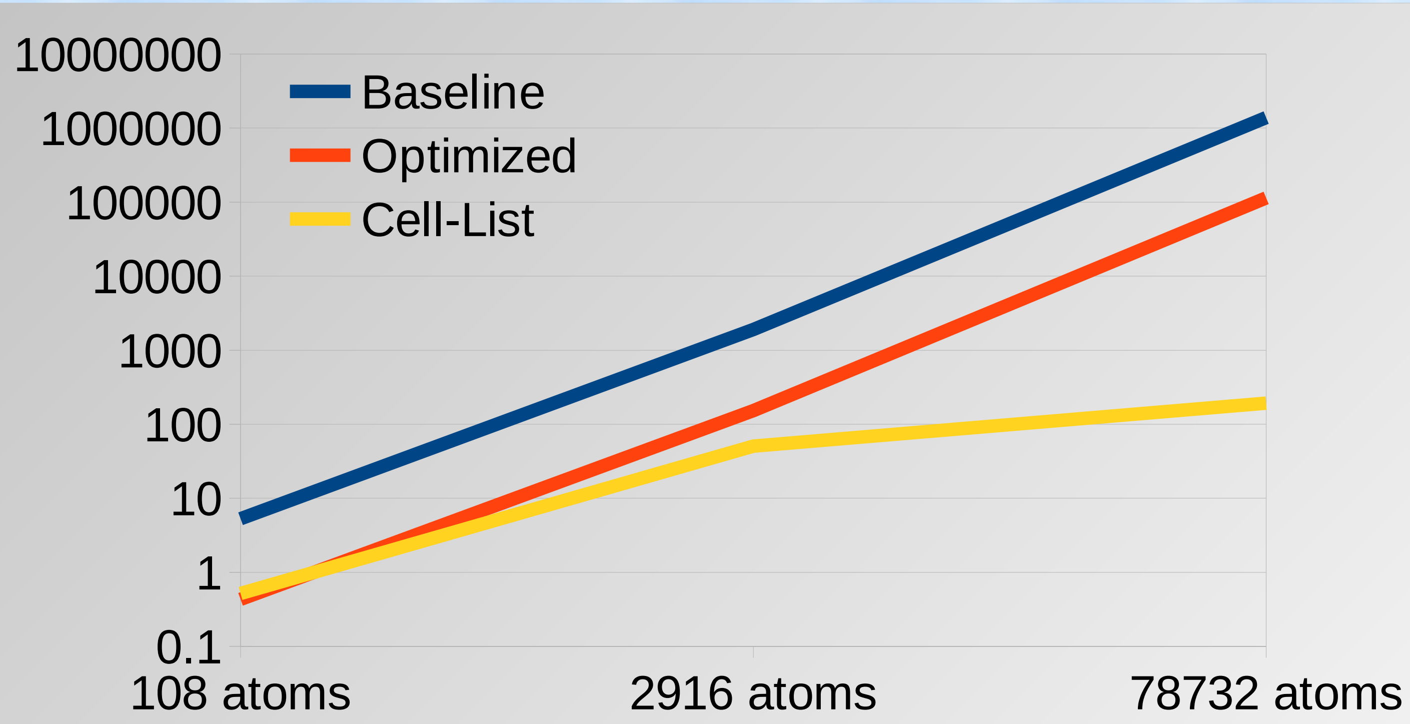
```
for(i=0; i < sys->npair; ++i) {
    cell_t *c1, *c2;
    c1=sys->clist + sys->plist[2*i];
    c2=sys->clist + sys->plist[2*i+1];

        for (int j=0; j < c1->natoms; ++j) {
            int ii=c1->idxlist[j];
            double rx1=sys->rx[ii];
            double ry1=sys->ry[ii];
            double rz1=sys->rz[ii];

            for(int k=0; k < c2->natoms; ++k) {
                double rx,ry,rz,rsq;
                int jj=c2->idxlist[k];
                rx=pbc(rx1 - sys->rx[jj], boxby2, sys->box);
                ry=pbc(ry1 - sys->ry[jj], boxby2, sys->box);
                ...
```

- 2916 atom time: 3.4s (4x faster), LAMMPS 2.7s

Scaling with System Size



- Cell list does not help (or hurt) much for small inputs, but is a huge win for larger problems => Lesson: always pay attention to scaling

What if optimization is not enough?

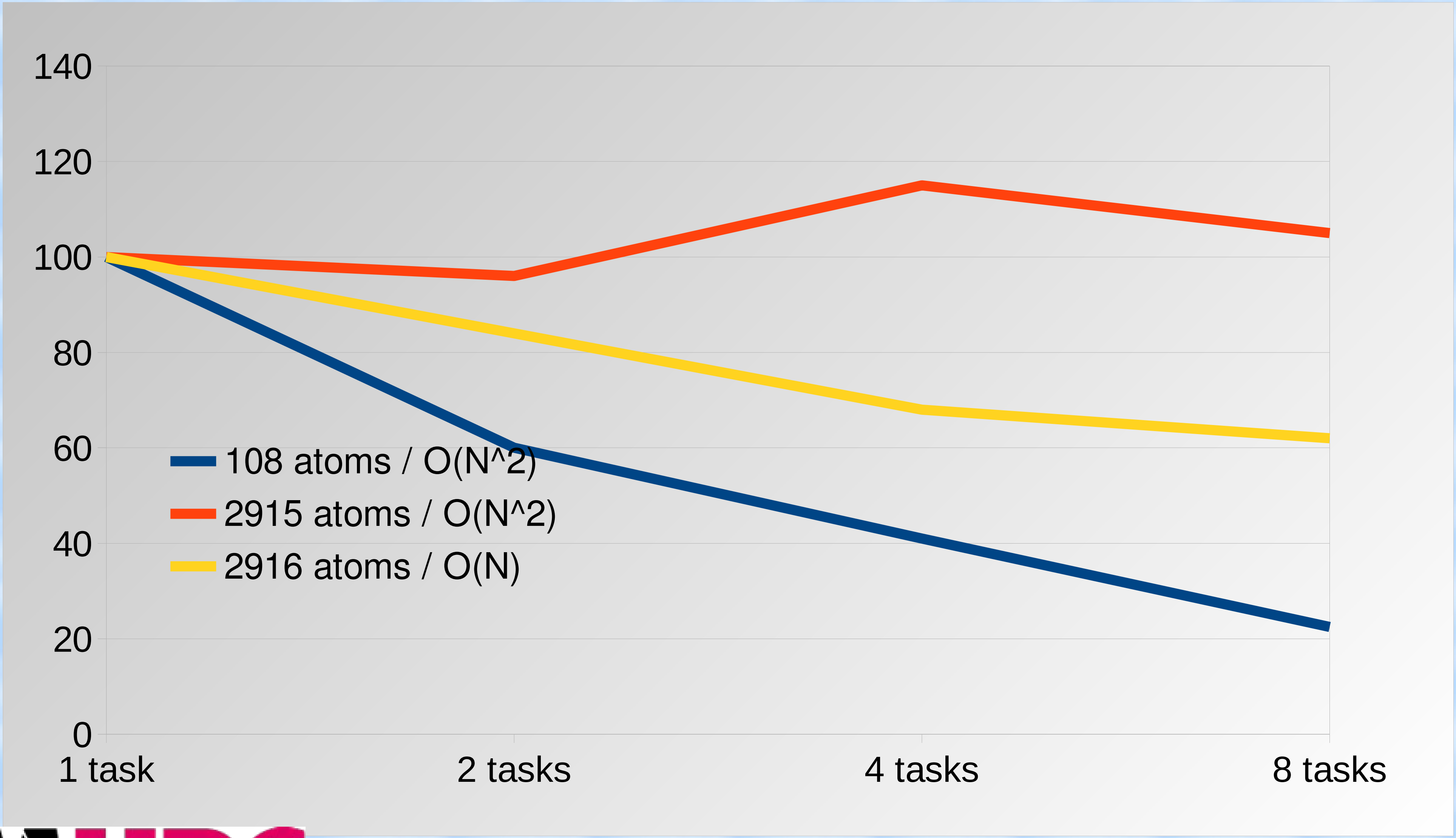
- Having linear scaling is nice, but twice the system size is still twice the work
  => Parallelization
- Simple MPI parallelization first
  - MPI is “share nothing” (replicated or distributed data)
  - Run the same code path with the same data but insert a few MPI calls
    - Broadcast positions from rank 0 to all before force()
    - Compute forces on different atoms for each rank
    - Collect (reduce) forces from all to rank 0 after force()

Replicated Data MPI Version

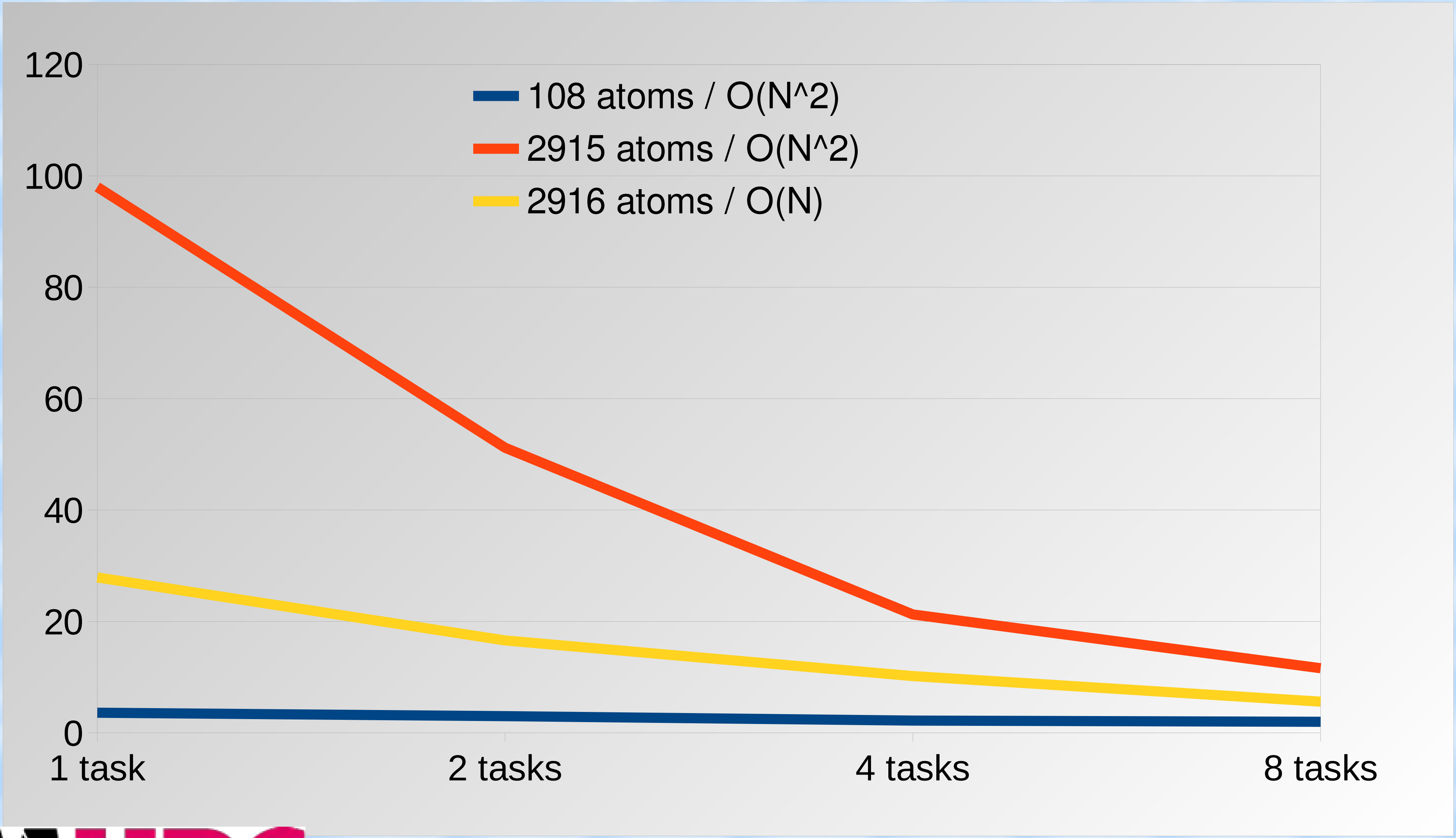
```
static void force(mdsys_t *sys) {
    double epot=0.0;
    azzero(sys->cx,sys->natoms); azzero(sys->cy,sys->natoms); azzero(sys->cz,sys->natoms);
    MPI_Bcast(sys->rx, sys->natoms, MPI_DOUBLE, 0, sys->mpicomm);
    MPI_Bcast(sys->ry, sys->natoms, MPI_DOUBLE, 0, sys->mpicomm);
    MPI_Bcast(sys->rz, sys->natoms, MPI_DOUBLE, 0, sys->mpicomm);
    for (i=0; i < sys->natoms-1; i += sys->nsize) {
        ii = i + sys->mpirank;
        if (ii >= (sys->natoms - 1)) break;
        for (j=i+1; i < sys->natoms; ++j) {
       [...]
                sys->cy[j] -= ry*ffac;
                sys->cz[j] -= rz*ffac;
    } }
    MPI_Reduce(sys->cx, sys->fx, sys->natoms, MPI_DOUBLE, MPI_SUM, 0, sys->mpicomm);
    MPI_Reduce(sys->cy, sys->fy, sys->natoms, MPI_DOUBLE, MPI_SUM, 0, sys->mpicomm);
    MPI_Reduce(sys->cz, sys->fz, sys->natoms, MPI_DOUBLE, MPI_SUM, 0, sys->mpicomm);
    MPI_Reduce(&epot, &sys->epot, 1, MPI_DOUBLE, MPI_SUM, 0, sys->mpicomm);
}
```

- Easy to implement, but lots of communication

MPI Parallel Efficiency



MPI Parallel Execution Times



OpenMP Parallelization

- OpenMP is directive based
  => code (can) work without them
- OpenMP can be added incrementally
- OpenMP only works in shared memory
  => multi-core processors
- OpenMP hides the calls to a threads library
  => less flexible, but less programming
- Caution: write access to shared data can easily lead to race conditions

Naive OpenMP Version

```
#if defined(_OPENMP)
#pragma omp parallel for default(shared) \
    private(i) reduction(+:epot)
#endif
    for(i=0; i < (sys->natoms)-1; ++i) {
        double rx1=sys->rx[i];
        double ry1=sys->ry[i];
        double rz1=sys->rz[i];
        [...]

               {
                    sys->fx[i] += rx*ffac;
                    sys->fy[i] += ry*ffac;
                    sys->fz[i] += rz*ffac;
                    sys->fx[j] -= rx*ffac;
                    sys->fy[j] -= ry*ffac;
                    sys->fz[j] -= rz*ffac;
                }
```

Each thread will work on different values of “i”

Race condition: “i” will be unique for each thread, but not “j”
=> multiple threads may write to the same location concurrently

Naive OpenMP Version

```
#if defined(_OPENMP)
#pragma omp parallel for default(shared) \
    private(i) reduction(+:epot)
#endif
    for(i=0; i < (sys->natoms)-1; ++i) {
        double rx1=sys->rx[i];
        double ry1=sys->ry[i];
        double rz1=sys->rz[i];
        [...]
```

Each thread will work on different values of “i”

```
#if defined(_OPENMP)
#pragma omp critical
#endif
                {
                    sys->fx[i] += rx*ffac;
                    sys->fy[i] += ry*ffac;
                    sys->fz[i] += rz*ffac;
                    sys->fx[j] -= rx*ffac;
                    sys->fy[j] -= ry*ffac;
                    sys->fz[j] -= rz*ffac;
                }
```

The “critical” directive will let only one thread at a time execute this block

Timings (108 atoms):
1 thread: 4.2s
2 threads: 7.1s
4 threads: 7.7s
8 threads: 8.6s

This is making it **slower** not faster!

OpenMP Improvements

- Use **omp atomic** to protect one instruction
  => faster, but requires hardware support
  108: 1T: 6.3s, 2T: 5.0s, 4T: 4.4s, 8T: 4.2s
  2916: 1T: 126s, 2T: 73s, 4T: 48s, 8T: 26s
  => some speedup, but noticable overhead
  => serial is faster than OpenMP with 1T
- Don't use Newton's 3rd Law => no race condition
  108: 1T: 6.5s, 2T: 3.7s, 4T: 2.3s, 8T: 2.1s
  2916: 1T: 213s, 2T: 106s, 4T: 53s, 8T: 21s
  => better scaling, but we lose 2x serial speed

MPI-like Approach with OpenMP

```
#if defined(_OPENMP)
#pragma omp parallel reduction(+:epot)
#endif
    {  double *fx, *fy, *fz;
#if defined(_OPENMP)
        int tid=omp_get_thread_num();
#else
        int tid=0;
#endif
        fx=sys->fx + (tid*sys->natoms); azzero(fx,sys->natoms);
        fy=sys->fy + (tid*sys->natoms); azzero(fy,sys->natoms);
        fz=sys->fz + (tid*sys->natoms); azzero(fz,sys->natoms);
        for(int i=0; i < (sys->natoms -1); i += sys->nthreads) {
            int ii = i + tid;
            if (ii >= (sys->natoms -1)) break;
            rx1=sys->rx[ii];
            ry1=sys->ry[ii];
            rz1=sys->rz[ii];
```

Thread Id is like MPI rank

sys->fx holds storage for one full fx array for each thread => race condition is eliminated.

MPI-like Approach with OpenMP (2)

- We need to write our own reduction:

```
#if defined (_OPENMP)
#pragma omp barrier
#endif
    i = 1 + (sys->natoms / sys->nthreads);
    fromidx = tid * i;
    toidx = fromidx + i;
    if (toidx > sys->natoms) toidx = sys->natoms;

    for (i=1; i < sys->nthreads; ++i) {
        int offs = i*sys->natoms;
        for (int j=fromidx; j < toidx; ++j) {
            sys->fx[j] += sys->fx[offs+j];
            sys->fy[j] += sys->fy[offs+j];
            sys->fz[j] += sys->fz[offs+j];
        }
    }
```

Need to make certain, all threads are done with computing forces

Use threads to parallelize the reductions

More OpenMP Timings

- The **omp parallel** region timings
  108: 1T: 3.5s, 2T: 2.5s, 4T: 2.2s, 8T: 2.5s
  2916: 1T: 103s, 2T: 53s, 4T: 19s, 8T: 10s
  => better speedup, 1T is about as fast as serial
  => scaling like no 3rd law, but speed 2x as fast
- This approach also works with cell lists:
  108: 1T: 4.3s, 2T: 3.1s, 4T: 2.4s, 8T: 2.9s
  2916: 1T: 28s, 2T: 15s, 4T: 8.9s, 8T: 4.1s
  => 6.8x speedup with 8 threads.
  62x faster than original code with 2916 atoms

Hybrid OpenMP/MPI Version

- With multi-core nodes, communication between MPI tasks becomes a problem
  => all communication has to us one link
  => reduced bandwidth, increased latency
- OpenMP and MPI parallelization are orthogonal and can be used at the same time
  Caution: don't call MPI from threaded region
- Parallel region OpenMP version is very similar to MPI version, so that would be easy to merge

Hybrid OpenMP/MPI Kernel

- MPI tasks are like GPU thread blocks
- Need to reduce forces/energies first across threads and then across all MPI tasks

```
[...]
      incr = sys->mpisize * sys->nthreads;
      /* self interaction of atoms in cell */
      for(n=0; n < sys->ncell; n += incr) {
          int i,j;
          const cell_t *c1;

          i = n + sys->mpirank*sys->nthreads + tid;
          if (i >= sys->ncell) break;
          c1=sys->clist + i;

          for (j=0; j < c1->natoms-1; ++j) {
 [...]
```

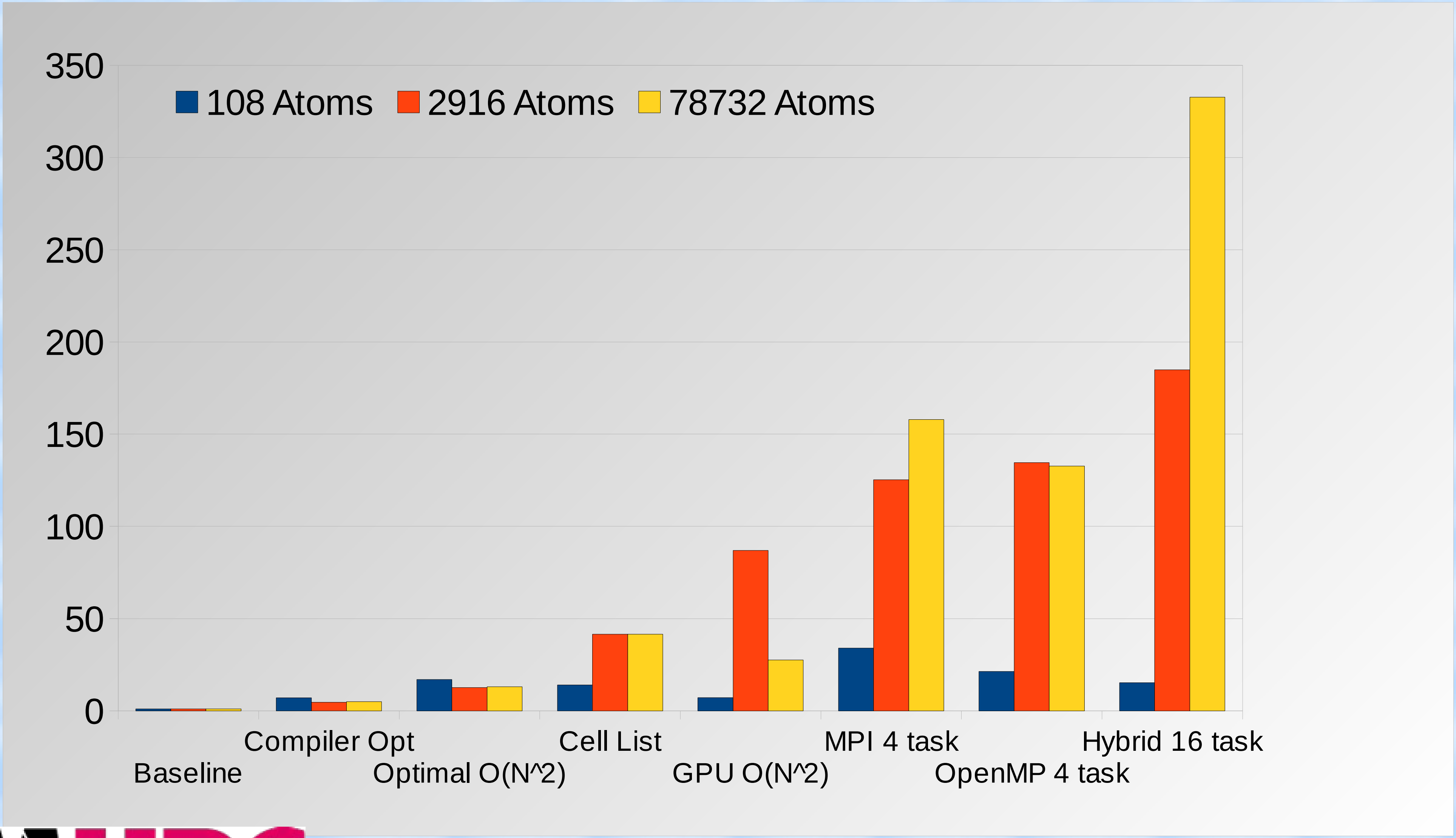
Hybrid OpenMP/MPI Timings

	2916 atoms system:	78732 atoms system:
Cell list serial code:	18s	50.1s
16 MPI x 1 Threads:	14s	19.8s
8 MPI x 2 Threads:	5.5s	8.9s
4 MPI x 4 Threads:	4.3s	8.2s
2 MPI x 8 Threads:	4.0s	7.3s
=> Best speedup:	4.5x	6.9x
=>Total speedup:	**185x**	**333x**

Two nodes with 2x quad-core

- Replicated data MPI is simple to implement but does not parallelize well for this kind of code

Total Speedup Comparison



LJMD Simulation Code

Conclusions

- Make sure that you exploit the physics of your problem well => Newton's 3rd law gives a 2x speedup for free (but interferes with threading!)
- Let the compiler help you (more readable code), but also make it easy to the compiler => unrolling, inlining can be offloaded
- Understand the properties of your hardware and adjust your code to match it
- For a large number of threads use simpler code

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Dr. Axel Kohlmeyer

Research Professor, Dept. of Mathematics
Associate Director, ICMS
College of Science and Technology
Temple University, Philadelphia

http://sites.google.com/site/akohlmey/

a.kohlmeyer@temple.edu

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