LJMD Case Study: Optimization and Parallelization

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Today's Show

0) Overture: the physics of the model

1) First Act: writing and optimizing a serial code

2) Intermezzo: improve scaling with system size

3) Second Act: MPI parallelization

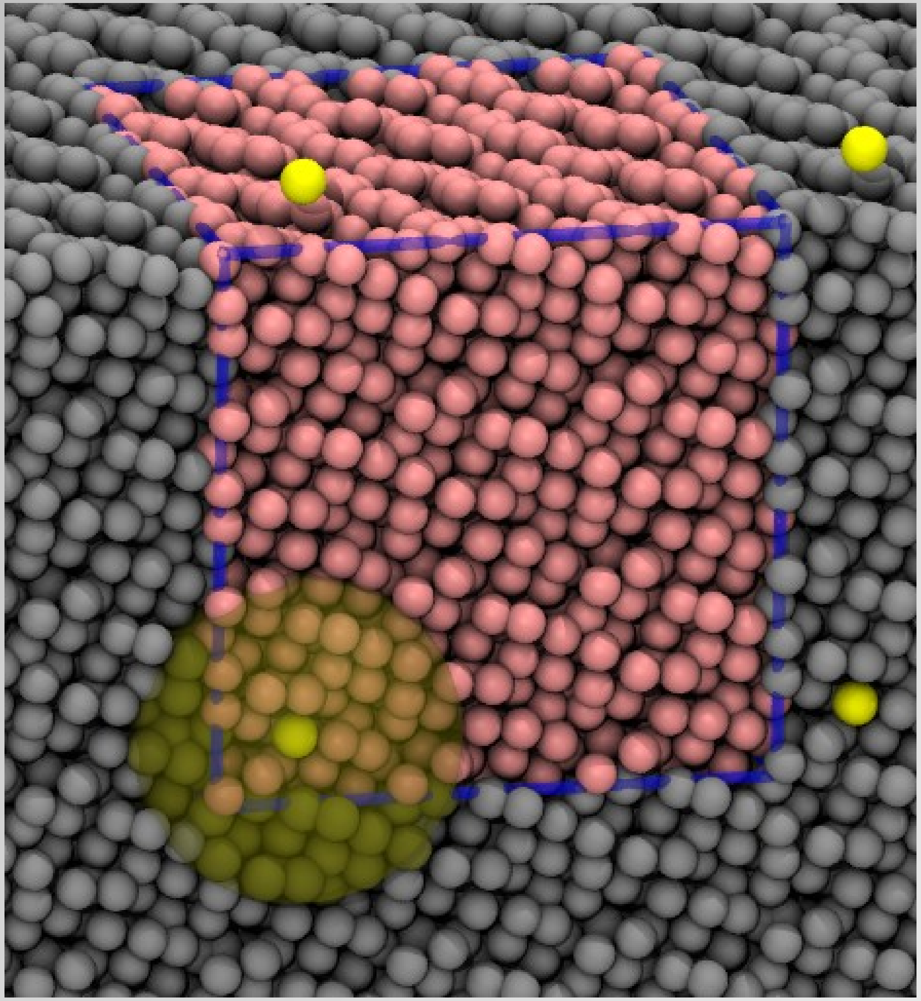
4) Third Act: OpenMP parallelization

5) Finale: Hybrid MPI/OpenMP parallelization

6) Encore: further options for improvement

7) Last dance: lessons learned

0) The Model for Liquid Argon



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

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

- 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 positions and velocities of the atoms

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

$$\vec{x}_i(t+\Delta t) = \vec{x}_i(t)+\vec{v}_i(t+\frac{\Delta t}{2})\Delta t$$

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

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

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

1) 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 in box with periodic boundary conditions

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
```

Step One: Compiler Optimization

- Use of pbc() is convenient, but costs 25% time
  => compiling with -O3 will inline it, no overhead
- 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 than 49s
- Now try more aggressive optimization options:
  -ffast-math -fexpensive-optimizations

  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

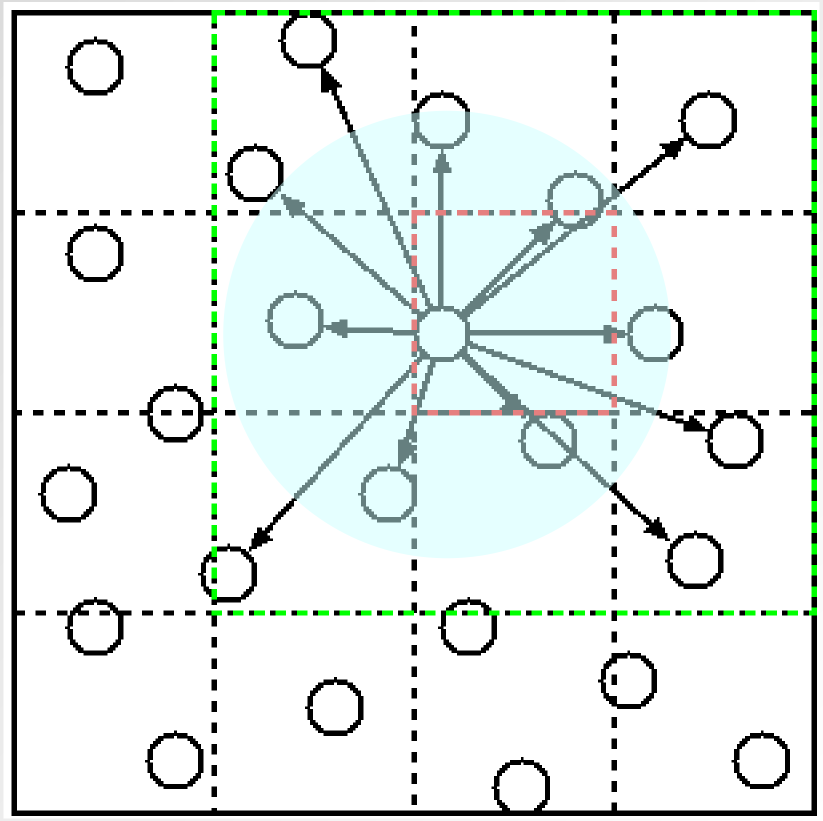
- Use the optimal compiler flags => ~5x faster but some of it: inlining, unrolling could be coded
- Use our knowledge of physics => ~2x faster since we need to compute only half the data.
- Use our knowledge of computer hardware => 1.35x faster. There could be more: vectorize

  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

2) Making it Scale with System Size

- Lets look at the algorithm again:
  We compute all distances between pairs
- But for larger systems not all pairs contribute and our effort is $O(N^2)$
- So we need a way to avoid looking at pairs that are too far away

  => Sort atoms into cell lists, which is O(N)



The Cell-List Variant

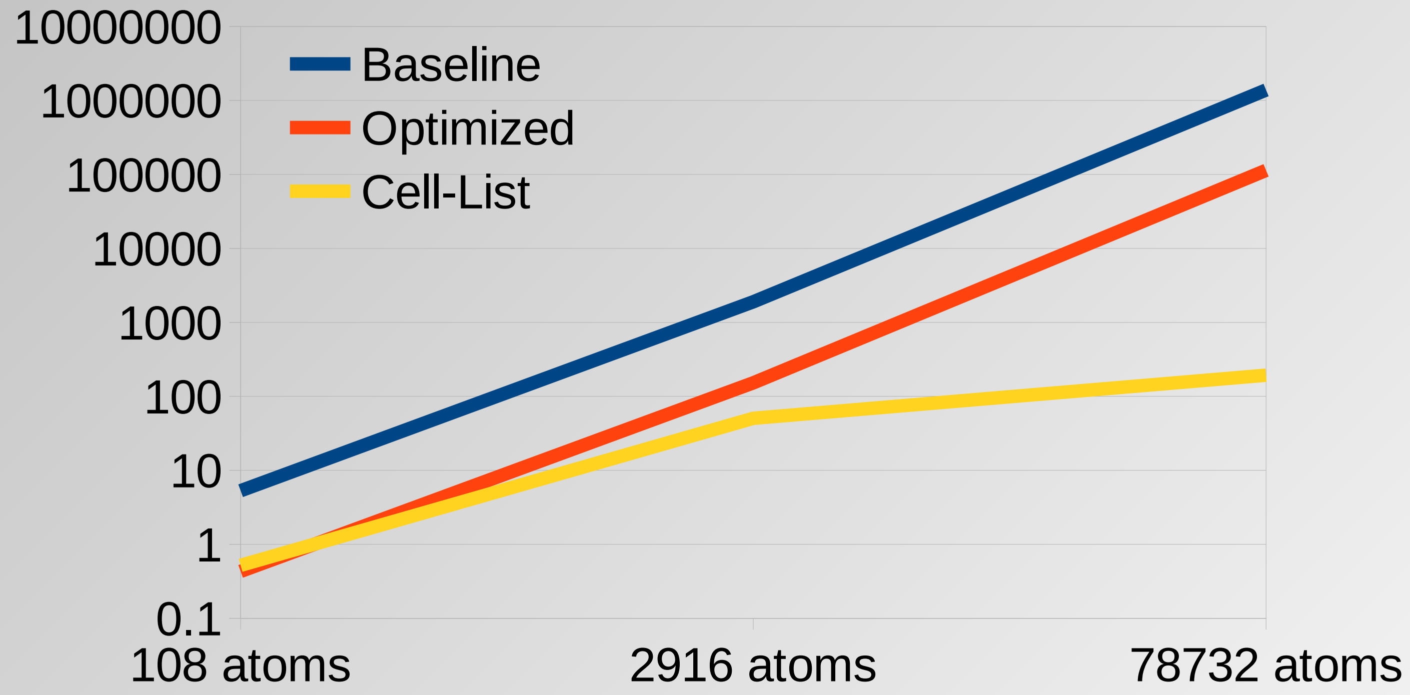
- At startup build a list of lists to store atom indices for atoms that “belong” to a cell
- Compute a list of pairs between cells which contain atoms within cutoff. Doesn't change!
- During MD sort atoms into cells
- Then loop over list of “close” pairs of cells *i* and *j*
- For pair of cells loop 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

3) What if optimization is not enough?

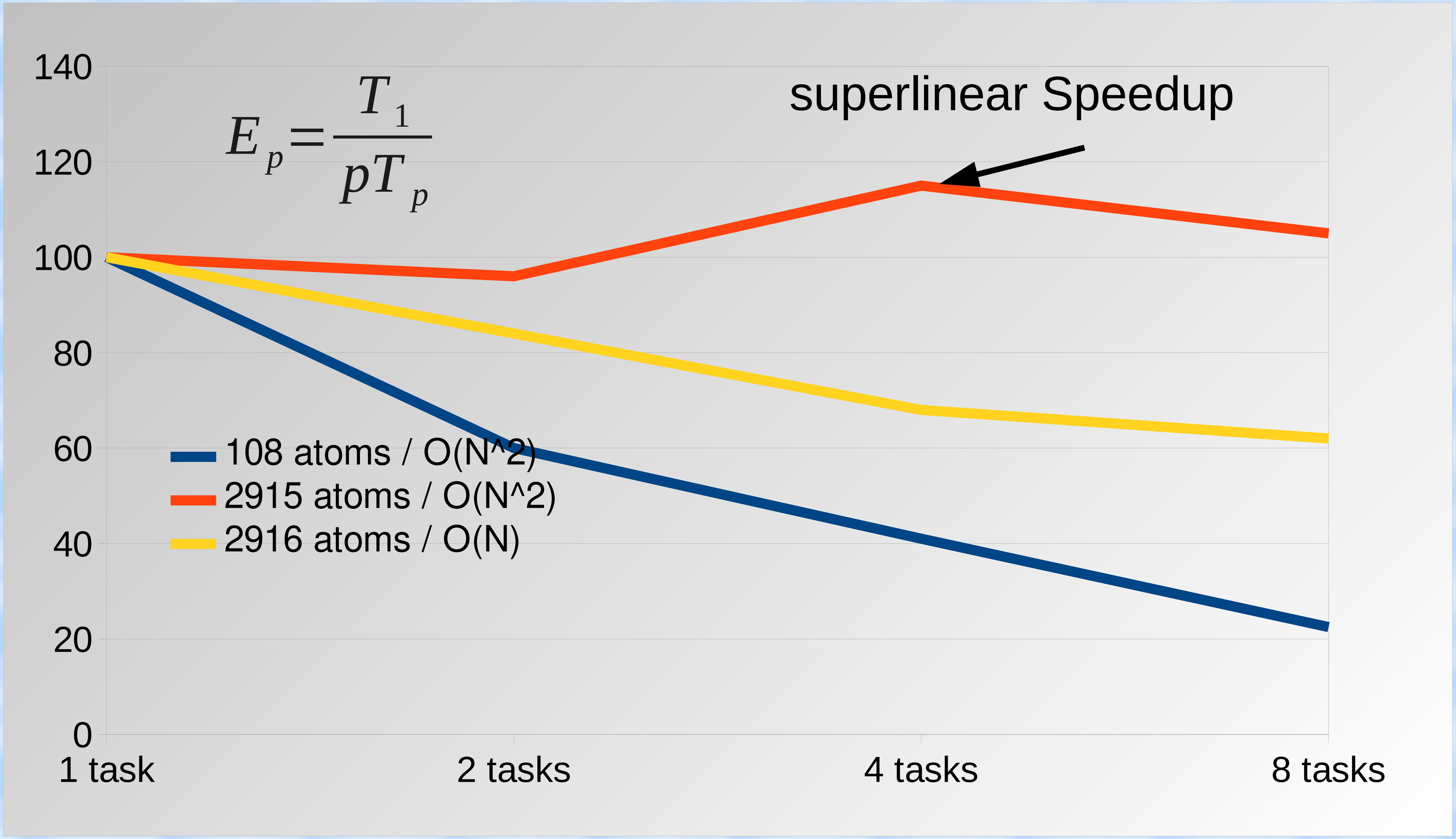
- Having linear scaling is nice, but twice the system size is <u>still</u> twice the work and takes twice the time. => Parallelization
- Simple MPI parallelization first
  - MPI is “share nothing” (replicated or distributed data)
  - Run the same code path with the same data but insert a few MPI calls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

Replicated Data MPI Version

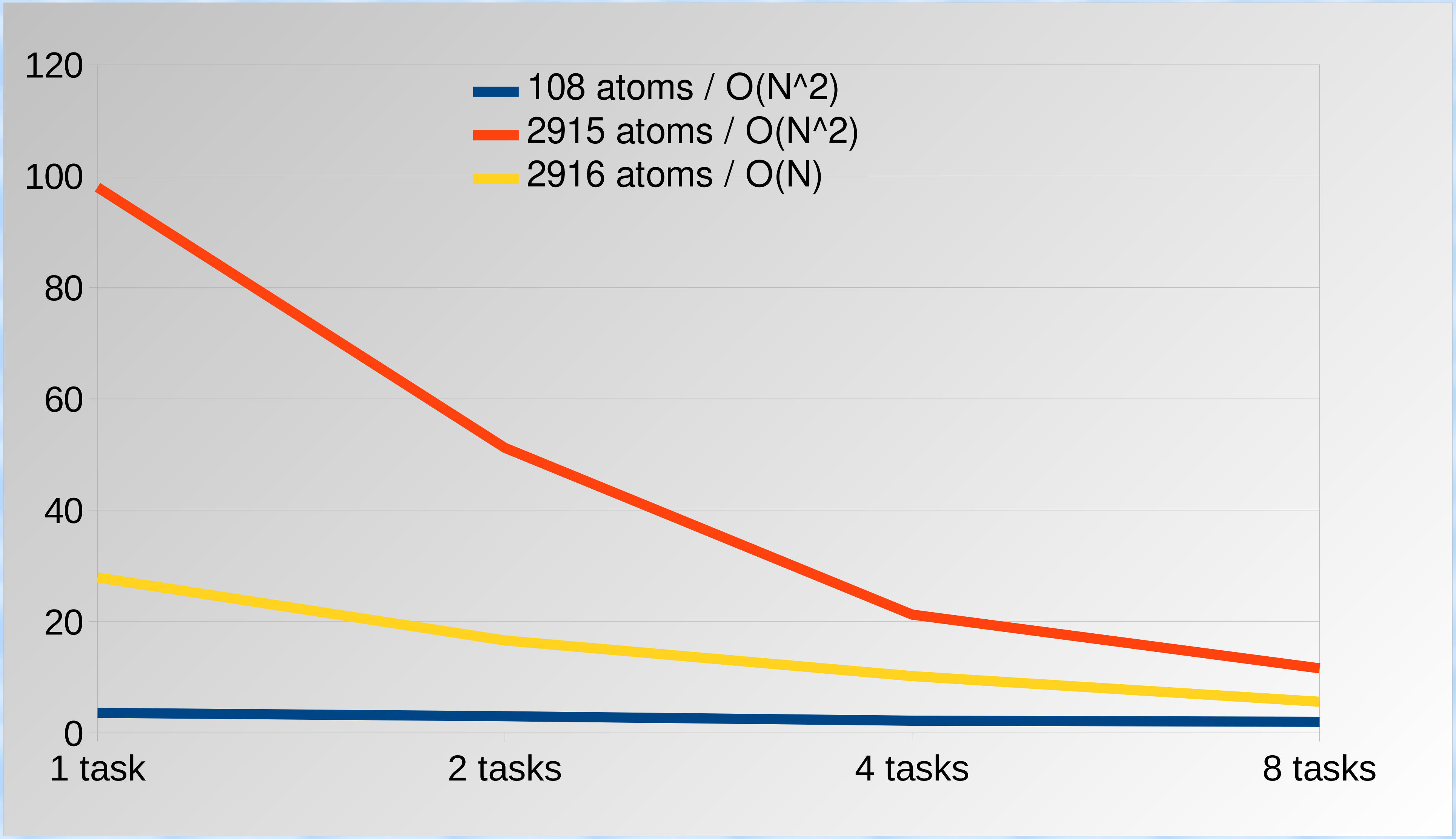
```
static void force(mdsys_t *sys) {
    double epot=0.0;
    azzero(sys->cx,sys->natoms); azzero(sys->cy,sys->natoms); azzero(sys->cz,sys->natoms);
    MPI_Bcast(sys->rx, sys->natoms, MPI_DOUBLE, 0, sys->mpicomm);
    MPI_Bcast(sys->ry, sys->natoms, MPI_DOUBLE, 0, sys->mpicomm);
    MPI_Bcast(sys->rz, 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


$$E_p = \frac{T_1}{pT_p}$$

MPI Parallel Execution Times



4) OpenMP Parallelization

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

Naive OpenMP Version

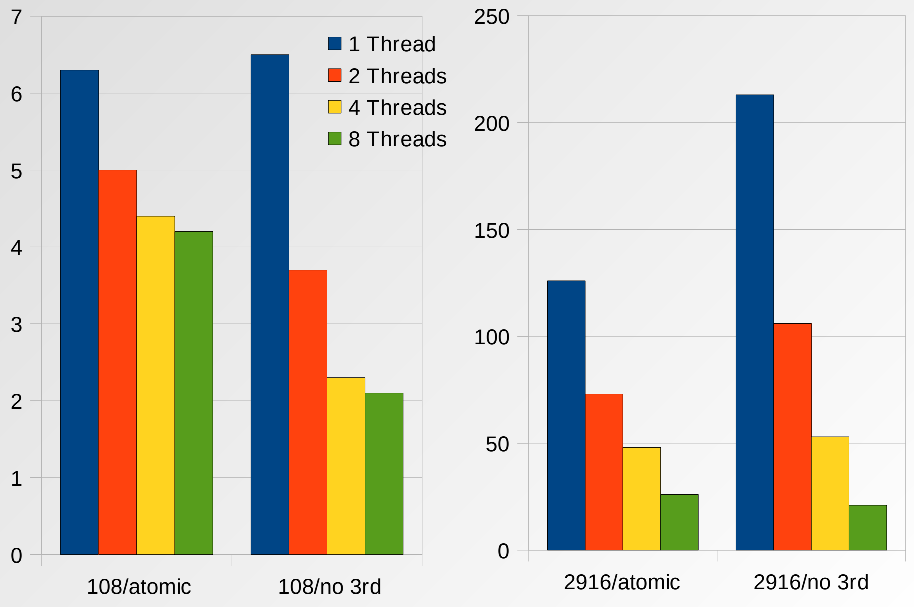
```
#if defined(_OPENMP)
#pragma omp parallel for default(shared) \
    private(i) reduction(+:epot)
#endif
    for(i=0; i < (sys->natoms)-1; ++i) {
        double rx1=sys->rx[i];
        double ry1=sys->ry[i];
        double rz1=sys->rz[i];
        [...]


          {
              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

Handling the Race Condition

- Use **omp critical** to let only one thread access => correct result but kills parallelism
- Use **omp atomic** to protect each force update => faster than 'critical' but slower with 1 thread
- No Newton's 3rd Law: => no race condition => better scaling but we lose 2x serial speed => need 8 threads to be faster than **atomic**



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; need to program reduction operation.

MPI-like Approach with OpenMP (2)

- OpenMP has no equivalent to MPI_Reduce():

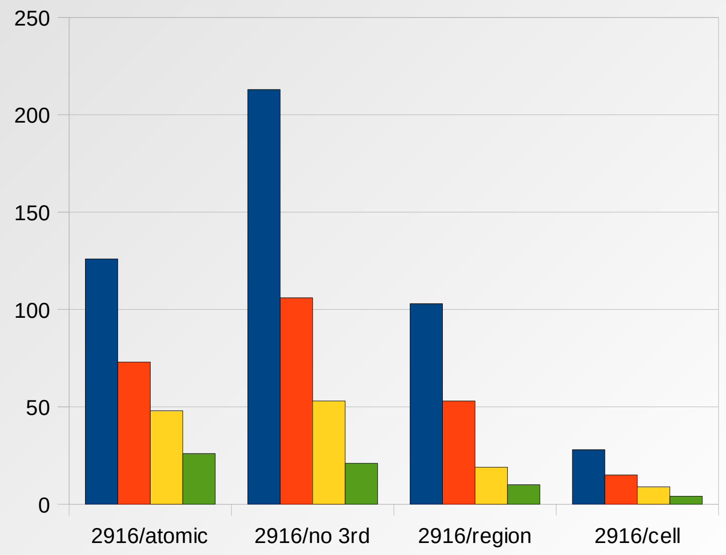
```
#if defined (_OPENMP)
#pragma omp barrier
#endif
    i = 1 + (sys->natoms / sys->nthreads);
    fromidx = tid * i;
    toidx = fromidx + i;
    if (toidx > sys->natoms) toidx = sys->natoms;

    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
  2916: 1T: 103s, 2T: 53s, 4T: 19s, 8T: 10s
  => better speedup, but serial is faster for 108,
  at 2916 atoms we are often beyond cutoff
- This approach also works with cell lists
  => with 8 threads:
  4.1s = 6.8x speedup vs.
  serial cell list version (28s).
  That is <u>**62x**</u> faster than
  the first naive serial version



5) Hybrid OpenMP/MPI Version

- With multi-core nodes, communication between MPI tasks becomes a problem
  => all communication has to use 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

- Now scatter loops over MPI tasks and threads
- Need to reduce forces/energies first across threads and then across all MPI tasks

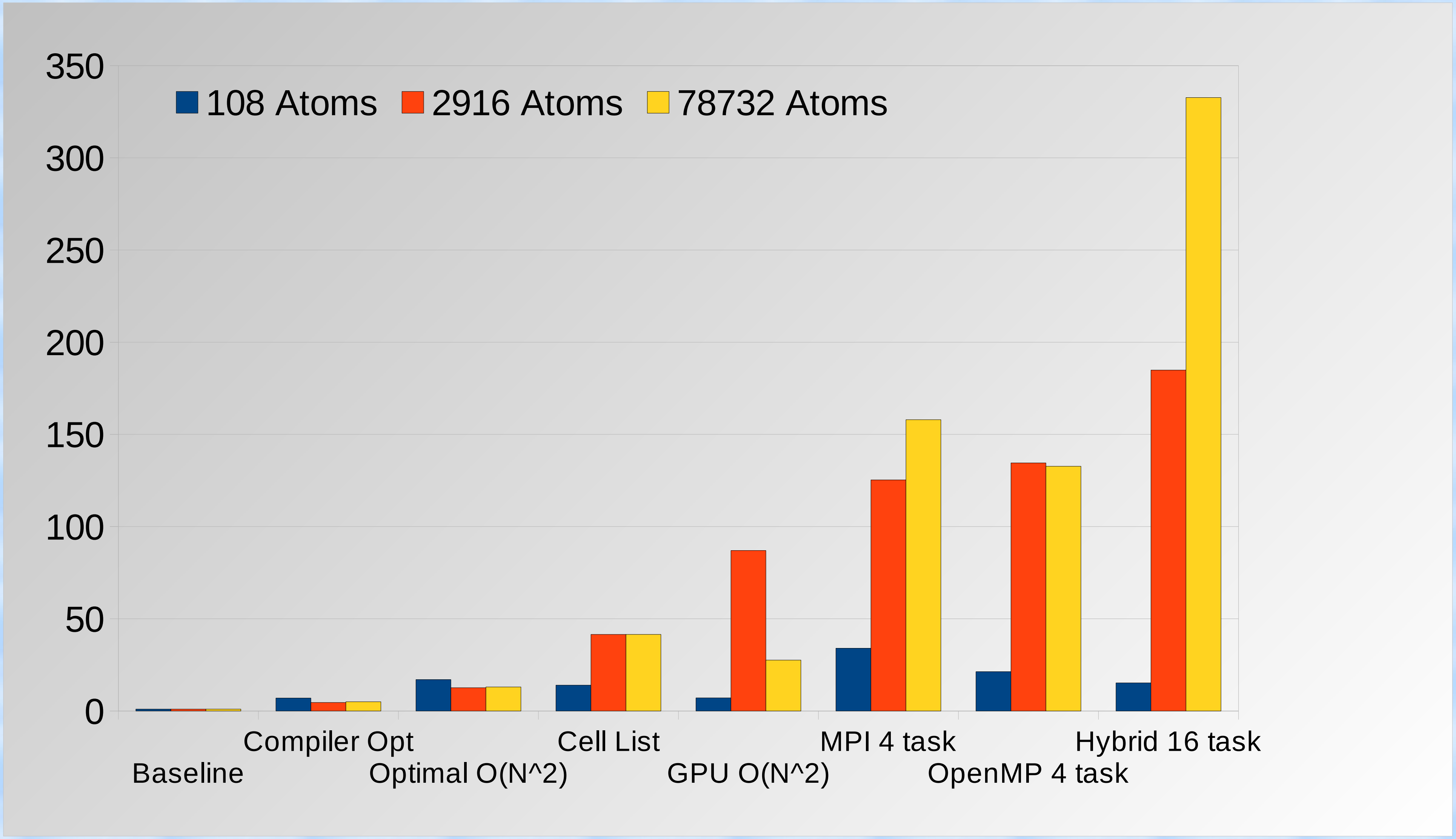
```
[...]
     incr = sys->mpisize * sys->nthreads;
     /* self interaction of atoms in cell */
     for(n=0; n < sys->ncell; n += incr) {
         int i,j;
         const cell_t *c1;

         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

Total Speedup Comparison



6) Further Options for Improvements

- Use domain decomposition
  => Better weak scaling, better cache locality
  => Complex communication (use LAMMPS)
- Use neighbor lists (aka Verlet lists)
  => Avoid even more distance computations
  => Increases memory use (use LAMMPS)
- Add vectorization support
  => Significant speedup with Intel compiler
  => Even more speedup with single precision
  => Increased code complexity (use LAMMPS)

7) 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!)
- Find strategies that have favorable scaling with system size; avoid unneded computations
- 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

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