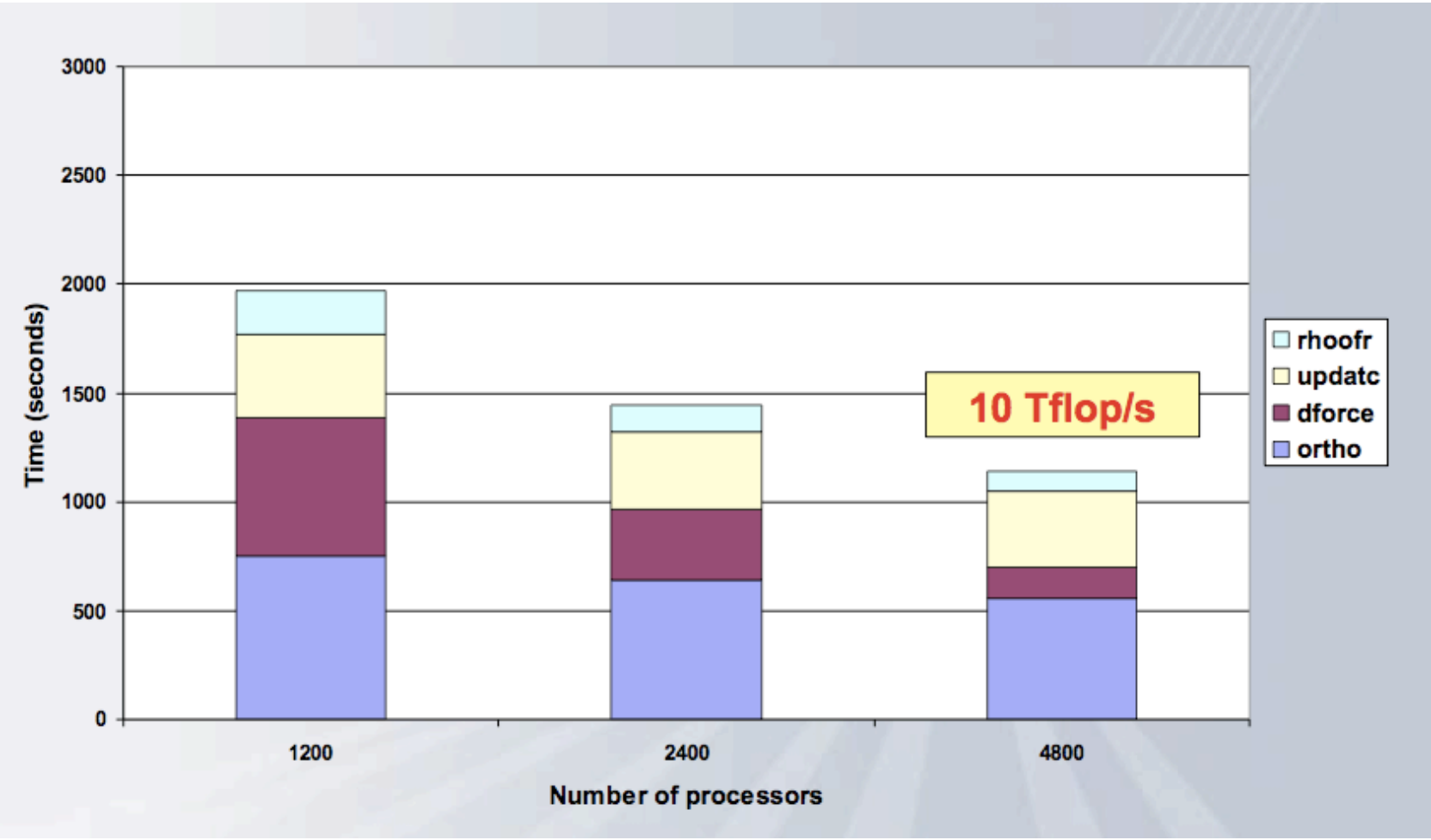
Quantum ESPRESSO

Notes on parallel computing



Parallel programming paradigms

Most modern electronic-structure code use one of the following approaches, or a combination of them:

- **MPI (Message Passing Interface) parallelization**
  Many processes are executed in parallel, one per processor, accessing their own set of variables. Access to variables on another processor is achieved via explicit calls to MPI libraries.

- **OpenMP parallelization**
  A single process spawns sub-processes (or "threads") on other processors that can access and process the variables of the code. Achieved with compiler directives and/or via call to "multi-threading" libraries like Intel MKL or IBM ESSL.

Quantum ESPRESSO exploits both MPI and OpenMP parallelization; the former is well-established, the latter is quickly stabilizing.

Comparison of parallel programming paradigms

MPI parallelization:

+ Portable to all architectures (as long as MPI libraries exist)

+ Can be very efficient (as long as MPI libraries are)

+ Can scale up to a large number of processors

– Requires significant code reorganization and rewriting

OpenMP parallelization:

+ Relatively easy to implement: requires modest code reorganization and rewriting

– Not very efficient: doesn't scale on more than a few processors. Interesting for multi-core CPU's or, in combination with MPI, for large parallel machines based on multi-core CPU's (e.g.: IBM BlueGene).

Relevant variables in PW-PP electronic-structure codes

N_w: number of plane waves (used in wavefunction expansion)
N_g: number of **G**-vectors (used in potential/charge density expansion)
N_1, N_2, N_3: dimensions of the FFT grid[1]
N_a: number of atoms in the unit cell or supercell
N_e: number of electron (Kohn-Sham) states (bands) used in the calculation
N_p: number of projectors in non-local pseudopotentials (summed over the cell)
N_k: number of **k**-points in the irreducible Brillouin Zone

Note that

$$N_w \propto V \quad \text{(size of the unit cell)}, \quad N_w \propto E_c^{3/2} \quad \text{(kinetic energy cutoff)}$$

and

$$N_g \sim N_1 \times N_2 \times N_3, \quad N_g \sim \alpha N_w$$

with $\alpha = 8$ for norm-conserving, $\alpha \sim 20$ for ultrasoft;

$$N_p \sim \beta N_a, \quad N_e \sim \gamma N_a \quad (\beta, \gamma \sim 10), \quad N_a << N_w.$$

[1] Note that there can be two distinct FFT grids with US PP

Time-consuming steps in PW-PP electronic-structure codes

- Calculation of density, $n(\mathbf{r}) = \sum |\psi(\mathbf{r})|^2$:
  FFT + linear algebra (matrix-matrix multiplication)

- Calculation of potential, $V(\mathbf{r}) = V_{xc}[n(r)] + V_H[n(\mathbf{r})]$:
  FFT + operations on real-space grid

- Iterative diagonalization (SCF) / electronic force (CP) calculation, $H\psi$ products:
  FFT + linear algebra (matrix-matrix multiplication)

- Subspace diagonalization (SCF) / Iterative orthonormalization of Kohn-Sham states (CP): diagonalization of $N_e \times N_e$ matrices + matrix-matrix multiplication

Basically: most CPU time spent in linear-algebra operations, implemented in BLAS and LAPACK libraries, and in FFT

Memory-consuming arrays in PW-PP electronic-structure codes

- **Wavefunctions** (Kohn-Sham orbitals):
  at least n_k arrays (at least 2 for CP) of size $N_w \times N_e$, plus a few more copies used as work space. If $n_k > 1$, arrays can be stored to disk and used one at the time, thus reducing memory usage, at the price of increased disk I/O

- **Charge density and potential**:
  several vectors with dimension N_g (in **G**-space) or $N_r = N_1 \times N_2 \times N_3$ (in **R**-space) each

- **Pseudopotential projectors**:
  a $N_w \times N_p$ array containing $\beta_i(\mathbf{G})$

- **Miscellaneous Matrices**:
  $N_e \times N_e$ arrays containing $\langle\psi_i|\psi_j\rangle$ products used in subspace diagonalization or iterative orthonormalization; $N_e \times N_p$ arrays containing $\langle\psi_i|\beta_j\rangle$ products

Required actions for effective parallelization of PW-PP electronic-structure codes

- **Balance load**:
  all processors should have the same load as much as possible

- **Reduce communications to the strict minimum**:
  communication is typically slower or much slower than computation!

- **Distribute all memory that grows with the size of the cell**:
  if you don't, you will run out of memory for large cells

- **Distribute all computation that grows with the size of the cell**:
  if you don't, sooner or later non-parallelized calculations will take most of the time (a practical demonstration of Amdhal's law)

The solution currently implemented in Quantum ESPRESSO introduces *several levels of parallelization*.

Parallelization level 1

- **Image** parallelization:
  Currently implemented only for NEB, but there are other cases where it could be useful. Images, i.e. points in the coordinate space, are distributed across n_{image} groups of CPUs. Example for 64 processors divided into $n_{image} = 4$ groups of 16 processors each:

  ```
  mpirun -np 64 pw.x -nimage 4 -inp input_file
  ```

  \+ potentially linear CPU scalability, limited by number of images:
  n_{image} *must be a divisor of the number of NEB images*
  \+ very modest communication requirements

  o load balancing fair to good: unlikely that all images take the same CPU

  – memory usage *does not scale* at all!

Good when usable, especially if the communication hardware is not so fast

Parallelization level 2

- **k-point** parallelization:
  k-points are distributed (if more than one) among n_{pool} *pools* of CPUs. Example for 16 processors divided into $n_{image} = 4$ image groups of $n_{pool} = 4$ pools of 4 processors each:

  ```
  mpirun -np 64 pw.x -nimage 4 -npool 4 -inp input_file
  ```

  \+ potentially linear scalability, limited by number of **k**-points:
  n_{pool} *must be a divisor of* N_k
  \+ modest communication requirements

  o load balancing fair to good

  – memory usage *does not scale* in practice

Good if one has **k**-points, especially if the communication hardware is not so fast

Parallelization level 3

- **Plane-wave** parallelization:
  wave-function coefficients are distributed among n_{PW} CPUs so that each CPU works on a subset of plane waves. The same is done on real-space grid points. This is the default parallelization scheme if other parallelization levels are not specified. In the example above:

  ```
  mpirun -np 64 pw.x -nimage 4 -npool 4 -inp input_file
  ```

  plane-wave parallelization is performed on groups of 4 processors.

  \+ high scalability of memory usage: the largest arrays are all distributed
  \+ good load balancing among different CPUs *if* n_{PW} *is a divisor of* N_3
  \+ excellent scalability, limited by the real-space 3D grid to $n_{PW} \leq N_3$
  – heavy and frequent intra-CPU communications, mainly in the 3D FFT

Best choice overall, if one has sufficiently fast communication hardware

Parallelization level 4

- **linear-algebra** parallelization:
  distribute and parallelize matrix diagonalization and matrix-matrix multiplications needed in iterative diagonalization (PWscf) or orthonormalization (CP). Introduces a *linear-algebra group* of n_{diag} processors as a subset of the plane-wave group. $n_{diag} = m^2$, where m is an integer such that $m^2 \leq n_{PW}$. Not used by default *(changed in new version)*. Should be set using the `-ndiag` or `-northo` command line option, e.g.:

  ```
  mpirun -np 64 pw.x -ndiag 25 -inp input_file
  ```

  \+ RAM is efficiently distributed: removes a major bottleneck in large systems
  \+ Increases speedup in large systems
  o Scaling tends to saturate: testing required to choose optimal value of n_{diag}

Home-made parallel algorithms are supplied, but `ScaLAPACK` works much better for serious calculations. Useful in large systems, when the RAM and CPU requirements of linear-algebra operations become a sizable share of the total.

Parallelization level 5

- **task group** parallelization:
  each plane-wave group of processors is split into n_{task} task groups of n_{FFT} processors, with $n_{task} \times n_{FFT} = n_{PW}$; each task group takes care of the FFT over N_e/n_t states. Used to extend scalability of FFT parallelization. Not set by default. Example for 4096 processors divided into $n_{image} = 8$ images of $n_{pool} = 2$ pools of $n_{PW} = 256$ processors, divided into $n_{task} = 8$ tasks of $n_{FFT} = 32$ processors each; subspace diagonalization performed on a subgroup of $n_{diag} = 144$ processors :

```
mpirun -np 4096 pw.x -nimage 8 -npool 2 -ntg 8 -ndiag 144 ...
```

Allows to extend scaling when the PW parallelization saturates: definitely needed if you want to run on more than ~ 100 processors.

Parallelization level 6

- **OpenMP** parallelization:

  explicit (with directives) parallelization of FFT is activated at compile time with preprocessing flag; currently implemented only for ESSL and FFTW. Requires an OpenMP-aware compiler,
  implicit (with libraries) parallelization with OpenMP-aware libraries: currently only ESSL and MKL

\+ Extends scaling

\- Danger of MPI-OpenMP conflicts!

To be used on large multicore machines (e.g. IBM BlueGene), in which several MPI instances running on the same node do not give very good performances.

Summary of parallelization levels in Quantum ESPRESSO

group	distributed quantities	communications	performances
image	NEB images	very low	linear CPU scaling, fair to good load balancing; does not distribute RAM
pool	$\mathbf{k}$-points	low	almost linear CPU scaling, fair to good load balancing; does not distribute RAM
plane-wave	PW, **G**-vector coefficients, **R**-space FFT arrays	high	good CPU scaling, good load balancing, distributes most RAM
task	FFT on electron states	high	improves load balancing
linear-algebra	subspace hamiltonians and constraints matrices	very high	improves scaling, distributes more RAM
OpenMP	FFT, libraries	intra-node	extends scaling on multicore machines

(Too) Frequently Asked Question
(that qualify you as a parallel newbie)

- How many processors can (or should) I use?
  It depends!

- It depends upon what??
  - Upon the kind of physical system you want to study: the larger the systems, the larger the number of processors you can or should use
  - Upon the factor driving you away from serial execution towards parallel execution: not enough RAM, too much CPU time needed, or both? If RAM is a problem, you need plane-wave parallelization
  - Upon the kind of machine you have: plane-wave parallelization is ineffective on more than $4 \div 8$ processors connected with cheap communication hardware

- So what should I do???
  You should benchmark your job with different numbers of processors, pools, image, task, linear algebra groups, taking into account the content of previous slides, until you find a satisfactory configuration for parallel execution.

Compiling and running in parallel

- **Compilation**: if you have a working parallel environment (compiler / libraries), `configure` will detect it and will attempt a parallel compilation by default. Beware serial-parallel compiler conflicts, signaled by lines like

  WARNING: serial/parallel compiler mismatch detected

  in the output of `configure`. Check for the following in `make.sys`:

  ```
  DFLAGS= ...-D__PARA -D__MPI ...
  MPIF90=mpif90 or any other parallel compiler
  ```

  For MPI-OpenMP parallelization, use
  `./configure --enable-openmp`
  verify the presence of `-D__OPENMP` in `DFLAGS`

  If `configure` doesn't detect a parallel machine as such, your parallel environment is either disfunctional (nonexistent or incomplete or not working properly) or exotic (in nonstandard locations or for strange machines) .

Compiling and running in parallel (2)

- **Execution**: beware the syntax! the total number of processor is sometimes an option of `mpirun` / `mpiexec` / whatever applies, sometimes it is set by the batch queueing system; `-nimage`, `-npool`, `-ndiag`, `-ntg` are options of Quantum ESPRESSO executables and should follow them.

  On some machines, you may need to supply input data using Quantum ESPRESSO option `-inp` *filename*; you may also need to supply optional arguments via "`mpirun -args` *'optional-arguments'*"

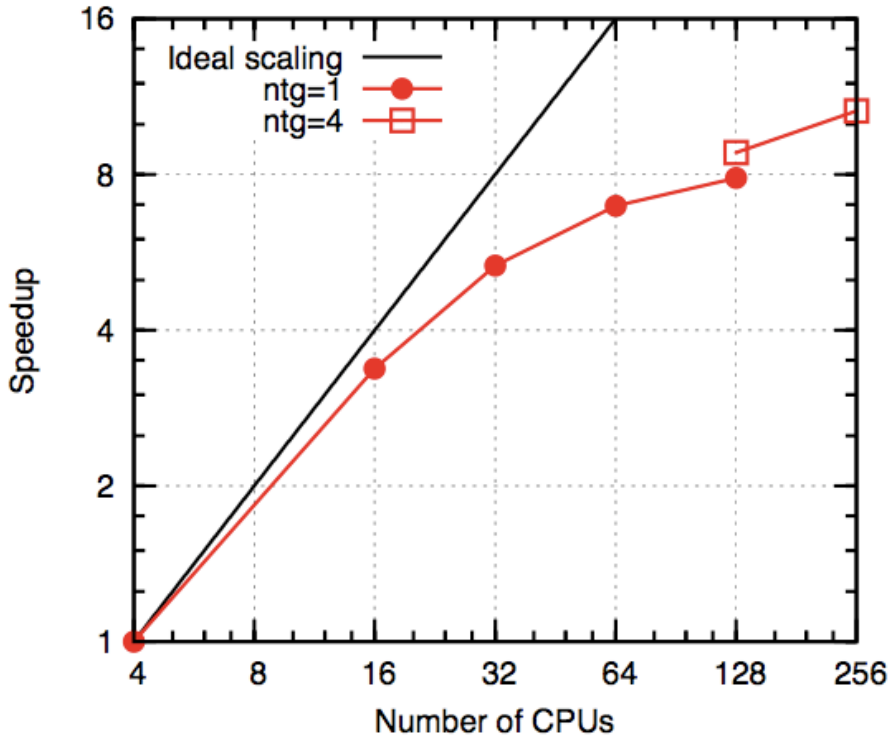
  Be careful not to make heavy I/O via NFS. Write to either a parallel file system (found only on expensive machines) or to local disks. In the latter case, check that all processors can access `pseudo_dir` and `outdir`. `PWscf`: use option `wf_collect` to collect final data files in a single place; consider using option `disk_io` to reduce I/O to the strict minimum.

  Mixed MPI-OpenMP parallelization should be used ONLY on machines (e.g. BlueGene) that allow you to control how many MPI processes run on a given node, and how many OpenMP threads.

Scalability for "small" systems

Typical speedup vs number of processors:

128 Water molecules (1024 electrons) in a cubic box 13.35 A side, Γ point.
`PWscf` code on a SP6 machine, MPI only.
ntg=1 parallelization on plane waves only
ntg=4 also on electron states

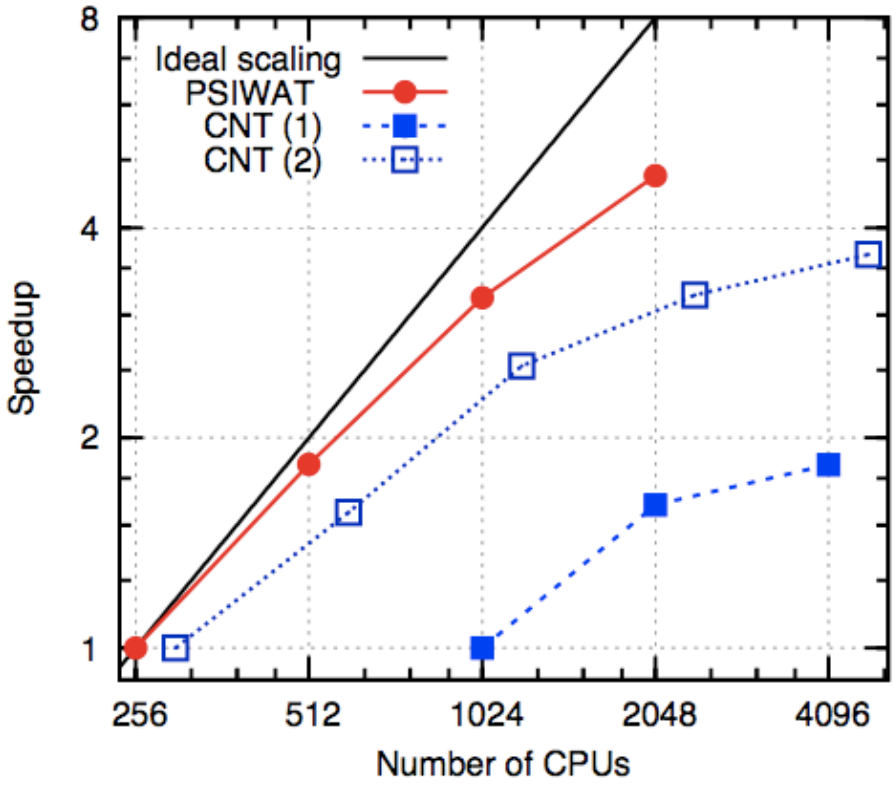


Scalability for "medium-size" systems

PSIWAT: Thiol-covered gold surface and water, 4 $\mathbf{k}-$*points,* $10.59 \times 20.53 \times 32.66$ A^3 *cell, 587 atoms, 2552 electrons.* `PWscf` *code on CRAY XT4, parallelized on plane waves, electron states,* $\mathbf{k}-$*points. MPI only.*

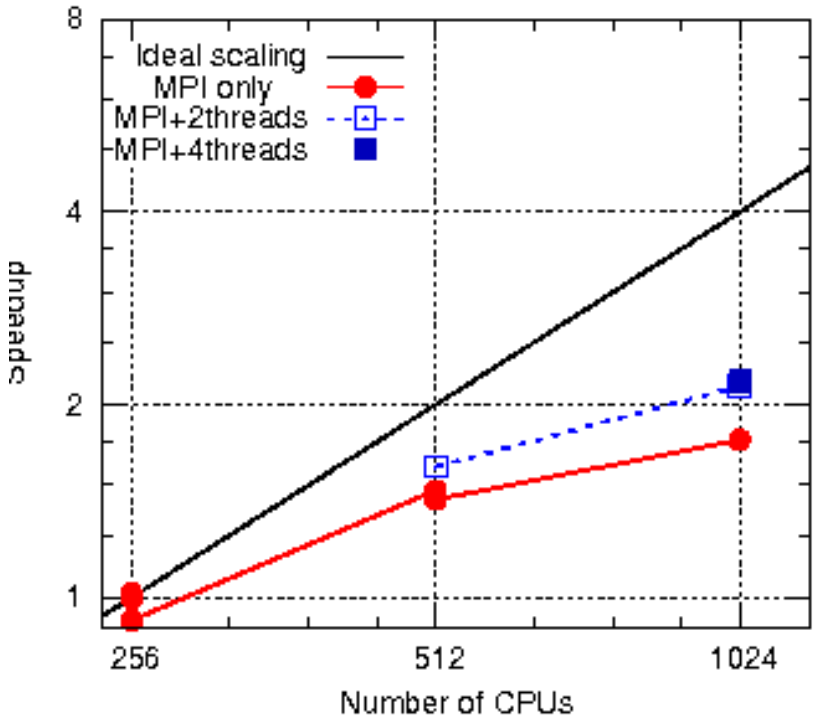
CNT(1): nanotube functionalized with porphyrins, Γ *point, 1532 atoms, 5232 electrons.* `PWscf` *code on CRAY XT4, parallelized on plane waves and electron states, MPI only.*

CNT(2): same system as for CNT(1). `CP` *code on a Cray XT3, MPI only.*



3D parallel distributed FFT is the main bottleneck. Additional parallelization levels (on electron states, on $\mathbf{k}-$points if available) allow to extend scalability.

Mixed MPI-OpenMP scalability



Fragment of an Aβ-peptide in water containing 838 atoms and 2312 electrons in a 22.1×22.9×19.9 A^3 cell, Γ-point. CP code on BlueGene/P, 4 processes per computing node.

Two models of graphene on Ir surface on a BlueGene/P using 4 processes per computing node. Execution times in s, initialization + 1 self-consistency step.

N cores	T cpu (wall) 443 atoms	T cpu (wall) 686 atoms
16384	740(772)	2861 (2915)
32768	441(515)	1962 (2014)
65536	327(483)	751 (1012)

(the large difference between CPU and wall time is likely due to I/O)