Optimization and Parallelization of a force field for silicon using OpenMP

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The force field by Lenosky and coworkers is the latest force field for silicon which is one of the most studied materials. It has turned out to be highly accurate in a large range of test cases. The optimization and parallelization of this force field using OpenMp and Fortan90 is described here. The optimized program allows us to handle a very large number of silicon atoms in large scale simulations. Since all the parallelization is hidden in a single subroutine that returns the total energies and forces, this subroutine can be called from within a serial program in an user friendly way.

I. PROGRAM SURVEY

Title of program: siliconiap
Computer hardware and operating system: Any shared memory computer running under Unix or Linux
Programming Language: Fortran90 with OpenMP compiler directives
Memory requirements: roughly 150 words per atom
No. of bits in a word: 64
No. of processors used: tested on up to 4 processors
Has the code been vectorized or parallelized: Parallelized with the OpenMP
No. of bytes in distributed program, including test data, etc: 50 000
Distribution format: Compressed tar file
Keywords: Silicon, Interatomic potential, Force field, Molecular dynamics
Nature of physical problem: condensed matter physics
Method of solution: Interatomic potential
Restrictions on the complexity of the problem: None
Typical running time: 30 µsec per step and per atom on a Compaq DEC Alpha
Unusual features of the program: None

II. INTRODUCTION

Due to its technological importance, silicon is one of the most studied materials. For small system sizes ab-initio density functional calculations [1] are the preferred approach. Unfortunately this kind of calculation becomes unfeasible for larger systems required to study problems such as interfaces or extended defects. For this type of calculations one resorts to force fields which are several orders of magnitude faster. Recent progress in the development of force fields has demonstrated that they can be a reliable tool for such studies. A highly accurate silicon force field has been developed by Lenosky and coworkers [6]. Its transferability has been demonstrated by extensive tests containing both bulk and cluster systems [6]. Its accuracy is in part due to the fact that second nearest neighbor interactions are included. This makes it unfortunately somewhat slower than force fields containing only nearest neighbor interactions. In the following a highly optimized parallel implementation of this force field will be presented that allows large scale calculations with this force field. The parallelization is achieved by using OpenMP, an emerging industry standard for medium size shared memory parallel computers.

Molecular dynamics calculations [2] have also been parallelized on distributed memory supercomputers [3]. This approach is considerably more complex than the one presented here. Since few researches have access to massively parallel supercomputers and are willing to overcome the complexities of doing molecular dynamics on such machines, medium scale parallelization [4] of molecular dynamics has an important place in practice.
III. CALLING THE SUBROUTINE

User friendliness was one of the major design goals in the development of this routine. Using Fortran90 made it possible to hide all the complexities in an object oriented fashion from the user. The calling sequence is just

\[
\text{call lenosky(nat, alat, rxyz, fxyz, ener, coord, ener_var, coord_var, count)}
\]

On input the user has to specify the number of atoms, \( \text{nat} \), the vector \( \text{alat} \) containing the 3 lattice constant of the orthorhombic periodic volume and the atomic positions \( \text{rxyz} \). The program then returns the total energy, \( \text{ener} \), the forces, \( \text{fxyz} \), the average coordination number, the variation of the energy per atom and of the coordination number as well as an counter that is increased in each call. In particular the user has not to supply any Verlet list.

Since the calculation of the forces is typically much more expensive than the update of the atomic positions in molecular dynamics or geometry optimizations, we expect that the subroutine will be called in most cases from within a serial program. In case the user is on a shared memory machine the subroutine will then nevertheless be executed in parallel if the program is compiled with the appropriate OpenMP options.

In addition the subroutine can of course also be used on a serial machine. In this case all the parallelization directives are considered by the compiler to be comments.

IV. CALCULATION OF THE VERLET LIST

The Verlet list gives all the atoms that are contained within the potential cutoff distance \( \text{cut} \) of any given atom. Typically the Verlet list consists of two integer arrays. The first array, called \( \text{lsta} \) in this work, points to the first/last neighbor position in the second array \( \text{lstb} \) that contains the numbering of the atoms that are neighbors. A straightforward implementation for a non-periodic system containing \( \text{nat} \) atoms is shown below. In this simple case the search through all atoms is sequential with respect to their numbering and it is redundant to give both the starting positions \( \text{lsta}(1, \text{iat}) \) and the ending position \( \text{lsta}(2, \text{iat}) \), since \( \text{lsta}(1, \text{iat}) = \text{lsta}(2, \text{iat} - 1) + 1 \). But in the more complicated linear scaling algorithm to be presented below, both will be needed.

\[
\begin{align*}
\text{indc} &= 0 \\
\text{do } 10 \text{ iat}=1, \text{nat} \\
\quad \text{starting position} \\
\quad &\text{lsta}(1, \text{iat}) = \text{indc} + 1 \\
\quad \text{do } 20 \text{ jat}=1, \text{nat} \\
\quad &\text{if } (\text{jat}.\ne.\text{iat}) \text{ then} \\
\quad &\quad \text{xrel1} = \text{rxyz}(1, \text{jat}) - \text{rxyz}(1, \text{iat}) \\
\quad &\quad \text{xrel2} = \text{rxyz}(2, \text{jat}) - \text{rxyz}(2, \text{iat}) \\
\quad &\quad \text{xrel3} = \text{rxyz}(3, \text{jat}) - \text{rxyz}(3, \text{iat}) \\
\quad &\quad \text{rr2} = \text{xrel1}**2 + \text{xrel2}**2 + \text{xrel3}**2 \\
\quad &\quad \text{if } (\text{rr2} \leq \text{cut}**2) \text{ then} \\
\quad &\quad &\text{indc} = \text{indc} + 1 \\
\quad &\text{nearest neighbor numbers} \\
\quad &\text{lstb}(\text{indc}) = \text{jat} \\
\quad &\text{endif} \\
\quad &20 \text{ continue} \\
\quad \text{ending position} \\
\quad &\text{lsta}(2, \text{iat}) = \text{indc} \\
\quad &10 \text{ continue}
\end{align*}
\]

This straightforward implementations has a quadratic scaling with respect to the numbers of atoms. Due to this scaling the calculation of the Verlet list starts to dominate the linear scaling calculation of the energies and forces for system sizes of more than 10 000 atoms. It is therefore good practice to calculate the Verlet list with a modified algorithm that has linear scaling as well.

To do this one first subdivides the system into boxes that have a side length that is equal to or larger than \( \text{cut} \) and then finds all the atoms that are contained in each box. The CPU time for this first step is less than 1 percent
of the entire Verlet list calculation. Hence this part was not parallelized. It could significantly affect the parallel performance according to Amdahl's law only if more than 50 processors are used. The largest SMP machines at our disposal had however only 4 processors.

To implement periodic boundary conditions all atoms within a distance cut of the boundary of the periodic volume are replicated on the opposite part as shown in Figure 1. This part is equally well less than 1 percent of the CPU time for the Verlet list for a 8000 atom system. Being a surface term it becomes even smaller for larger systems. Consequently it wasn’t parallelized either.

After these two preparing steps one has to search only among all the atoms in the reference cell containing the atom for which one wants to find its neighbors as well as all the atoms in the cells neighboring this reference cell (26 cells in 3 dimensions). This implies that starting and ending positions lsta for the atoms 1 to nat are not calculated in a sequential way, necessitating, as mentioned before, separate starting and ending positions in the array lsta. The corresponding parallel code is shown below. The indices l1, l2, l3 refer to the cells, icell(l1, l2, l3, 0) contains the number of atoms in cell l1, l2, l3 and icell(l1, l2, l3, *) their numbering. The array rel saves the relative positions and distances that will again be needed in the loop calculating the forces and energies. Each thread has its own starting position iam * myspace + 1 in the shared memory space lstb and these starting positions are uniformly distributed. This approach allows the different threads to work independently. The resulting speedup is much higher than the one that one would obtain by calculating in the parallel version an array lstb that is identical to the one from the serial version. If there are on the average more neighbors than expected (24 by default) the allocated space becomes too small. In this case the array lstb is deallocated and a new larger version is allocated. This check for sufficient memory requires some minimal amount of coordination among the processors and is implemented by a critical section. If a reallocation is necessary, a message is written into an file to alert the user of the inefficiency due to the need of a second calculation of the Verlet list.

```fortran
allocate(lsta(2,nat))
nnbrx=24
2345  nnbrx=3*nnbrx/2
allocate(lstb(nnbrx*nat),rel(5,nnbrx*nat))
indlstx=0

!$omp parallel &
!$omp private(iat,cut2,iam,ii,indlst,l1,l2,l3,myspace,npr) &
!$omp shared(indlstx,nat,nn,nnbrx,ncx,l11,l12,l13,icell,lsta,lstb,lay, &
!$omp rel,rxyz,cut,myspaceout)
```

FIG. 1. Illustration of the construction of the cell structure necessary for a linear scaling calculation of the nearest neighbor list for a 2-dimensional case. The periodic volume is indicated by the dark background. The bright cells are replicated dark cells.
npr=1

iam=0

cut2=cut**2

myspace=(nat*nnbrx)/npr

if (iam.eq.0) myspaceout=myspace

! Verlet list, relative positions
ndlst=0

6000,13=0,113-1
6000,12=0,112-1
6000,11=0,111-1
6000,i=1,icell(0,11,12,13)
iat=icell(ii,11,12,13)

indeat=iam*myspace+indlst+1

call sublistiat(iat,nn,ncx,111,112,113,11,12,13,myspace, &
    rxyz,icell,lstb(iam*myspace+1),lay,rel(1,iam*myspace+1),cut2,indlst)

endlst=iam*myspace+indlst

6600 continue
6000 continue

!$omp critical

indlstx=max(indlstx,indlst)

!$omp end critical

!$omp end parallel

if (indlstx.gt.myspaceout) then
    write(10,*) count,'NNBRX too small', nnbrx
    deallocate(lstb,rel)
    goto 2345
endif

subroutine sublistiat(iat,nn,ncx,111,112,113,11,12,13,myspace, &
    rxyz,icell,lstb,lay,rel,cut2,indlst)

implicit real*8 (a-h,o-z)
dimension rxyz(3,nn),lay(nn),icell(0:ncx,-1:ll1,-1:ll2,-1:ll3), &
lstb(0:myspace-1),rel(5,0:myspace-1)

do 6363,k3=ll3-1,ll3+1
    do 6363,k2=ll2-1,ll2+1
        do 6363,k1=ll1-1,ll1+1
            do 6363,jj=1,icell(0,k1,k2,k3)
                jat=icell(jj,k1,k2,k3)
                if (jat.eq.iat) goto 6363
                xrel= rxyz(1,iat)-rxyz(1,jat)
                yrel= rxyz(2,iat)-rxyz(2,jat)
                zrel= rxyz(3,iat)-rxyz(3,jat)
                rr2=xrel**2 + yrel**2 + zrel**2
                if (rr2 .le. cut2) then
indlst = min(indlst, myspace-1)
lstb(indlst) = lay(jat)

\[ tt = \sqrt{rr2} \]

tti = 1.d0/tt
rel(1, indlst) = xrel * tti
rel(2, indlst) = yrel * tti
rel(3, indlst) = zrel * tti
rel(4, indlst) = tt
rel(5, indlst) = tti

indlst = indlst + 1

endif
6363 continue
return
end

V. CALCULATION OF THE ENERGIES AND FORCES

The computationally most important part taking some 80 percent of the CPU time is the calculation of the energies and forces. The energy expression for the Lenosky force field is given by

\[ E = \sum_{i,j} \phi(r_{ij}) + \sum_{i} U \left( \sum_{j} \rho(r_{ij}) + \sum_{j,k} f(r_{ik}) g(\cos(\theta_{jik})) \right) \]  

All the functions (\(\phi\), \(U\), \(\rho\), \(f\), \(g\)) in this energy expression are given by cubic splines. The subroutine for evaluating the cubic spline is listed below. The case that the argument is outside the cubic spline interval \([tmin, tmax]\) is rare and unimportant for performance considerations. The important cubic spline case is characterized by many dependencies. In the case of such dependencies the latency of the functional unit pipeline comes into play and reduces the attainable speed. A latency of some 20 cycles comes from the first two statements (tt=(x-tmin)*hi ; klo=tt) alone, requiring arithmetic operations and a floating point to integer conversion. For this reason the calculation of tt was taken out of the (most likely occurring) else block to overlap its evaluation with the evaluation of the if clauses. To further speed up the evaluation of the splines the structure of the energy expression was exploited. In the computationally most important loop over \(j\) and \(k\) two splines (\(f(r_{ik})\) and \(g(\cos(\theta_{jik}))\)) have to be evaluated. Inlining by hand the subroutine splint for both evaluations and calculating alternatingly one step of the first spline evaluation and one step of the second spline evaluation introduces two independent streams. This reduces the effect of latencies and boosts speed. Compilers are not able to do these complex type of optimizations. The best performance after these optimizations was obtained with low level compiler optimization flags (-O3 -qarch=pwr3 -qtune-pwr3 on IBM Power3, -O2 on the Compaq DEC Alpha, -O2 -xW on Intel Pentium4)

subroutine splint(ya,y2a,tmin,tmax,hsixth,h2sixth,hi,n,x,y,yp)
implicit real*8 (a-h,o-z)
dimension y2a(0:n-1),ya(0:n-1)

! interpolate if the argument is outside the cubic spline interval \([tmin,tmax]\)
\[ tt = (x-tmin)*hi \]
if (x.lt.tmin) then
\[ yp = hi*(ya(1)-ya(0)) - & ( y2a(1)+2.d0*y2a(0) )*hsixth \]
y = ya(0) + (x-tmin)*yp
else if (x.gt.tmax) then
\[ yp = hi*(ya(n-1)-ya(n-2)) + & ( 2.d0*y2a(n-1)+y2a(n-2) )*hsixth \]
y = ya(n-1) + (x-tmax)*yp
else
! otherwise evaluate cubic spline

else
The final single processor performance for the entire subroutine is 460 Mflops on a Compaq DEC Alpha at 833 MHz, 300 Mflops on a IBM Power3 at 350 MHz and 550 Mflops on a Pentium 4. In order to obtain a high parallel speedup in this central part of the subroutine the threads are completely decoupled. This was done by introducing private copies for each thread to accumulate the energies `tener` and forces `txyz`. The global energy and force are summed up in an additional loop at the end of the parallel region in a critical section.

```fortran
klo=tt
khi=klo+1
ya_klo=ya(klo)
y2a_klo=y2a(klo)
b=tt-klo
a=1.d0-b
ya_khi=ya(khi)
y2a_khi=y2a(khi)
b2=b*b
y=a*ya_klo
yp=ya_khi-ya_klo
a2=a*a
cof1=a2-1.d0
cof2=b2-1.d0
y=y+b*ya_khi
yp=hi*yp
cof3=3.d0*b2
cof4=3.d0*a2
cof1=a*cof1
cof2=b*cof2
cof3=cof3-1.d0
cof4=cof4-1.d0
yt1=cof1*y2a_klo
yt2=cof2*y2a_khi
ypt1=cof3*y2a_khi
ypt2=cof4*y2a_klo
y=y + (yt1+yt2)*h2sixth
yp=yp + ( ypt1 - ypt2 )*hsixth
endif
return
end

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```
allocate(txyz(3,nat),f2ij(3,npjx),f3ij(3,npjx),f3ik(3,npjx))

if (iam.eq.0) then
  ener=0.d0
  ener2=0.d0
  coord=0.d0
  coord2=0.d0
  do 121,iat=1,nat
    fxyz(1,iat)=0.d0
    fxyz(2,iat)=0.d0
  121  fxyz(3,iat)=0.d0
  endif

  lot=nat/npr+.999999999999d0
  iat1=iam*lot+1
  iat2=min((iam+1)*lot,nat)
  call subfeniat(iat1,iat2,nat,lsta,lstb,rel,ener,ener2, &
                 coord,coord2,nnbrx,txyz,f2ij,f3ij,f3ik,istop)

ener=ener+tener
ener2=ener2+tener2
coord=coord+tcoord
coord2=coord2+tcoord2
istopg=istopg+istop

do 8093,iat=1,nat
  fxyz(1,iat)=fxyz(1,iat)+txyz(1,iat)
  fxyz(2,iat)=fxyz(2,iat)+txyz(2,iat)
  fxyz(3,iat)=fxyz(3,iat)+txyz(3,iat)
8093 continue

deallocate(txyz,f2ij,f3ij,f3ik)

else

  iat1=1
  iat2=nat
  allocate(f2ij(3,npjx),f3ij(3,npjx),f3ik(3,npjx))
  call subfeniat(iat1,iat2,nat,lsta,lstb,rel,ener,ener2, &
                 coord,coord2,nnbrx,fxyz,f2ij,f3ij,f3ik,istop)
  deallocate(f2ij,f3ij,f3ik)
endif

! SERIAL CASE

ener_var=ener2/nat-(ener/nat)**2
coord_var=coord2/nat-coord**2

deallocate(rxyz,icell,lay,lsta,lstb,rel)

end

subroutine subfeniat(iat1,iat2,nat,lsta,lstb,rel,tener,tener2, &
tcoord, tcoord2, nnbrx, txyz, f2ij, npjx, f3ij, npjkx, f3ik, istop)
implicit real*8 (a-h, o-z)
dimension lsta(2, nat), lstb(nnbrx*nat), rel(5, nnbrx*nat), txyz(3, nat)
dimension f2ij(3, npjx), f3ij(3, npjkx), f3ik(3, npjkx)

initialize data ........

! create temporary private scalars for reduction sum on energies and
tener=0.d0
tener2=0.d0
tcoord=0.d0
tcoord2=0.d0
istop=0
do 121, iat=1, nat
  txyz(1, iat)=0.d0
  txyz(2, iat)=0.d0
  txyz(3, iat)=0.d0
121

! calculation of forces, energy

do 1000, iat=iat1, iat2
  dens2=0.d0
  dens3=0.d0
  jcnt=0
  jkcnt=0
  coord_iat=0.d0
  ener_iat=0.d0
  do 2000, jbr=1, lsta(1, iat), lsta(2, iat)
    jat=lstb(jbr)
    jcnt=jcnt+1
    if (jcnt.gt.npjx) then
      write(6,*) 'WARNING: enlarge npjx'
      istop=1
    endif
    fxij=rel(1, jbr)
    fyij=rel(2, jbr)
    fzij=rel(3, jbr)
    rij=rel(4, jbr)
    sij=rel(5, jbr)

! coordination number calculated with soft cutoff between first and
! second nearest neighbor
if (rij.le.2.36d0) then
  coord_iat=coord_iat+1.d0
else if (rij.ge.3.83d0) then
  coord_iat=coord_iat+1.d0
else
  x=(rij-2.36d0)*(1.d0/(3.83d0-2.36d0))
  coord_iat=coord_iat+(2*x+1.d0)*(x-1.d0)**2
endif

! pairpotential term
  call splint(cof_phi, dof_phi, tmin_phi, tmax_phi, &
        hsixth_phi, h2sixth_phi, hi_phi, 10, rij, e_phi, ep_phi)
  ener_iat=ener_iat+(e_phi*.5d0)
txyz(1,iat)=txyz(1,iat)-fxij*(ep_phi*.5d0)
txyz(2,iat)=txyz(2,iat)-fyij*(ep_phi*.5d0)
txyz(3,iat)=txyz(3,iat)-fzij*(ep_phi*.5d0)
txyz(1,jat)=txyz(1,jat)+fxij*(ep_phi*.5d0)
txyz(2,jat)=txyz(2,jat)+fyij*(ep_phi*.5d0)
txyz(3,jat)=txyz(3,jat)+fzij*(ep_phi*.5d0)

! 2 body embedding term
    call splint(cof_rho,dof_rho,tmin_rho,tmax_rho, &
               hsi6th_rho,h2si6th_rho,hi_rho,11,rij,rho,rhop)
dens2=dens2+rho
f2ij(1,jcnt)=fxij*rhop
f2ij(2,jcnt)=fyij*rhop
f2ij(3,jcnt)=fzij*rhop

! 3 body embedding term
    call splint(cof_fff,dof_fff,tmin_fff,tmax_fff, &
               hsi6th_fff,h2si6th_fff,hi_fff,10,rij,fij,fijp)
do 3000,kbr=lsta(1,iat),lsta(2,iat)
kat=lstb(kbr)
if (kat.lt.jat) then
jkcnt=jkcnt+1
if (jkcnt.gt.npjkx) then
write(6,*) 'WARNING: enlarge npjkx'
istop=1
endif

! begin optimized version
    rik=rel(4,kbr)
    if (rik.gt.tmax_fff) then
fikp=0.d0 ; fik=0.d0
    gijk=0.d0 ; gjikp=0.d0 ; sik=0.d0
    costheta=0.d0 ; fxik=0.d0 ; fyik=0.d0 ; fzik=0.d0
else if (rik.lt.tmin_fff) then
    fxik=rel(1,kbr)
    fyik=rel(2,kbr)
    fzik=rel(3,kbr)
    costheta=fxij*fxik+fyij*fyik+fzij*fzik
    sik=rel(5,kbr)
    fikp=hi_fff*(cof_fff(1)-cof_fff(0)) - &
         (dof_fff(1)+2.d0*dof_fff(0))*h6th_fff
    fik=cof_fff(0) + (rik-tmin_fff)*fikp
    tt_fff=(costheta-tmin_fff)*hi_fff
    if (costheta.gt.tmax_fff) then
gijk=hi_fff*(cof_fff(8-1)-cof_fff(8-2)) + &
     (2.d0*dof_fff(8-1)+dof_fff(8-2))*h6th_fff
    gjik=cof_fff(8-1) + (costheta-tmax_fff)*gijkp
else
    klo_fff=tt_fff
    khi_fff=klo_fff+1
    cof_fff_klo=cof_fff(klo_fff)
    dof_fff_klo=dof_fff(klo_fff)
    b_fff=tt_fff-klo_fff
    a_fff=1.d0-b_fff
    cof_fff_khi=cof_fff(khi_fff)

enddo
dof_ggg_khi = dof_ggg(khi_ggg)
b2_ggg = b_ggg * b_ggg
gjik = a_ggg * cof_ggg_klo
gjkp = cof_ggg_khi - cof_ggg_klo
a2_ggg = a_ggg * a_ggg
cof1_ggg = a2_ggg - 1.d0
cof2_ggg = b2_ggg - 1.d0
gjik = gjik + b_ggg * cof_ggg_khi
gjkp = hi_ggg * gjkp
cof3_ggg = 3.d0 * b2_ggg
cof4_ggg = 3.d0 * a2_ggg
cof1_ggg = a_ggg * cof1_ggg
cof2_ggg = b_ggg * cof2_ggg
cof3_ggg = cof3_ggg - 1.d0
cof4_ggg = cof4_ggg - 1.d0
yt1_ggg = cof1_ggg * dof_ggg_klo
ty2_ggg = cof2_ggg * dof_ggg_khi
ypt1_ggg = cof3_ggg * dof_ggg_khi
ypt2_ggg = cof4_ggg * dof_ggg_klo
gjik = gjik + (yt1_ggg + yt2_ggg) * h2sixth_ggg
gjkp = gjkp + (ypt1_ggg - ypt2_ggg) * hsixth_ggg
endif
else
fxik = rel(1, kbr)
tt_fff = rik - tmin_fff
costheta = fxij * fxik
fyik = rel(2, kbr)
tt_fff = tt_fff * hi_fff
costheta = costheta + fyij * fyik
fzik = rel(3, kbr)
klo_fff = tt_fff
costheta = costheta + fzij * fzik
sik = rel(5, kbr)
tt_ggg = (costheta - tmin_ggg) * hi_ggg
if (costheta.gt.tmax_ggg) then
gjkp = hi_ggg * (cof_ggg(8-1) - cof_ggg(8-2)) + &
(2.d0 * dof_ggg(8-1) + dof_ggg(8-2)) * hsixth_ggg
gjik = cof_ggg(8-1) + (costheta - tmax_ggg) * gjkp
khi_fff = klo_fff + 1
cof_fff_klo = cof_fff(klo_fff)
dof_fff_klo = dof_fff(klo_fff)
b_fff = tt_fff - klo_fff
a_fff = 1.d0 - b_fff
cof_fff_khi = cof_fff(khi_fff)
dof_fff_khi = dof_fff(khi_fff)
b2_fff = b_fff * b_fff
fik = a_fff * cof_fff_klo
fikp = cof_fff_khi - cof_fff_klo
a2_fff = a_fff * a_fff
cof1_fff = a2_fff - 1.d0
cof2_fff = b2_fff - 1.d0
fik = fik + b_fff * cof_fff_khi
fikp = hi_fff * fikp
cof3_fff = 3.d0 * b2_fff
cof4_fff = 3.d0 * a2_fff
cof1_fff = a_fff * cof1_fff
cof2_fff = b_fff * cof2_fff
cof3_fff = cof3_fff - 1.d0
cof4_fff = cof4_fff - 1.d0
yt1_fff = cof1_fff * dof_fff_klo
yt2_fff = cof2_fff * dof_fff_khi
ypt1_fff = cof3_fff * dof_fff_khi
ypt2_fff = cof4_fff * dof_fff_klo
fik = fik + (yt1_fff + yt2_fff) * h2sixth_fff
fikp = fikp + (ypt1_fff - ypt2_fff) * hsixth_fff
else
  klo_ggg = tt_ggg
  khi_ggg = klo_ggg + 1
  khi_fff = klo_fff + 1
  cof_ggg_klo = cof_ggg(klo_ggg)
  cof_fff_klo = cof_fff(klo_fff)
  dof_ggg_klo = dof_ggg(klo_ggg)
  dof_fff_klo = dof_fff(klo_fff)
  b_ggg = tt_ggg - klo_ggg
  b_fff = tt_fff - klo_fff
  a_ggg = 1.d0 - b_ggg
  a_fff = 1.d0 - b_fff
  cof_ggg_khi = cof_ggg(khi_ggg)
  cof_fff_khi = cof_fff(khi_fff)
  dof_ggg_khi = dof_ggg(khi_ggg)
  dof_fff_khi = dof_fff(khi_fff)
  b2_ggg = b_ggg * b_ggg
  b2_fff = b_fff * b_fff
  gjik = a_ggg * cof_ggg_klo
  fik = a_fff * cof_fff_klo
  gjikp = cof_ggg_khi - cof_ggg_klo
  fikp = cof_fff_khi - cof_fff_klo
  a2_ggg = a_ggg * a_ggg
  a2_fff = a_fff * a_fff
  cof1_ggg = a2_ggg - 1.d0
  cof1_fff = a2_fff - 1.d0
  cof2_ggg = b2_ggg - 1.d0
  cof2_fff = b2_fff - 1.d0
  gjik = gjik + b_ggg * cof_ggg_khi
  fik = fik + b_fff * cof_fff_khi
  gjikp = h1_ggg * gjikp
  fikp = h1_fff * fikp
  cof3_ggg = 3.d0 * b2_ggg
  cof3_fff = 3.d0 * b2_fff
  cof4_ggg = 3.d0 * a2_ggg
  cof4_fff = 3.d0 * a2_fff
  cof1_ggg = a_ggg * cof1_ggg
  cof1_fff = a_fff * cof1_fff
  cof2_ggg = b_ggg * cof2_ggg
  cof2_fff = b_fff * cof2_fff
  cof3_ggg = cof3_ggg - 1.d0
  cof3_fff = cof3_fff - 1.d0
  cof4_ggg = cof4_ggg - 1.d0
  cof4_fff = cof4_fff - 1.d0
  yt1_ggg = cof1_ggg * dof_ggg_klo
  yt1_fff = cof1_fff * dof_fff_klo
  yt2_ggg = cof2_ggg * dof_ggg_khi
  yt2_fff = cof2_fff * dof_fff_khi
yt2_fff=cof2_fff*dof_fff_khi
ypt1_ggg=cof3_ggg*dof_ggg_khi
ypt1_fff=cof3_fff*dof_fff_khi
ypt2_ggg=cof4_ggg*dof_ggg_klo
ypt2_fff=cof4_fff*dof_fff_klo
gjik=gjik + (yt1_ggg+yt2_ggg)*h2sixth_ggg
fik=fik + (yt1_fff+yt2_fff)*h2sixth_fff
gjikp=gjikp + ( ypt1_ggg - ypt2_ggg )*hsixth_ggg
fikp=fikp + ( ypt1_fff - ypt2_fff )*hsixth_fff
endif
endif
! end optimized version

tt=fij*fik
dens3=dens3+tt*gjik

t1=fijp*fik*ggik

t2=sij*(tt*ggikp)
f3ij(1,jkcnt)=fxij*t1 + (fxik-fxij*costheta)*t2
f3ij(2,jkcnt)=fyij*t1 + (fyik-fyij*costheta)*t2
f3ij(3,jkcnt)=fzij*t1 + (fzik-fzij*costheta)*t2

t3=fikp*fij*ggik

t4=sik*(tt*ggikp)
f3ik(1,jkcnt)=fxik*t3 + (fxij-fxik*costheta)*t4
f3ik(2,jkcnt)=fyik*t3 + (fyij-fyik*costheta)*t4
f3ik(3,jkcnt)=fzik*t3 + (fzik-fzik*costheta)*t4
endif

3000 continue
2000 continue
dens=dens2+dens3
call splint(cof_uuu,dof_uuu,tmin_uuu,tmax_uuu, &
hsixth_uuu,h2sixth_uuu,hi_uuu,8,dens,e_uuu,ep_uuu)
ener_iat=ener_iat+e_uuu

! Only now ep_uu is known and the forces can be calculated, lets loop again
jcnt=0
jkcnt=0
do 2200,jbr=1sta(1,iat),1sta(2,iat)
jat=1stb(jbr)
jcnt=jcnt+1

! 3 body embedding term

do 3300,kbr=1sta(1,iat),1sta(2,iat)
kat=1stb(kbr)
if (kat.lt.jat) then
jkcnt=jcnt+1
txyz(1,iat)=txyz(1,iat)-ep_uuu*f2ij(1,jcnt)
txyz(2,iat)=txyz(2,iat)-ep_uuu*f2ij(2,jcnt)
txyz(3,iat)=txyz(3,iat)-ep_uuu*f2ij(3,jcnt)
txyz(1,jat)=txyz(1,jat)+ep_uuu*f2ij(1,jcnt)
txyz(2,jat)=txyz(2,jat)+ep_uuu*f2ij(2,jcnt)
txyz(3,jat)=txyz(3,jat)+ep_uuu*f2ij(3,jcnt)
! 3 body embedding term

t_xyz(3, iat) = t_xyz(3, iat) - \epsilon_{uuu} * (f_{3ij}(3, jkcnt) + f_{3ik}(3, jkcnt))

\begin{align*}
t_{xyz}(1, jat) &= t_{xyz}(1, jat) + \epsilon_{uuu} \cdot f_{3ij}(1, jkcnt) \\
t_{xyz}(2, jat) &= t_{xyz}(2, jat) + \epsilon_{uuu} \cdot f_{3ij}(2, jkcnt) \\
t_{xyz}(3, jat) &= t_{xyz}(3, jat) + \epsilon_{uuu} \cdot f_{3ij}(3, jkcnt) \\
t_{xyz}(1, kat) &= t_{xyz}(1, kat) + \epsilon_{uuu} \cdot f_{3ik}(1, jkcnt) \\
t_{xyz}(2, kat) &= t_{xyz}(2, kat) + \epsilon_{uuu} \cdot f_{3ik}(2, jkcnt) \\
t_{xyz}(3, kat) &= t_{xyz}(3, kat) + \epsilon_{uuu} \cdot f_{3ik}(3, jkcnt)
\end{align*}

endif

3300 continue
2200 continue

tener = tener + ener_iat

tener2 = tener2 + ener_iat**2

tcoord = tcoord + coord_iat
	coord2 = tcoord2 + coord_iat**2

1000 continue

return
end

In addition to the energy and the forces the program still returns the coordination number as well as the variance of the energy per atom and the coordination number. The coordination number is calculated using a soft cutoff between the first and second nearest neighbor distance. These extra calculations are very cheap and not visible as an increase in the CPU time.

VI. PARALLEL PERFORMANCE RESULTS

Table I shows the final overall speedups obtained by the program. The results were obtained for an 8000 atom system, but the CPU time per call and atom is nearly independent of system size.

Table I. Timings in µsec for a combined evaluation of the forces and the energy per particle as well as the corresponding speedups (in parentheses) on an IBM SP3 based on a 375 MHz Power3 processor, on a Compaq SC 232 based on a 833Mhz EV67 processor and on an Intel Pentium4 biprocessor at 2 GHz

| number of processors | IBM Power3 | Compaq EV67 | Intel P4 |
|----------------------|------------|-------------|----------|
| 1                    | 46         | 30          | 25       |
| 2                    | 21 (1.9)   | 16 (1.9)    | 13 (1.9) |
| 4                    | 13 (3.5)   | 8.6 (3.5)   |          |
| 8                    | 7.7 (6.0)  |             |          |
Obtaining such high speedups was not straightforward. Only the Compaq Fortran90 compiler was able to use in the original version of the program the OpenMP 'parallel do' directive to obtain a good speedup. Both the IBM compiler and the Intel compiler failed. In order to get the performances of Table I, it was necessary to encapsulate the workload of the different threads into the subroutines 'sublstias' and 'subfen', which amounts to doing the parallelization quasi by hand. Using allocatable arrays in connection with OpenMP turned also out to be tricky. Because of these problems, the parallelization was much more painful that one might expect for a shared memory model.

VII. CONCLUSIONS

The results show that simulations for very large silicon systems are feasible on relatively cheap serial or parallel computers accessible to a large number of researches.

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[1] W. Kohn, Rev. Mod. Phys., 718, 1253 (1999)
[2] M. Allen and D. Tildesley, Computer Simulations of Liquids, Claredon Press, Oxford, 1987
[3] D. Beazley and P. Lomdahl, Parallel Computing 20, 173 (1994);
[4] R. Couturier and C. Chipot, Comp. Phys. Commun. 14, 49 (2000);
[5] R. Hockney and J. Eastwood, Computer Simulations using Particles, McGraw Hill, New York, 1981
[6] T. J. Lenosky, B. Sadigh, E. Alonso, V. Bulatov, T. Diaz de la Rubia, J. Kim, A.F. Voter adn J. D. Kress, Modelling Simul. Mater. Sci. Eng. 8, 825 (2000);
[7] S. Goedecker, A. Hoisie, Performance Optimization of numerically intensive codes, SIAM publishing company, Philadelphia, USA 2001 (ISBN 0-89871-484-2)