CSCI596 Assignment 4—Hybrid MPI+OpenMP Parallel Molecular Dynamics

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CSCI-596 assignment4
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1. source code of hmd.c：

```
/*--------------------------------------------------------------------------
Program pmd.c performs parallel molecular-dynamics for Lennard-Jones
systems using the Message Passing Interface (MPI) standard.
--------------------------------------------------------------------------*/
#include "hmd.h"

/*--------------------------------------------------------------------------*/
int main(int argc, char **argv) {
/*--------------------------------------------------------------------------*/
   double cpu1;

   MPI_Init(&argc,&argv); /* Initialize the MPI environment */
   MPI_Comm_rank(MPI_COMM_WORLD, &sid);    /* My processor ID */
   /* Vector index of this processor */
   vid[0] = sid/(vproc[1]*vproc[2]);
   vid[1] = (sid/vproc[2])%vproc[1];
   vid[2] = sid%vproc[2];

   omp_set_num_threads(nthrd);
   init_params();

   set_topology();
   init_conf();
   atom_copy();
   compute_accel(); /* Computes initial accelerations */

   cpu1 = MPI_Wtime();
   for (stepCount=1; stepCount<=StepLimit; stepCount++) {
      single_step();
      if (stepCount%StepAvg == 0) eval_props();
   }
   cpu = MPI_Wtime() - cpu1;
   if (sid == 0) printf("CPU & COMT = %le %le\n",cpu,comt);

   MPI_Finalize(); /* Clean up the MPI environment */
```

```
  return 0;
}

/*-------------------------------------------------------------------------*/
void init_params() {
/*-------------------------------------------------------------------------
Initializes parameters.
-------------------------------------------------------------------------*/
  int a;
  double rr,ri2,ri6,r1;
  FILE *fp;

  /* Read control parameters */
  fp = fopen("pmd.in","r");
  fscanf(fp,"%d%d%d",&InitUcell[0],&InitUcell[1],&InitUcell[2]);
  fscanf(fp,"%le",&Density);
  fscanf(fp,"%le",&InitTemp);
  fscanf(fp,"%le",&DeltaT);
  fscanf(fp,"%d",&StepLimit);
  fscanf(fp,"%d",&StepAvg);
  fclose(fp);

  /* Compute basic parameters */
  DeltaTH = 0.5*DeltaT;
  for (a=0; a<3; a++) al[a] = InitUcell[a]/pow(Density/4.0,1.0/3.0);
  if (sid == 0) printf("al = %e %e %e\n",al[0],al[1],al[2]);

  /* Compute the # of cells for linked cell lists */
  for (a=0; a<3; a++) {
    lc[a] = al[a]/RCUT;

    /* Size of cell block that each thread is assigned */
    thbk[a] = lc[a]/vthrd[a];
    /* # of cells = integer multiple of the # of threads */
    lc[a] = thbk[a]*vthrd[a]; /* Adjust # of cells/MPI process */

    rc[a] = al[a]/lc[a];
  }
  if (sid == 0) {
    printf("lc = %d %d %d\n",lc[0],lc[1],lc[2]);
    printf("rc = %e %e %e\n",rc[0],rc[1],rc[2]);
  }

  /* Constants for potential truncation */
```

```
   rr = RCUT*RCUT; ri2 = 1.0/rr; ri6 = ri2*ri2*ri2; r1=sqrt(rr);
   Uc = 4.0*ri6*(ri6 - 1.0);
   Duc = -48.0*ri6*(ri6 - 0.5)/r1;
}

/*----------------------------------------------------------------------*/
void set_topology() {
/*----------------------------------------------------------------------
Defines a logical network topology.  Prepares a neighbor-node ID table,
nn, & a shift-vector table, sv, for internode message passing.  Also
prepares the node parity table, myparity.
----------------------------------------------------------------------*/
   /* Integer vectors to specify the six neighbor nodes */
   int iv[6][3] = {
      {-1,0,0}, {1,0,0}, {0,-1,0}, {0,1,0}, {0,0,-1}, {0,0,1}
   };
   int ku,a,k1[3];

   /* Set up neighbor tables, nn & sv */
   for (ku=0; ku<6; ku++) {
      /* Vector index of neighbor ku */
      for (a=0; a<3; a++)
         k1[a] = (vid[a]+iv[ku][a]+vproc[a])%vproc[a];
      /* Scalar neighbor ID, nn */
      nn[ku] = k1[0]*vproc[1]*vproc[2]+k1[1]*vproc[2]+k1[2];
      /* Shift vector, sv */
      for (a=0; a<3; a++) sv[ku][a] = al[a]*iv[ku][a];
   }

   /* Set up the node parity table, myparity */
   for (a=0; a<3; a++) {
      if (vproc[a] == 1)
         myparity[a] = 2;
      else if (vid[a]%2 == 0)
         myparity[a] = 0;
      else
         myparity[a] = 1;
   }
}

/*----------------------------------------------------------------------*/
void init_conf() {
/*----------------------------------------------------------------------
r are initialized to face-centered cubic (fcc) lattice positions.
```

```
rv are initialized with a random velocity corresponding to Temperature.
-------------------------------------------------------------------------*/
   double c[3],gap[3],e[3],vSum[3],gvSum[3],vMag;
   int j,a,nX,nY,nZ;
   double seed;
   /* FCC atoms in the original unit cell */
   double origAtom[4][3] = {{0.0, 0.0, 0.0}, {0.0, 0.5, 0.5},
                            {0.5, 0.0, 0.5}, {0.5, 0.5, 0.0}};

   /* Set up a face-centered cubic (fcc) lattice */
   for (a=0; a<3; a++) gap[a] = al[a]/InitUcell[a];
   n = 0;
   for (nZ=0; nZ<InitUcell[2]; nZ++) {
      c[2] = nZ*gap[2];
      for (nY=0; nY<InitUcell[1]; nY++) {
         c[1] = nY*gap[1];
         for (nX=0; nX<InitUcell[0]; nX++) {
            c[0] = nX*gap[0];
            for (j=0; j<4; j++) {
               for (a=0; a<3; a++)
                  r[n][a] = c[a] + gap[a]*origAtom[j][a];
               ++n;
            }
         }
      }
   }
   /* Total # of atoms summed over processors */
   MPI_Allreduce(&n,&nglob,1,MPI_INT,MPI_SUM,MPI_COMM_WORLD);
   if (sid == 0) printf("nglob = %d\n",nglob);

   /* Generate random velocities */
   seed = 13597.0+sid;
   vMag = sqrt(3*InitTemp);
   for(a=0; a<3; a++) vSum[a] = 0.0;
   for(j=0; j<n; j++) {
      RandVec3(e,&seed);
      for (a=0; a<3; a++) {
         rv[j][a] = vMag*e[a];
         vSum[a] = vSum[a] + rv[j][a];
      }
   }
   MPI_Allreduce(vSum,gvSum,3,MPI_DOUBLE,MPI_SUM,MPI_COMM_WORLD);

   /* Make the total momentum zero */
```

```
   for (a=0; a<3; a++) gvSum[a] /= nglob;
   for (j=0; j<n; j++)
      for(a=0; a<3; a++) rv[j][a] -= gvSum[a];
}

/*----------------------------------------------------------------------*/
void single_step() {
/*----------------------------------------------------------------------
r & rv are propagated by DeltaT using the velocity-Verlet scheme.
----------------------------------------------------------------------*/
   int i,a;

   half_kick(); /* First half kick to obtain v(t+Dt/2) */
   for (i=0; i<n; i++) /* Update atomic coordinates to r(t+Dt) */
      for (a=0; a<3; a++) r[i][a] = r[i][a] + DeltaT*rv[i][a];
   atom_move();
   atom_copy();
   compute_accel(); /* Computes new accelerations, a(t+Dt) */
   half_kick(); /* Second half kick to obtain v(t+Dt) */
}

/*----------------------------------------------------------------------*/
void half_kick() {
/*----------------------------------------------------------------------
Accelerates atomic velocities, rv, by half the time step.
----------------------------------------------------------------------*/
   int i,a;
   for (i=0; i<n; i++)
      for (a=0; a<3; a++) rv[i][a] = rv[i][a]+DeltaTH*ra[i][a];
}

/*----------------------------------------------------------------------*/
void atom_copy() {
/*----------------------------------------------------------------------
Exchanges boundary-atom coordinates among neighbor nodes:    Makes
boundary-atom list, LSB, then sends & receives boundary atoms.
----------------------------------------------------------------------*/
   int kd,kdd,i,ku,inode,nsd,nrc,a;
   int nbnew = 0; /* # of "received" boundary atoms */
   double com1;

/* Main loop over x, y & z directions starts-------------------------*/

   for (kd=0; kd<3; kd++) {
```

```
/* Make a boundary-atom list, LSB--------------------------------*/

/* Reset the # of to-be-copied atoms for lower&higher directions */
for (kdd=0; kdd<2; kdd++) lsb[2*kd+kdd][0] = 0;

/* Scan all the residents & copies to identify boundary atoms */
for (i=0; i<n+nbnew; i++) {
   for (kdd=0; kdd<2; kdd++) {
      ku = 2*kd+kdd; /* Neighbor ID */
      /* Add an atom to the boundary-atom list, LSB, for neighbor ku
           according to bit-condition function, bbd */
      if (bbd(r[i],ku)) lsb[ku][++(lsb[ku][0])] = i;
   }
}

/* Message passing-----------------------------------------------*/

com1=MPI_Wtime(); /* To calculate the communication time */

/* Loop over the lower & higher directions */
for (kdd=0; kdd<2; kdd++) {

   inode = nn[ku=2*kd+kdd]; /* Neighbor node ID */

   /* Send & receive the # of boundary atoms-----------------------*/

   nsd = lsb[ku][0]; /* # of atoms to be sent */

   /* Even node: send & recv */
   if (myparity[kd] == 0) {
      MPI_Send(&nsd,1,MPI_INT,inode,10,MPI_COMM_WORLD);
      MPI_Recv(&nrc,1,MPI_INT,MPI_ANY_SOURCE,10,
                  MPI_COMM_WORLD,&status);
   }
   /* Odd node: recv & send */
   else if (myparity[kd] == 1) {
      MPI_Recv(&nrc,1,MPI_INT,MPI_ANY_SOURCE,10,
                  MPI_COMM_WORLD,&status);
      MPI_Send(&nsd,1,MPI_INT,inode,10,MPI_COMM_WORLD);
   }
   /* Single layer: Exchange information with myself */
   else
      nrc = nsd;
```

```
      /* Now nrc is the # of atoms to be received */

      /* Send & receive information on boundary atoms-----------------*/

      /* Message buffering */
      for (i=1; i<=nsd; i++)
        for (a=0; a<3; a++) /* Shift the coordinate origin */
          dbuf[3*(i-1)+a] = r[lsb[ku][i]][a]-sv[ku][a];

      /* Even node: send & recv */
      if (myparity[kd] == 0) {
        MPI_Send(dbuf,3*nsd,MPI_DOUBLE,inode,20,MPI_COMM_WORLD);
        MPI_Recv(dbufr,3*nrc,MPI_DOUBLE,MPI_ANY_SOURCE,20,
                 MPI_COMM_WORLD,&status);
      }
      /* Odd node: recv & send */
      else if (myparity[kd] == 1) {
        MPI_Recv(dbufr,3*nrc,MPI_DOUBLE,MPI_ANY_SOURCE,20,
                 MPI_COMM_WORLD,&status);
        MPI_Send(dbuf,3*nsd,MPI_DOUBLE,inode,20,MPI_COMM_WORLD);
      }
      /* Single layer: Exchange information with myself */
      else
        for (i=0; i<3*nrc; i++) dbufr[i] = dbuf[i];

      /* Message storing */
      for (i=0; i<nrc; i++)
        for (a=0; a<3; a++) r[n+nbnew+i][a] = dbufr[3*i+a];

      /* Increment the # of received boundary atoms */
      nbnew = nbnew+nrc;

      /* Internode synchronization */
      MPI_Barrier(MPI_COMM_WORLD);

    } /* Endfor lower & higher directions, kdd */

    comt += MPI_Wtime()-com1; /* Update communication time, COMT */

} /* Endfor x, y & z directions, kd */

/* Main loop over x, y & z directions ends--------------------------*/

/* Update the # of received boundary atoms */
```

```
  nb = nbnew;
}

/*----------------------------------------------------------------------*/
void compute_accel() {
/*----------------------------------------------------------------------
Given atomic coordinates, r[0:n+nb-1][], for the extended (i.e.,
resident & copied) system, computes the acceleration, ra[0:n-1][], for
the residents.
----------------------------------------------------------------------*/
  int i,j,a,lc2[3],lcyz2,lcxyz2,mc[3],c,mc1[3],c1;
  //int bintra;
  double rrCut,lpe;
  double lpe_td[nthrd]
  /* Reset the potential & forces */
  lpe = 0.0;
  for( i=0; i<nthrd; i ++) lpe_td[i]= 0.0;
  for (i=0; i<n; i++) for (a=0; a<3; a++) ra[i][a] = 0.0;

  /* Make a linked-cell list, lscl--------------------------------------*/

  for (a=0; a<3; a++) lc2[a] = lc[a]+2;
  lcyz2 = lc2[1]*lc2[2];
  lcxyz2 = lc2[0]*lcyz2;

  /* Reset the headers, head */
  for (c=0; c<lcxyz2; c++) head[c] = EMPTY;

  /* Scan atoms to construct headers, head, & linked lists, lscl */

  for (i=0; i<n+nb; i++) {
    for (a=0; a<3; a++) mc[a] = (r[i][a]+rc[a])/rc[a];

    /* Translate the vector cell index, mc, to a scalar cell index */
    c = mc[0]*lcyz2+mc[1]*lc2[2]+mc[2];

    /* Link to the previous occupant (or EMPTY if you're the 1st) */
    lscl[i] = head[c];

    /* The last one goes to the header */
    head[c] = i;
  } /* Endfor atom i */

  /* Calculate pair interaction-----------------------------------------*/
```

```
    rrCut = RCUT*RCUT;

#pragma omp parallel private(a,mc,c,mc1,c1,i,j)
{
        double dr[3],rr,ri2,ri6,r1,fcVal,f,vVal;
    int std,vtd[3],mofst[3];

    std = omp_get_thread_num();
    vtd[0] = std/(vthrd[1]*vthrd[2]);
    vtd[1] = (std/vthrd[2])%vthrd[1];
    vtd[2] = std%vthrd[2];
    for (a=0; a<3; a++)
        mofst[a] = vtd[a]*thbk[a];

    /* Scan inner cells */
    //for (mc[0]=1; mc[0]<=lc[0]; (mc[0])++)
    //for (mc[1]=1; mc[1]<=lc[1]; (mc[1])++)
    //for (mc[2]=1; mc[2]<=lc[2]; (mc[2])++) {
    for (mc[0]=mofst[0]+1; mc[0]<=mofst[0]+thbk[0]; (mc[0])++)
    for (mc[1]=mofst[1]+1; mc[1]<=mofst[1]+thbk[1]; (mc[1])++)
    for (mc[2]=mofst[2]+1; mc[2]<=mofst[2]+thbk[2]; (mc[2])++){

        /* Calculate a scalar cell index */
        c = mc[0]*lcyz2+mc[1]*lc2[2]+mc[2];
        /* Skip this cell if empty */
        if (head[c] == EMPTY) continue;

        /* Scan the neighbor cells (including itself) of cell c */
        for (mc1[0]=mc[0]-1; mc1[0]<=mc[0]+1; (mc1[0])++)
        for (mc1[1]=mc[1]-1; mc1[1]<=mc[1]+1; (mc1[1])++)
        for (mc1[2]=mc[2]-1; mc1[2]<=mc[2]+1; (mc1[2])++) {

            /* Calculate the scalar cell index of the neighbor cell */
            c1 = mc1[0]*lcyz2+mc1[1]*lc2[2]+mc1[2];
            /* Skip this neighbor cell if empty */
            if (head[c1] == EMPTY) continue;

            /* Scan atom i in cell c */
            i = head[c];
            while (i != EMPTY) {

                /* Scan atom j in cell c1 */
                j = head[c1];
```

```
            while (j != EMPTY) {

               /* No calculation with itself */
               if (j != i) {
                  /* Logical flag: intra(true)- or inter(false)-pair atom */
                  //bintra = (j < n);

                  /* Pair vector dr = r[i] - r[j] */
                  for (rr=0.0, a=0; a<3; a++) {
                     dr[a] = r[i][a]-r[j][a];
                     rr += dr[a]*dr[a];
                  }

                  /* Calculate potential & forces for intranode pairs (i < j)
                        & all the internode pairs if rij < RCUT; note that for
                        any copied atom, i < j */
                 // if (i<j && rr<rrCut) {
               if(rr<rrCut){
                     ri2 = 1.0/rr; ri6 = ri2*ri2*ri2; r1 = sqrt(rr);
                     fcVal = 48.0*ri2*ri6*(ri6-0.5) + Duc/r1;
                     vVal = 4.0*ri6*(ri6-1.0) - Uc - Duc*(r1-RCUT);
                    // if (bintra) lpe += vVal; else lpe += 0.5*vVal;
                     lpe_td[std] += 0.5*vVal;
                     for (a=0; a<3; a++) {
                        f = fcVal*dr[a];
                        ra[i][a] += f;
                       // if (bintra) ra[j][a] -= f;
                     }
                  }
               } /* Endif not self */

               j = lscl[j];
            } /* Endwhile j not empty */

            i = lscl[i];
         } /* Endwhile i not empty */

      } /* Endfor neighbor cells, c1 */

   } /* Endfor central cell, c */

}//end parallel section

// thread reduction
```

```
for(i=0;i<nthrd;i++)    lpe += lpe_td[i];

   /* Global potential energy */
   MPI_Allreduce(&lpe,&potEnergy,1,MPI_DOUBLE,MPI_SUM,MPI_COMM_WORLD);
}

/*----------------------------------------------------------------------*/
void eval_props() {
/*----------------------------------------------------------------------
Evaluates physical properties: kinetic, potential & total energies.
----------------------------------------------------------------------*/
   double vv,lke;
   int i,a;

   /* Total kinetic energy */
   for (lke=0.0, i=0; i<n; i++) {
      for (vv=0.0, a=0; a<3; a++) vv += rv[i][a]*rv[i][a];
      lke += vv;
   }
   lke *= 0.5;
   MPI_Allreduce(&lke,&kinEnergy,1,MPI_DOUBLE,MPI_SUM,MPI_COMM_WORLD);

   /* Energy paer atom */
   kinEnergy /= nglob;
   potEnergy /= nglob;
   totEnergy = kinEnergy + potEnergy;
   temperature = kinEnergy*2.0/3.0;

   /* Print the computed properties */
   if (sid == 0) printf("%9.6f %9.6f %9.6f %9.6f\n",
                        stepCount*DeltaT,temperature,potEnergy,totEnergy);
}

/*----------------------------------------------------------------------*/
void atom_move() {
/*----------------------------------------------------------------------
Sends moved-out atoms to neighbor nodes and receives moved-in atoms
from neighbor nodes.    Called with n, r[0:n-1] & rv[0:n-1], atom_move
returns a new n' together with r[0:n'-1] & rv[0:n'-1].
----------------------------------------------------------------------*/

/* Local variables-------------------------------------------------

mvque[6][NBMAX]: mvque[ku][0] is the # of to-be-moved atoms to neighbor
```

```
  ku; MVQUE[ku][k>0] is the atom ID, used in r, of the k-th atom to be
  moved.
-----------------------------------------------------------------------*/
  int mvque[6][NBMAX];
  int newim = 0; /* # of new immigrants */
  int ku,kd,i,kdd,kul,kuh,inode,ipt,a,nsd,nrc;
  double com1;

  /* Reset the # of to-be-moved atoms, MVQUE[][0] */
  for (ku=0; ku<6; ku++) mvque[ku][0] = 0;

  /* Main loop over x, y & z directions starts-----------------------*/

  for (kd=0; kd<3; kd++) {

    /* Make a moved-atom list, mvque-----------------------------------*/

    /* Scan all the residents & immigrants to list moved-out atoms */
    for (i=0; i<n+newim; i++) {
      kul = 2*kd   ; /* Neighbor ID */
      kuh = 2*kd+1;
      /* Register a to-be-copied atom in mvque[kul|kuh][] */
      if (r[i][0] > MOVED_OUT) { /* Don't scan moved-out atoms */
        /* Move to the lower direction */
        if (bmv(r[i],kul)) mvque[kul][++(mvque[kul][0])] = i;
        /* Move to the higher direction */
        else if (bmv(r[i],kuh)) mvque[kuh][++(mvque[kuh][0])] = i;
      }
    }

    /* Message passing with neighbor nodes-----------------------------*/

    com1 = MPI_Wtime();

    /* Loop over the lower & higher directions-------------------------*/

    for (kdd=0; kdd<2; kdd++) {

      inode = nn[ku=2*kd+kdd]; /* Neighbor node ID */

      /* Send atom-number information-----------------------------------*/

      nsd = mvque[ku][0]; /* # of atoms to-be-sent */
```

```
/* Even node: send & recv */
if (myparity[kd] == 0) {
   MPI_Send(&nsd,1,MPI_INT,inode,110,MPI_COMM_WORLD);
   MPI_Recv(&nrc,1,MPI_INT,MPI_ANY_SOURCE,110,
                MPI_COMM_WORLD,&status);
}
/* Odd node: recv & send */
else if (myparity[kd] == 1) {
   MPI_Recv(&nrc,1,MPI_INT,MPI_ANY_SOURCE,110,
                MPI_COMM_WORLD,&status);
   MPI_Send(&nsd,1,MPI_INT,inode,110,MPI_COMM_WORLD);
}
/* Single layer: Exchange information with myself */
else
   nrc = nsd;
/* Now nrc is the # of atoms to be received */

/* Send & receive information on boundary atoms-----------------*/

/* Message buffering */
for (i=1; i<=nsd; i++)
   for (a=0; a<3; a++) {
      /* Shift the coordinate origin */
      dbuf[6*(i-1)   +a] = r [mvque[ku][i]][a]-sv[ku][a];
      dbuf[6*(i-1)+3+a] = rv[mvque[ku][i]][a];
      r[mvque[ku][i]][0] = MOVED_OUT; /* Mark the moved-out atom */
   }

/* Even node: send & recv, if not empty */
if (myparity[kd] == 0) {
   MPI_Send(dbuf,6*nsd,MPI_DOUBLE,inode,120,MPI_COMM_WORLD);
   MPI_Recv(dbufr,6*nrc,MPI_DOUBLE,MPI_ANY_SOURCE,120,
                MPI_COMM_WORLD,&status);
}
/* Odd node: recv & send, if not empty */
else if (myparity[kd] == 1) {
   MPI_Recv(dbufr,6*nrc,MPI_DOUBLE,MPI_ANY_SOURCE,120,
                MPI_COMM_WORLD,&status);
   MPI_Send(dbuf,6*nsd,MPI_DOUBLE,inode,120,MPI_COMM_WORLD);
}
/* Single layer: Exchange information with myself */
else
   for (i=0; i<6*nrc; i++) dbufr[i] = dbuf[i];
```

```
            /* Message storing */
            for (i=0; i<nrc; i++)
               for (a=0; a<3; a++) {
                  r [n+newim+i][a] = dbufr[6*i   +a];
                  rv[n+newim+i][a] = dbufr[6*i+3+a];
               }

            /* Increment the # of new immigrants */
            newim = newim+nrc;

            /* Internode synchronization */
            MPI_Barrier(MPI_COMM_WORLD);

         } /* Endfor lower & higher directions, kdd */

         comt=comt+MPI_Wtime()-com1;

      } /* Endfor x, y & z directions, kd */

      /* Main loop over x, y & z directions ends--------------------------*/

      /* Compress resident arrays including new immigrants */

      ipt = 0;
      for (i=0; i<n+newim; i++) {
         if (r[i][0] > MOVED_OUT) {
            for (a=0; a<3; a++) {
               r [ipt][a] = r [i][a];
               rv[ipt][a] = rv[i][a];
            }
            ++ipt;
         }
      }

      /* Update the compressed # of resident atoms */
      n = ipt;
   }

   /*----------------------------------------------------------------------
   Bit condition functions:

   1. bbd(ri,ku) is .true. if coordinate ri[3] is in the boundary to
            neighbor ku.
   2. bmv(ri,ku) is .true. if an atom with coordinate ri[3] has moved out
```

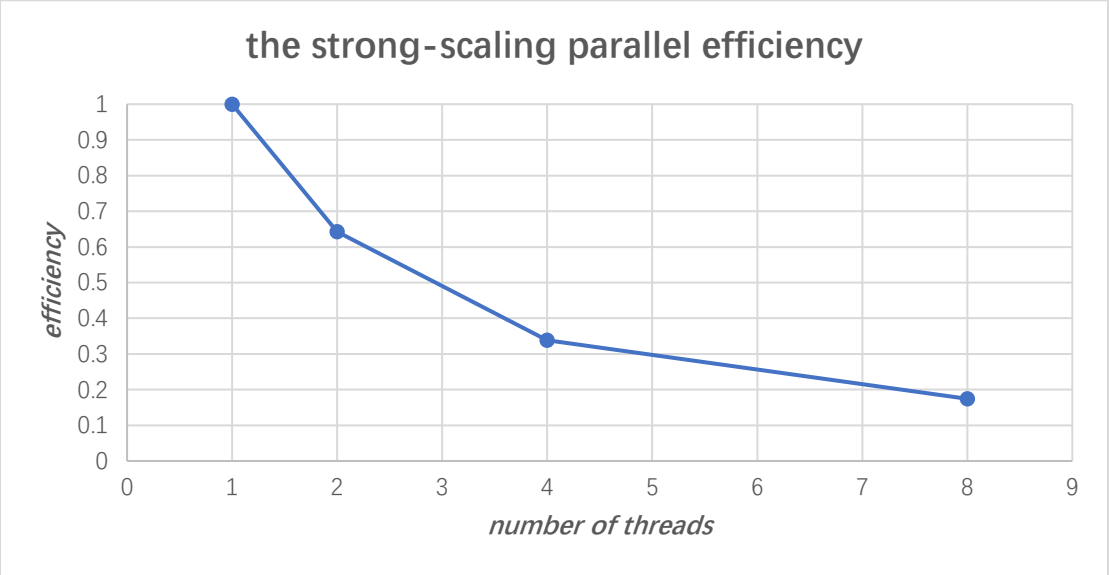
```
        to neighbor ku.
-------------------------------------------------------------------------*/
int bbd(double* ri, int ku) {
   int kd,kdd;
   kd = ku/2; /* x(0)|y(1)|z(2) direction */
   kdd = ku%2; /* Lower(0)|higher(1) direction */
   if (kdd == 0)
      return ri[kd] < RCUT;
   else
      return al[kd]-RCUT < ri[kd];
}
int bmv(double* ri, int ku) {
   int kd,kdd;
   kd = ku/2; /* x(0)|y(1)|z(2) direction */
   kdd = ku%2; /* Lower(0)|higher(1) direction */
   if (kdd == 0)
      return ri[kd] < 0.0;
   else
      return al[kd] < ri[kd];
}
```

2. output:

```
youzhiqu@hpcl118:/auto/dr-std/an2/youzhiqu$ srun -n 2 ./hmd
al = 4.103942e+01 4.103942e+01 2.051971e+01
lc = 16 16 8
rc = 2.564964e+00 2.564964e+00 2.564964e+00
nglob = 55296
 0.050000  0.877345 -5.137153 -3.821136
 0.100000  0.462056 -4.513097 -3.820013
 0.150000  0.510836 -4.587287 -3.821033
 0.200000  0.527457 -4.611958 -3.820772
 0.250000  0.518668 -4.598798 -3.820796
 0.300000  0.529023 -4.614343 -3.820808
 0.350000  0.532890 -4.620133 -3.820798
 0.400000  0.536070 -4.624899 -3.820794
 0.450000  0.539725 -4.630387 -3.820799
 0.500000  0.538481 -4.628514 -3.820792
CPU & COMT = 1.222426e+01 1.104946e-01
```

3. the strong-scaling parallel efficiency

A	B	C
time	number of threads	efefficiency
36.90344	1	1
28.70776	2	0.642743
27.26838	4	0.338335
26.45132	8	0.174393




```
youzhiqu@hpcl119:/auto/dr-std/an2/youzhiqu$ srun -n 1 ./hmd1
al = 4.103942e+01 4.103942e+01 4.103942e+01
lc = 16 16 16
rc = 2.564964e+00 2.564964e+00 2.564964e+00
nglob = 55296
CPU & COMT = 3.690344e+01 4.278564e-02
youzhiqu@hpcl119:/auto/dr-std/an2/youzhiqu$ srun -n 1 ./hmd2
al = 4.103942e+01 4.103942e+01 4.103942e+01
lc = 16 16 16
rc = 2.564964e+00 2.564964e+00 2.564964e+00
nglob = 55296
CPU & COMT = 2.870776e+01 4.933786e-02
youzhiqu@hpcl119:/auto/dr-std/an2/youzhiqu$ srun -n 1 ./hmd4
al = 4.103942e+01 4.103942e+01 4.103942e+01
lc = 16 16 16
rc = 2.564964e+00 2.564964e+00 2.564964e+00
nglob = 55296
CPU & COMT = 2.726838e+01 4.921603e-02
youzhiqu@hpcl119:/auto/dr-std/an2/youzhiqu$ srun -n 1 ./hmd8
al = 4.103942e+01 4.103942e+01 4.103942e+01
lc = 16 16 16
rc = 2.564964e+00 2.564964e+00 2.564964e+00
nglob = 55296
CPU & COMT = 2.645132e+01 5.426192e-02
```