Assignment04

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1.

modifications are marked with ####

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;
```

```c
  /* 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,rrCut,fcVal,lpe,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 for parallel cell*/  // #####

      //Thresd 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];
}
```

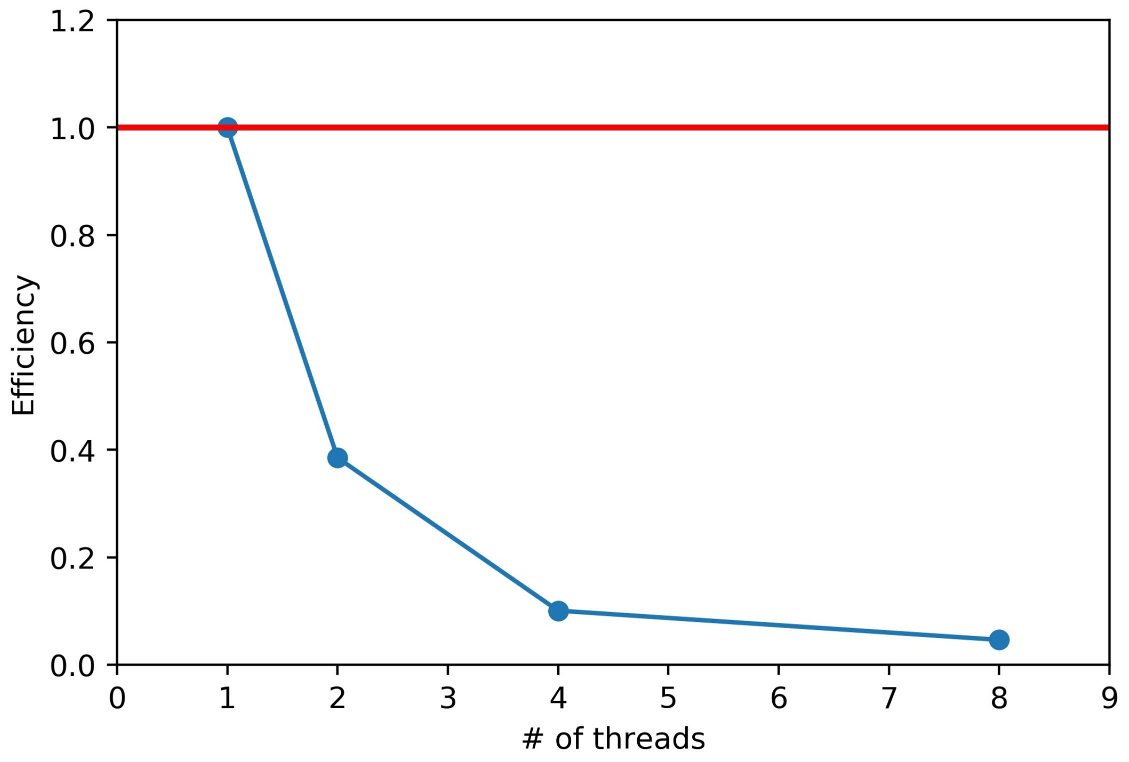
2.

hmd.out :

```
----------------------------------------
Begin SLURM Prolog Wed 10 Oct 2018 09:12:09 PM PDT
Job ID:          2019069
Username:        liangsiq
Accountname:     lc_an2
Name:            hmd.sl
Partition:       quick
Nodes:           hpc[1118-1119]
TasksPerNode:    1(x2)
CPUSPerTask:     4
TMPDIR:          /tmp/2019069.quick
SCRATCHDIR:      /staging/scratch/2019069
Cluster:         uschpc
HSDA Account:    false
End SLURM Prolog
----------------------------------------
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 = 7.283849e+00 5.137362e-01
```

3.

Plot:


Efficiency
# of threads
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5
6
7
8
9