# CSCI596 Assignment 3—Parallel Molecular Dynamics

Youzhi Qu
CSCI-596 assignment3
Prof. Aiichiro Nakano

## Part I—Asynchronous Messages

**Source code:**

**pmd_irecv.c:**

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

	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;
		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 */

        MPI_Irecv(&nrc, 1, MPI_INT, MPI_ANY_SOURCE, 10,
            MPI_COMM_WORLD, &request);
        MPI_Send(&nsd, 1, MPI_INT, inode, 10, MPI_COMM_WORLD);
        MPI_Wait(&request, &status);
        /* Now nrc is the # of atoms to be received */

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

        MPI_Irecv(dbufr, 3 * nrc, MPI_DOUBLE, MPI_ANY_SOURCE, 20,
            MPI_COMM_WORLD, &request);
        /* 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];
        MPI_Send(dbuf, 3 * nsd, MPI_DOUBLE, inode, 20, MPI_COMM_WORLD);
        MPI_Wait(&request, &status);

        /* 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;
```

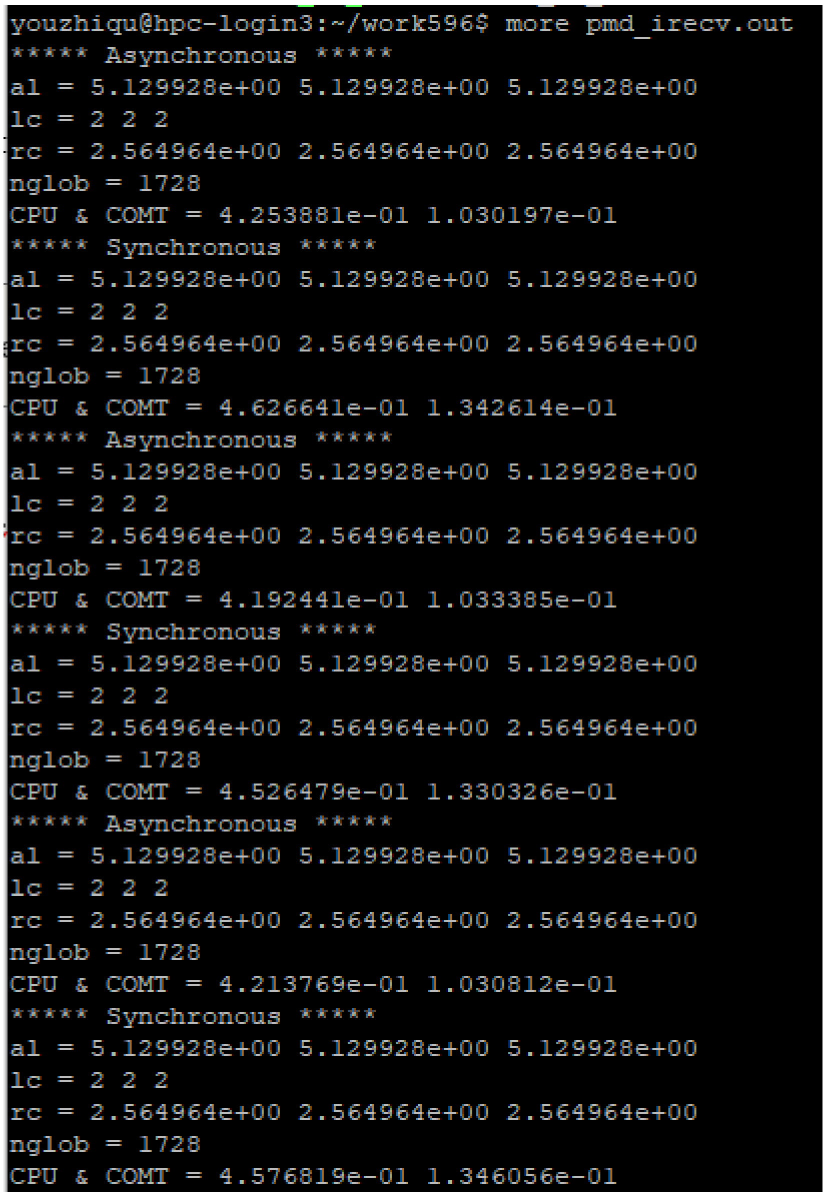
```
            /* Internode synchronization */
            MPI_Barrier(MPI_COMM_WORLD);

        } /* 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 dr[3], rr, ri2, ri6, r1, rrCut, fcVal, f, vVal, lpe;

    /* Reset the potential & forces */
    lpe = 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;

    /* 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])++) {

                /* 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) {
                                        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;
                                                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 */

                /* 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 */

        MPI_Irecv(&nrc, 1, MPI_INT, MPI_ANY_SOURCE, 110,
            MPI_COMM_WORLD, &request);
        MPI_Send(&nsd, 1, MPI_INT, inode, 110, MPI_COMM_WORLD);
        MPI_Wait(&request, &status);

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

        /* Send & receive information on boundary atoms-----------------*/
        MPI_Irecv(dbufr, 6 * nrc, MPI_DOUBLE, MPI_ANY_SOURCE, 120,
            MPI_COMM_WORLD, &request);

        /* 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 */
            }

        MPI_Send(dbuf, 6 * nsd, MPI_DOUBLE, inode, 120, MPI_COMM_WORLD);
        MPI_Wait(&request, &status);


        /* 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];
}
```

**pmd_irecv.c program runs faster.**
**timing data:**



```
youzhiqu@hpc-login3:~/work596$ more pmd_irecv.out
***** Asynchronous *****
al = 5.129928e+00 5.129928e+00 5.129928e+00
lc = 2 2 2
rc = 2.564964e+00 2.564964e+00 2.564964e+00
nglob = 1728
CPU & COMT = 4.253881e-01 1.030197e-01
***** Synchronous *****
al = 5.129928e+00 5.129928e+00 5.129928e+00
lc = 2 2 2
rc = 2.564964e+00 2.564964e+00 2.564964e+00
nglob = 1728
CPU & COMT = 4.626641e-01 1.342614e-01
***** Asynchronous *****
al = 5.129928e+00 5.129928e+00 5.129928e+00
lc = 2 2 2
rc = 2.564964e+00 2.564964e+00 2.564964e+00
nglob = 1728
CPU & COMT = 4.192441e-01 1.033385e-01
***** Synchronous *****
al = 5.129928e+00 5.129928e+00 5.129928e+00
lc = 2 2 2
rc = 2.564964e+00 2.564964e+00 2.564964e+00
nglob = 1728
CPU & COMT = 4.526479e-01 1.330326e-01
***** Asynchronous *****
al = 5.129928e+00 5.129928e+00 5.129928e+00
lc = 2 2 2
rc = 2.564964e+00 2.564964e+00 2.564964e+00
nglob = 1728
CPU & COMT = 4.213769e-01 1.030812e-01
***** Synchronous *****
al = 5.129928e+00 5.129928e+00 5.129928e+00
lc = 2 2 2
rc = 2.564964e+00 2.564964e+00 2.564964e+00
nglob = 1728
CPU & COMT = 4.576819e-01 1.346056e-01
```

## Part II—Communicators

**Source code:**

**pmd_split.c:**

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

void calc_pv() {
   double lpv[NBIN],pv[NBIN],dv,v;
   int i;

   dv = VMAX/NBIN;    // Bin size
```

```
  for (i=0; i<NBIN; i++) lpv[i] = 0.0; // Reset local histogram
  for (i=0; i<n; i++) {
    v = sqrt(pow(rv[i][0],2)+pow(rv[i][1],2)+pow(rv[i][2],2));
    lpv[v/dv < NBIN ? (int)(v/dv) : NBIN-1] += 1.0;
  }
  MPI_Allreduce(lpv,pv,NBIN,MPI_DOUBLE,MPI_SUM,workers);
  MPI_Allreduce(&n,&nglob,1,MPI_INT,MPI_SUM,workers);
  for (i=0; i<NBIN; i++) pv[i] /= (dv*nglob);    // Normalization
  if (sid == 0) {
    for (i=0; i<NBIN; i++) fprintf(fpv,"%le %le\n",i*dv,pv[i]);
    fprintf(fpv,"\n");
  }
}
/*--------------------------------------------------------------------*/
int main(int argc, char **argv) {
/*--------------------------------------------------------------------*/
  double cpu1;
  int i,a;

  MPI_Init(&argc,&argv); /* Initialize the MPI environment */
  //MPI_Comm_rank(MPI_COMM_WORLD, &sid);   /* My processor ID */

  MPI_Comm_rank(MPI_COMM_WORLD,&gid); //Global rank
  md = gid%2; // = 1 (MD workers) or 0 (analysis workers) color is 2
  MPI_Comm_split(MPI_COMM_WORLD,md,0,&workers);
  MPI_Comm_rank(workers,&sid); // Rank in workers

  /* Vector index of this processor */
  vid[0] = sid/(vproc[1]*vproc[2]);
  vid[1] = (sid/vproc[2])%vproc[1];
  vid[2] = sid%vproc[2];

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

  init_params();
  if (md) {
    set_topology();
    init_conf();
    atom_copy();
    compute_accel();
    }
    else
        if (sid == 0) fpv = fopen("pv.dat","w");

    cpu1 = MPI_Wtime();
    for (stepCount=1; stepCount<=StepLimit; stepCount++) {
        //single_step();
        //if (stepCount%StepAvg == 0) eval_props();
        if (md) single_step();
        if (stepCount%StepAvg == 0) {
            if (md) {
                //Send # of atoms, n, to rank gid-1 in MPI_COMM_WORLD
                MPI_Send(&n, 1, MPI_INT, gid - 1, 1000, MPI_COMM_WORLD);
                //Send velocities of n atoms to rank gid-1 in MPI_COMM_WORLD
                for(i = 0; i < n; i++)
                    for(a = 0; a < 3; a++)
                        dbuf[3*i+a] = rv[i][a];
                MPI_Send(dbuf, 3*n, MPI_DOUBLE, gid - 1, 2000, MPI_COMM_WORLD);
                eval_props();
            }
            else {
                //Receive # of atoms, n, from rank gid+1 in MPI_COMM_WORLD
                MPI_Recv(&n, 1, MPI_INT, gid + 1, 1000, MPI_COMM_WORLD, &status);
                //Receive velocities of n atoms from rank gid+1 in MPI_COMM_WORLD
                MPI_Recv(dbufr, 3*n, MPI_DOUBLE, gid + 1, 2000, MPI_COMM_WORLD,
&status);
                for(i = 0; i < n; i++)
                    for(a = 0; a < 3; a++)
                        rv[i][a] = dbufr[3*i+a];
                calc_pv();
            }
        }
    }
    cpu = MPI_Wtime() - cpu1;
    //if (sid == 0) printf("CPU & COMT = %le %le\n",cpu,comt);
    if(md && sid == 0)
        printf("CPU & COMT = %le %le\n", cpu, comt);
    if(!md && sid == 0)
        fclose(fpv);

    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;
      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,workers);
    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,workers);

    /* 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 */

   MPI_Irecv(&nrc,1,MPI_INT,MPI_ANY_SOURCE,10,
                  workers,&request);

   MPI_Send(&nsd,1,MPI_INT,inode,10,workers);
   MPI_Wait(&request, &status);

   // /* 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-----------------*/
```

```
        MPI_Irecv(dbufr,3*nrc,MPI_DOUBLE,MPI_ANY_SOURCE,20,
                  workers,&request);
        /* 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];

        MPI_Send(dbuf,3*nsd,MPI_DOUBLE,inode,20,workers);
        MPI_Wait(&request, &status);

        // /* 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(workers);

      } /* 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 dr[3],rr,ri2,ri6,r1,rrCut,fcVal,f,vVal,lpe;

  /* Reset the potential & forces */
  lpe = 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;

/* 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])++) {

   /* 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) {
                 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;
                 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 */

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

/*--------------------------------------------------------------------*/
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,workers);
```

```
   /* 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 */

  MPI_Irecv(&nrc,1,MPI_INT,MPI_ANY_SOURCE,110,
               workers,&request);
  MPI_Send(&nsd,1,MPI_INT,inode,110,workers);
  MPI_Wait(&request, &status);

  // /* 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-----------------*/

   MPI_Irecv(dbufr,6 * nrc,MPI_DOUBLE,MPI_ANY_SOURCE,120,
                  workers,&request);
     /* 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 */
        }
   MPI_Send(dbuf,6 * nsd,MPI_DOUBLE,inode,120,workers);
   MPI_Wait(&request, &status);

// /* 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(workers);
```

```
      } /* 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];
}
```

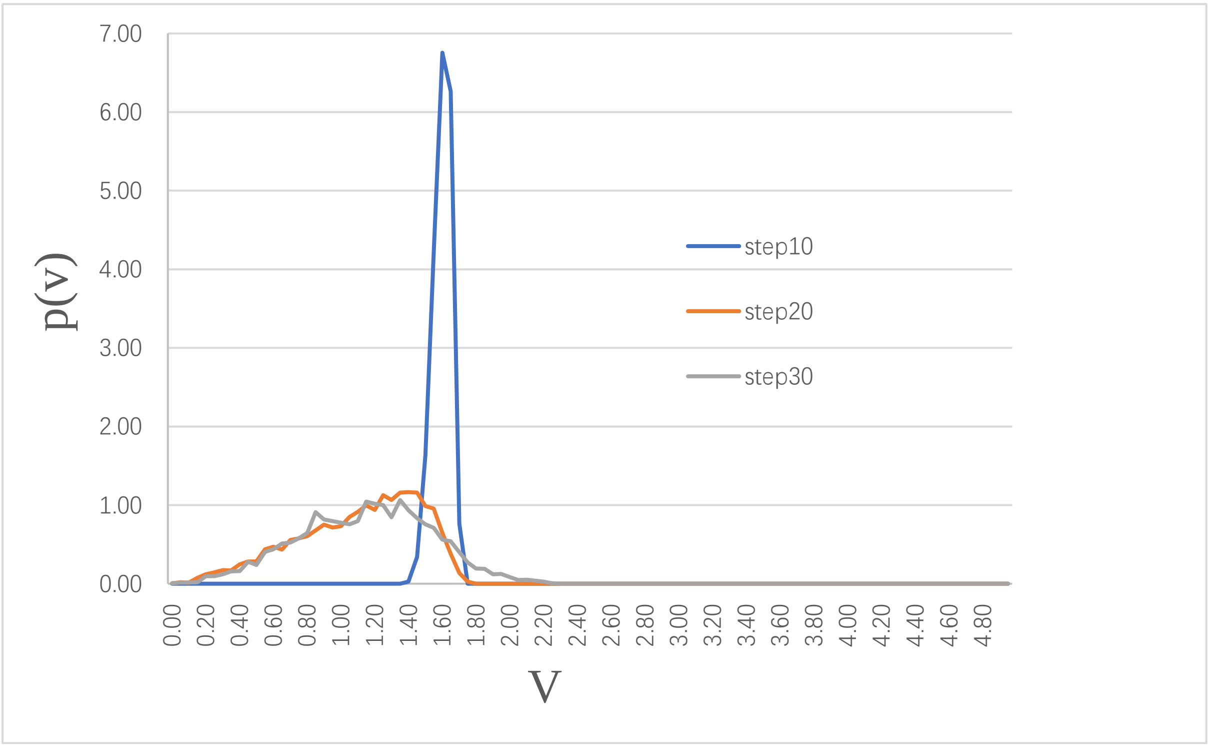
**pmd_split.h:**

```
/*----------------------------------------------------------------------
pmd.h is an include file for a parallel MD program, pmd.c.
----------------------------------------------------------------------*/
#include <stdio.h>
#include <math.h>
#include "mpi.h"

/* Constants------------------------------------------------------------

NMAX = Maximum # of atoms per processor
NEMAX = Maximum # of augmented (= resident + copied) atoms
NDBUF = Size of a double-precision buffer, dbuf
        > 6*(# of boundary atoms for each neighbor)
NBMAX = Maximum # of copied boundary atoms per neighbor.
NCLMAX = Maximum # of cells per processor.
RCUT = Potential cut-off length
MOVED_OUT: Signifies a moved-out resident atom in function atom_move.
EMPTY: Signifies the end of a linked list.
----------------------------------------------------------------------*/
#define NMAX 100000
#define NEMAX 200000
#define NDBUF 300000
#define NBMAX 100000
#define NCLMAX 100000
#define RCUT 2.5
#define MOVED_OUT -1.0e10
#define EMPTY -1
/* Constants for the random number generator */
#define D2P31M 2147483647.0
#define DMUL 16807.0

#define VMAX 5.0    // Max. velocity value to construct a velocity histogram
#define NBIN 100    // # of bins in the histogram
/* Variables------------------------------------------------------------
```

```
al[0|1|2] = Box length per processor in the x|y|z direction.
n = # of resident atoms in this processor.
nb = # of copied boundary atoms from neighbors.
nglob = Total # of atoms summed over processors.
r[NEMAX][3]: r[i][0|1|2] is the x|y|z coordinate of atom i (including
   the copied atoms).
rv[NEMAX][3]: rv[i][0|1|2] is the x|y|z velocity of atom i (including
   the copied atoms).
ra[NMAX][3]: ra[i][0|1|2] is the x|y|z acceleration on atom i.
dbuf[NDBUF]: Buffer for sending double-precision data
dbufr[NDBUF]:                   receiving
vproc[0|1|2] = # of processors in the x|y|z direction.
nproc = # of processors = vproc[0]*vproc[1]*vproc[2].
sid = Sequential processor ID.
vid[3] = Vector processor ID;
   sid = vid[0]*vproc[1]*vproc[2] + vid[1]*vproc[2] + vid[2].
NN[6]: NN[ku] is the node ID of the neighbor specified by a neighbor.
   index, ku.   The neighbor index is defined as:
   ku = 0: xlow    (West );
          1: xhigh (East );
          2: ylow    (South);
          3: yhigh (North);
          4: zlow    (Down );
          5: zhigh (Up      ).
sv[6][3]: sv[ku][] is the shift vector to the ku-th neighbor.
myparity[0|1|2] = Parity of vector processor ID in the x|y|z direction.
lsb[6][NBMAX]: lsb[ku][0] is the total # of boundary atoms to be sent
   to neighbor ku; lsb[ku][k] is the atom ID, used in r, of the k-th
   atom to be sent.
status: Returned by MPI message-passing routines.
cpu: Elapsed wall-clock time in seconds.
comt: Communication time in seconds.
lc[3]: lc[0|1|2] is the # of cells in the x|y|z direction.
rc[3]: rc[0|1|2] is the length of a cell in the x|y|z direction.
lscl[NEMAX]: Linked cell lists.
head[NCLMAX]: Headers for the linked cell lists.
kinEnergy = Kinetic energy.
potEnergy = Potential energy.
totEnergy = Total energy.
temperature = Current temperature.
stepCount = Current time step.
----------------------------------------------------------------------*/
double al[3];
```

```
int n, nb, nglob;
double r[NEMAX][3], rv[NEMAX][3], ra[NMAX][3];
double dbuf[NDBUF], dbufr[NDBUF];
int vproc[3] = { 2,2,2 }, nproc = 8;
int sid, vid[3], nn[6], myparity[3];
double sv[6][3];
int lsb[6][NBMAX];
MPI_Status status;
MPI_Request request;
double cpu, comt;
int head[NCLMAX], lscl[NEMAX], lc[3];
double rc[3];
double kinEnergy, potEnergy, totEnergy, temperature;
int stepCount;
double DeltaTH;         /* Half the time step */
double Uc, Duc;         /* Potential cut-off parameters */

FILE *fpv;

int gid, md;
MPI_Comm workers;

/* Input data-----------------------------------------------------------

Control data: pmd.in.
---------------------------------------------------------------------*/
int InitUcell[3];      /* Number of unit cells per processor */
double Density;         /* Number density of atoms (in reduced unit) */
double InitTemp;        /* Starting temperature (in reduced unit) */
double DeltaT;          /* Size of a time step (in reduced unit) */
int StepLimit;          /* Number of time steps to be simulated */
int StepAvg;            /* Reporting interval for statistical data */

/* Functions & function prototypes-----------------------------------*/

double SignR(double v, double x) { if (x > 0) return v; else return -v; }
double Dmod(double a, double b) {
      int n;
      n = (int)(a / b);
      return (a - b * n);
}
double RandR(double *seed) {
      *seed = Dmod(*seed*DMUL, D2P31M);
      return (*seed / D2P31M);
}
void RandVec3(double *p, double *seed) {
        double x, y, s = 2.0;
        while (s > 1.0) {
                x = 2.0*RandR(seed) - 1.0; y = 2.0*RandR(seed) - 1.0; s = x * x + y * y;
        }
        p[2] = 1.0 - 2.0*s; s = 2.0*sqrt(1.0 - s); p[0] = s * x; p[1] = s * y;
}

void init_params();
void set_topology();
void init_conf();
void single_step();
void half_kick();
void atom_copy();
void compute_accel();
void eval_props();
void atom_move();
int bbd(double* ri, int ku);
int bmv(double* ri, int ku);
/*------------------------------------------------------------------*/
```

**the plot of calculated PDFs at time steps 10, 20, and 30:**


p(v)
step10
step20
step30
V