

```

1  #include <stdio.h>
2  #include <math.h>
3  #include <float.h>
4  #include <stdlib.h>
5  #include <string.h>
6  #include <time.h>
7  #include <mpi.h>
8
9  int Np ;
10 int Np_d = 100; /* Default number of particles*/
11
12 float total_time ;
13 float time_d = 60; /* Default simulation time*/
14
15 float dt;
16 float dt_d = 0.02; /* Default time step*/
17
18 float m = 10.0; /* mass */
19 int range = 20; /* range for position generation */
20
21 int rank, size; /* world rank and size*/
22
23 typedef struct {
24     float x, y, z;
25 } Pos; /* struct for position co-ordinates*/
26 Pos *position;
27
28 typedef struct {
29     float vx, vy, vz;
30 } Vel; /* struct for velocity */
31 Vel *velocity;
32
33 typedef struct {
34     float ax, ay, az;
35 } Acc; /* struct for acceleration */
36 Acc *a;
37
38 int lengths[3] = { 1, 1, 1 };
39 const MPI_Aint displacements[3] = { 0, sizeof(float), sizeof(float)*2 };
40 MPI_Datatype types[3] = { MPI_FLOAT, MPI_FLOAT, MPI_FLOAT }; /* to create MPI data types
41 for position, velocity and acceleration */
42 MPI_Datatype POSITION;
43 MPI_Datatype VELOCITY;
44
45 int start, end, *sendcounts, *displs; /* variables to control imbalanced scatter/gather*/
46
47 void P_r(int number_of_particles, int size, int rank, int *start, int *end, int
48 *sendcounts, int *displs )
49 {
50     int r = (number_of_particles)%size;
51     int s = 0;
52
53     for (int p = 0; p < size; p++)
54     {
55         sendcounts[p] = ((number_of_particles)/size); /* array of number of particles
56 assigned for current rank*/
57         if (r > 0) {
58             sendcounts[p] = sendcounts[p] + 1;
59             r--;
60         }
61
62         displs[p] = s; /*start boundary of particles in current rank */
63         s += sendcounts[p];
64     }
65
66     if (rank == (size-1))
67     {
68         *start = displs[rank];
69         *end = number_of_particles;
70     }
71     else
72     {
73         *start = displs[rank]; /* start n end in case of parallelizing loops*/
74         *end = displs[rank+1];
75     }
76 }
77
78 void generate_pos_vel() /* Function to initialize position and velocity*/
79 {
80     for (int i = 0; i < Np; i++)
81     {
82         position[i].x = (rand()/((double) RAND_MAX + 1)) * range;
83         position[i].y = (rand()/((double) RAND_MAX + 1)) * range;
84         position[i].z = (rand()/((double) RAND_MAX + 1)) * range;
85     }
86 }

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82         velocity[i].vx= ((double) rand()/RAND_MAX*2.0-1.0)*0.0001;
83         velocity[i].vy= ((double) rand()/RAND_MAX*2.0-1.0)*0.0001;
84         velocity[i].vz= ((double) rand()/RAND_MAX*2.0-1.0)*0.0001;
85     }
86 }
87
88 void cal_acceleration() /* function to calculate resultant acceleration of current
particle in particular dt*/
{
89     float del_x,del_y,del_z,invr,invr3,f;
90
91     for(int i=0;i<sendcounts[rank];i++)
92     {
93         a[i].ax = 0.0;
94         a[i].ay = 0.0;
95         a[i].az = 0.0;
96         for(int j=0;j<Np;j++)
97         {
98             if((i+(displs[rank])) != j)
99             {
100                 del_x = position[i+(displs[rank])].x - position[j].x;
101                 del_y = position[i+(displs[rank])].y - position[j].y;
102                 del_z = position[i+(displs[rank])].z - position[j].z;
103                 invr = 1.0 /
sqrt((del_x*del_x)+(del_y*del_y)+(del_z*del_z)+DBL_EPSILON);
104                 invr3 = pow(invr,3);
105                 f = m*invr3;
106
107                 a[i].ax += f*del_x;
108                 a[i].ay += f*del_y;
109                 a[i].az += f*del_z;
110             }
111         }
112     }
113 }
114
115 void cal_vel() /* function to calculate resultant velocity of current particle in
particular dt*/
{
116     for (int i = 0; i < sendcounts[rank]; i++)
117     {
118         velocity[i+(displs[rank])].vx += (dt*a[i].ax);
119         velocity[i+(displs[rank])].vy += (dt*a[i].ay);
120         velocity[i+(displs[rank])].vz += (dt*a[i].az);
121     }
122 }
123
124 void cal_position() /* function to update position of particles from resultant velocity
and acceleration*/
{
125     for (int i = 0; i < sendcounts[rank]; i++)
126     {
127         position[i+(displs[rank])].x +=
(dt*velocity[i+(displs[rank])].vx)+(0.5*dt*dt*a[i].ax);
128         position[i+(displs[rank])].y +=
(dt*velocity[i+(displs[rank])].vy)+(0.5*dt*dt*a[i].ay);
129         position[i+(displs[rank])].z +=
(dt*velocity[i+(displs[rank])].vz)+(0.5*dt*dt*a[i].az);
130     }
131 }
132
133 void write_p() /* function to write the updated positions at all time steps*/
{
134     FILE *fp1 = fopen("pos.txt", "a");
135     for(int i=0; i<Np; i++)
136     {
137         fprintf(fp1,"%f %f %f \n",position[i].x,position[i].y,position[i].z);
138     }
139     fprintf(fp1,"\n");
140     fclose(fp1);
141 }
142
143 void sim() /* function to start n particle simulation*/
{
144     MPI_Bcast(position,Np,POSITION,0,MPI_COMM_WORLD);
145     MPI_Bcast(velocity,Np,VELOCITY,0,MPI_COMM_WORLD);
146
147     int iterations = total_time / dt;
148
149     for(int t=0;t<iterations;t++)
150     {
151         cal_acceleration();
152         cal_vel();
153         cal_position();
154     }
155 }

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159
160 MPI_Allgather(position+(displs[rank]), sendcounts[rank], POSITION, position, sendcounts, displs,
    POSITION, MPI_COMM_WORLD);
161
162 MPI_Allgather(velocity+(displs[rank]), sendcounts[rank], VELOCITY, velocity, sendcounts, displs,
    VELOCITY, MPI_COMM_WORLD);
163
164     if(rank==0)
165     { write_p(); }
166 }
167
168 int main(int argc, char **argv)
169 {
170     srand(time(0));
171     MPI_Init(&argc, &argv); /* Initiate MPI*/
172
173     MPI_Barrier(MPI_COMM_WORLD);
174     double tcal = MPI_Wtime(); /* Computation start time*/
175
176     if (argc >= 2)
177         Np = atoi(argv[1]);
178     else
179         Np = Np_d;
180
181     if (argc >= 3)
182         total_time = atoi(argv[2]); /* user input through command line arguments */
183     else
184         total_time = time_d;
185
186     if (argc >= 4)
187         dt = atof(argv[3]);
188     else
189         dt = dt_d;
190
191     MPI_Comm_size(MPI_COMM_WORLD, &size); /* size and rank of MPI*/
192     MPI_Comm_rank(MPI_COMM_WORLD, &rank);
193
194     MPI_Type_create_struct(3, lengths, displacements, types, &POSITION);
195     MPI_Type_commit(&POSITION); /*committing user
defined MPI data types*/
196
197     MPI_Type_create_struct(3, lengths, displacements, types, &VELOCITY);
198     MPI_Type_commit(&VELOCITY);
199
200     sendcounts = malloc(sizeof(int)*size); /* allocating memory for arrays*/
201     displs = malloc(sizeof(int)*size);
202
203     P_r(Np, size, rank, &start, &end, sendcounts, displs); /* calling function to calculate send
counts and displacements*/
204
205     position = (Pos *) malloc(Np * sizeof(Pos)); /* allocating memory for structs*/
206     velocity = (Vel *) malloc(Np * sizeof(Vel));
207     a = (Acc *) malloc(sendcounts[rank] * sizeof(Acc));
208
209     if (rank == 0)
210     {
211         generate_pos_vel(); /* initializing position and velocity in root process*/
212
213         FILE *fp = fopen("pos.txt", "w"); /*writing initial positions*/
214         for(int i=0; i<Np; i++)
215         {
216             fprintf(fp, "%f %f %f \n", position[i].x, position[i].y, position[i].z);
217         }
218         fprintf(fp, "\n");
219         fclose(fp);
220     }
221
222     sim(); /* function call for particle simulation */
223
224     MPI_Barrier(MPI_COMM_WORLD);
225     double elapsedt = MPI_Wtime() - tcal; /* computational time taken to complete the
process*/
226
227     if (rank==0)
228     {
229         printf("Np=%d, Total time= %f, dt=%f \n", Np, total_time, dt);
230         printf("run time = %f \n", elapsedt);
231     }
232
233     MPI_Finalize();
234 }
235

```