

# FDPS講習会

## サンプルコード編

細野 七月

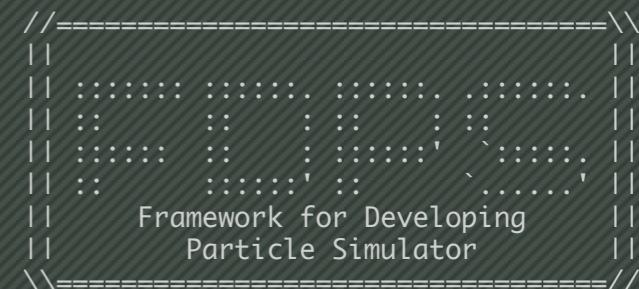
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2016/07/06 FDPS講習会

## コード構成

## ●ユーザーが書くべきもの

- `#include <particle_simulator.h>`
  - 粒子クラスと必要なメンバ関数
  - 相互作用関数
  - 時間積分ルーチン
  - I/O (粒子クラスのI/Oと、FileHeaderクラス)



# サンプルコード

- ## ● 今回のサンプルコードの内容

# 流体 (Smoothed Particle Hydrodynamics)

重力 (w/ and w/o Phantom-GRAPE (Tanikawa+, 2011; 2012))

- 本スライドでは、重力を計算するコードを取り上げて解説する。

- ・時間積分法はleap-frog法
  - ・初期条件はその場生成(ファイル読み込みではない)
  - ・ファイル構成

# user-defined.hpp

# nbody.cpp



# user-defined.hpp

1 lines (151 LOC) | 3.95 KB

```
1 #pragma once
2 class FileHeader{
3 public:
4     PS::S64 n_body;
5     PS::F64 time;
6     PS::S32 readAscii(FILE * fp) {
7         fscanf(fp, "%lf\n", &time);
8         fscanf(fp, "%lld\n", &n_body);
9         return n_body;
10    }
11    void writeAscii(FILE* fp) const {
12        fprintf(fp, "%e\n", time);
13        fprintf(fp, "%lld\n", n_body);
14    }
15 };
16
17 class FPGrav{
18 public:
19     PS::S64 id;
20     PS::F64 mass;
21     PS::F64vec pos;
22     PS::F64vec vel;
23     PS::F64vec acc;
24     PS::F64 note;
```

# user-defined.hpp

1 lines (151 SLOC) | 3.95 KB

```
1 #pragma once
2 class FileHeader{ クラス
3 public:
4     PS::S64 n_body;
5     PS::F64 time;
6     PS::S32 readAscii(FILE * fp) {
7         fscanf(fp, "%lf\n", &time);
8         fscanf(fp, "%lld\n", &n_body);
9         return n_body;
10    }
11    void writeAscii(FILE* fp) const {
12        fprintf(fp, "%e\n", time);
13        fprintf(fp, "%lld\n", n_body);
14    }
15 };
16
17 class FPGrav{
18 public:
19     PS::S64 id;
20     PS::F64 mass;
21     PS::F64vec pos;
22     PS::F64vec vel;
23     PS::F64vec acc;
24 }
```

# user-defined.hpp

111 lines (151 SLOC) | 5.95 KB

```
1 #pragma once
2 class FileHeader{
3 public:
4     PS::S64 n_body;
5     PS::F64 time;
6     PS::S32 readAscii(FILE * fp) {
7         fscanf(fp, "%lf\n", &time);
8         fscanf(fp, "%lld\n", &n_body);
9         return n_body;
10    }
11    void writeAscii(FILE* fp) const {
12        fprintf(fp, "%e\n", time);
13        fprintf(fp, "%lld\n", n_body);
14    }
15};
```

```
17 class FPGrav{
18 public:
19     PS::S64 id;
20     PS::F64 mass;
21     PS::F64vec pos;
22     PS::F64vec vel;
23     PS::F64vec acc;
```

FileHeaderクラス

```
16  
17 class FPGrav{  
18 public:  
19     PS::S64    id;  
20     PS::F64    mass;  
21     PS::F64vec pos;  
22     PS::F64vec vel;  
23     PS::F64vec acc;  
24     PS::F64    pot;  
25  
26     static PS::F64 eps;  
27  
28     PS::F64vec getPos() const {  
29         return pos;  
30     }  
31  
32     PS::F64 getCharge() const {  
33         return mass;  
34     }  
35  
36     void copyFromFP(const FPGrav & fp){  
37         mass = fp.mass;  
38         pos  = fp.pos;  
39     }  
40  
41     void copyFromForce(const FPGrav & force) {  
42         acc = force.acc;  
43         pot = force.pot;  
44     }
```

## 粒子クラス

```
16  
17 class FPGrav{  
18 public:  
19     PS::S64    id;  
20     PS::F64    mass;  
21     PS::F64vec pos;      粒子物理量  
22     PS::F64vec vel;  
23     PS::F64vec acc;  
24     PS::F64    pot;  
25  
26     static PS::F64 eps;  
27  
28     PS::F64vec getPos() const {  
29         return pos;  
30     }  
31  
32     PS::F64 getCharge() const {  
33         return mass;  
34     }  
35  
36     void copyFromFP(const FPGrav & fp){  
37         mass = fp.mass;  
38         pos  = fp.pos;  
39     }  
40  
41     void copyFromForce(const FPGrav & force) {  
42         acc = force.acc;  
43         pot = force.pot;  
44     }
```

```
19 PS::S64    id;
20 PS::F64    mass;
21 PS::F64vec pos;
22 PS::F64vec vel;
23 PS::F64vec acc;
24 PS::F64    pot;
25
26 static PS::F64 eps;
27
28 PS::F64vec getPos() const {
29     return pos;
30 }
31
32 PS::F64 getCharge() const {
33     return mass;
34 }
35
36 void copyFromFP(const FPGrav & fp){
37     mass = fp.mass;
38     pos  = fp.pos;
39 }
40
41 void copyFromForce(const FPGrav & force) {
42     acc = force.acc;
43     pot = force.pot;
44 }
45
46 void clear() {
47     acc = 0.0;
```

FDPSにデータを渡すための  
メンバ関数

## I/Oメンバ関数

```
44
45
46 void clear() {
47     acc = 0.0;
48     pot = 0.0;
49 }
50
51 void writeAscii(FILE* fp) const {
52     fprintf(fp, "%lld\t%g\t%g\t%g\t%g\t%g\t%g\t%g\n",
53             this->id, this->mass,
54             this->pos.x, this->pos.y, this->pos.z,
55             this->vel.x, this->vel.y, this->vel.z);
56 }
57
58 void readAscii(FILE* fp) {
59     fscanf(fp, "%lld\t%lf\t%lf\t%lf\t%lf\t%lf\t%lf\t%lf\n",
60             &this->id, &this->mass,
61             &this->pos.x, &this->pos.y, &this->pos.z,
62             &this->vel.x, &this->vel.y, &this->vel.z);
63 }
64
65 };
66
67
68 #ifdef ENABLE_PHANTOM_GRAPE_X86
69
70
71 template <class TParticle>
```

&this->vel.x, &this->vel.y, &this->vel.z);

相互作用

## テンプレート関数

(w/ Phantom-GRAPE)

```
#ifdef ENABLE_PHANTOM_GRAPE_X86

template <class TParticleJ>
void CalcGravity(const FPGrav * iptcl,
                 const PS::S32 ni,
                 const TParticleJ * jptcl,
                 const PS::S32 nj,
                 FPGrav * force) {
    const PS::S32 nipipe = ni;
    const PS::S32 njpipe = nj;
    PS::F64 (*xi)[3] = (PS::F64 (*)[3])malloc(sizeof(PS::F64) * nipipe * PS::DIMENSION);
    PS::F64 (*ai)[3] = (PS::F64 (*)[3])malloc(sizeof(PS::F64) * nipipe * PS::DIMENSION);
    PS::F64 *pi      = (PS::F64 *)malloc(sizeof(PS::F64) * nipipe);
    PS::F64 (*xj)[3] = (PS::F64 (*)[3])malloc(sizeof(PS::F64) * njpipe * PS::DIMENSION);
    PS::F64 *mj      = (PS::F64 *)malloc(sizeof(PS::F64) * njpipe);
    for(PS::S32 i = 0; i < ni; i++) {
        xi[i][0] = iptcl[i].getPos()[0];
        xi[i][1] = iptcl[i].getPos()[1];
        xi[i][2] = iptcl[i].getPos()[2];
        ai[i][0] = 0.0;
        ai[i][1] = 0.0;
        ai[i][2] = 0.0;
```

```
96     xj[j][2] = jptcl[j].getPos()[2];
97     mj[j]    = jptcl[j].getCharge();
98     xj[j][0] = jptcl[j].pos[0];
99     xj[j][1] = jptcl[j].pos[1];
100    xj[j][2] = jptcl[j].pos[2];
101    mj[j]    = jptcl[j].mass;
102
103    PS::S32 devid = PS::Comm::getThreadNum();
104    g5_set_xmjMC(devid, 0, nj, xj, mj);
105    g5_set_nMC(devid, nj);
106    g5_calculate_force_on_xMC(devid, xi, ai, pi, ni);
107    for(PS::S32 i = 0; i < ni; i++) {
108        force[i].acc[0] += ai[i][0];
109        force[i].acc[1] += ai[i][1];
110        force[i].acc[2] += ai[i][2];
111        force[i].pot    -= pi[i];
112    }
113    free(xi);
114    free(ai);
115    free(pi);
116    free(xj);
117    free(mj);
118}
119
120 #else
121
122 template <class TParticle>
123 void CalcGravity(const FPGrav * ep_i,
124                  const PS::S32 n_in
```

```
21
22 template <class TParticleJ>
23 void CalcGravity(const FPGrav * ep_i,
24                 const PS::S32 n_ip,
25                 const TParticleJ * ep_j,
26                 const PS::S32 n_jp,
27                 FPGrav * force) {
28
29     PS::F64 eps2 = FPGrav::eps * FPGrav::eps;
30
31     for(PS::S32 i = 0; i < n_ip; i++){
32         PS::F64vec xi = ep_i[i].getPos();
33         PS::F64vec ai = 0.0;
34         PS::F64 poti = 0.0;
35
36         for(PS::S32 j = 0; j < n_jp; j++){
37             PS::F64vec rij = xi - ep_j[j].getPos();
38             PS::F64 r3_inv = rij * rij + eps2;
39             PS::F64 r_inv = 1.0/sqrt(r3_inv);
40             r3_inv = r_inv * r_inv;
41             r_inv *= ep_j[j].getCharge();
42             r3_inv *= r_inv;
43             ai -= r3_inv * rij;
44             poti -= r_inv;
45         }
46         force[i].acc += ai;
47         force[i].pot += poti;
48     }
49
50 #endif
```

相互作用  
テンプレート関数  
(w/o Phantom-GRAPE)

```

21 template <class TParticleJ>
22
23 void CalcGravity(const FPGrav * ep_i,
24                  const PS::S32 n_ip,
25                  const TParticleJ * ep_j,
26                  const PS::S32 n_jp,
27                  FPGrav * force) {
28
29     PS::F64 eps2 = FPGrav::eps * FPGrav::eps;
30
31     for(PS::S32 i = 0; i < n_ip; i++){
32         PS::F64vec xi = ep_i[i].getPos();
33         PS::F64vec ai = 0.0;
34         PS::F64 poti = 0.0;
35
36         for(PS::S32 j = 0; j < n_jp; j++){
37             PS::F64vec rij = xi - ep_j[j].getPos();
38             PS::F64 r3_inv = rij * rij + eps2;
39             PS::F64 r_inv = 1.0/sqrt(r3_inv);
40             r3_inv = r_inv * r_inv;
41             r_inv *= ep_j[j].getCharge();
42             r3_inv *= r_inv;
43             ai -= r3_inv * rij;
44             poti -= r_inv;
45         }
46         force[i].acc += ai;
47         force[i].pot += poti;
48     }
49
50 #endif

```

相互作用

テンプレート関数

(w/o Phantom-GRAPE)

```

21 template <class TParticleJ>
22 void CalcGravity(const FPGrav * ep_i,
23                  const PS::S32 n_ip,
24                  const TParticleJ * ep_j,
25                  const PS::S32 n_jp,
26                  FPGrav * force) {
27
28     PS::F64 eps2 = FPGrav::eps * FPGrav::eps;
29
30     for(PS::S32 i = 0; i < n_ip; i++){
31         PS::F64vec xi = ep_i[i].getPos();
32
33         PS::F64vec ai = 0.0;
34
35         PS::F64 poti = 0.0;
36
37         for(PS::S32 j = 0; j < n_jp; j++){
38             PS::F64vec rij = xi - ep_j[j].getPos();
39
40             PS::F64 r3_inv = rij * rij + eps2;
41
42             PS::F64 r_inv = 1.0/sqrt(r3_inv);
43
44             r3_inv = r_inv * r_inv;
45
46             r_inv *= ep_j[j].getCharge();
47
48             r3_inv *= r_inv;
49
50             ai -= r3_inv * rij;
51
52             poti -= r_inv;
53
54         }
55
56         force[i].acc += ai;
57
58         force[i].pot += poti;
59
60     }
61
62 }
63
64 #endif

```

相互作用

テンプレート関数

(w/o Phantom-GRAPE)

# 相互作用template関数

- 本当は2つ(Super Particleからの寄与と通常Particleからの寄与)書く必要がある。
- 今回はどうちらも相互作用形としては同じなので、templateを使って1つで済ます。



# nbody.cpp

```
1 #include<iostream>
2 #include<fstream>
3 #include<unistd.h>
4 #include<sys/stat.h>
5 #include<particle_simulator.hpp>
6 #ifdef ENABLE_PHANTOM_GRAPE_X86
7 #include <gp5util.h>
8 #endif
9 #ifdef ENABLE_GPU_CUDA
10 #define MULTI_WALK
11 #include"force_gpu_cuda.hpp"
12 #endif
13 #include "user-defined.hpp"
14
15 void makeColdUniformSphere(const PS::F64 mass_glb,
16                             const PS::S64 n_glb,
17                             const PS::S64 n_loc,
18                             PS::F64 *& mass,
19                             PS::F64vec *& pos,
20                             PS::F64vec *& vel,
21                             const PS::F64 eng = -0.25,
22                             const PS::S32 seed = 0) {
23
24     assert(n_glb > 0);
25
26     PS::F64 pi = 3.141592653589793;
27     PS::F64 r = sqrt(mass_glb / (4.0 * pi * n_loc));
28     PS::F64 x0 = 0.0;
29     PS::F64 y0 = 0.0;
30     PS::F64 z0 = 0.0;
31
32     for(PS::S32 i = 0; i < n_glb; i++) {
33         PS::F64 phi = 2.0 * pi * rand(seed) / n_loc;
34         PS::F64 theta = pi * rand(seed) / n_glb;
35
36         PS::F64 x = r * sin(theta) * cos(phi);
37         PS::F64 y = r * sin(theta) * sin(phi);
38         PS::F64 z = r * cos(theta);
39
40         pos[i] = PS::F64vec(x, y, z);
41
42         PS::F64 vx = 0.0;
43         PS::F64 vy = 0.0;
44         PS::F64 vz = 0.0;
45
46         if(eng < 0.0) {
47             vx = -sqrt(-2.0 * log(1.0 - rand(seed)));
48             vy = -sqrt(-2.0 * log(1.0 - rand(seed))) * sin(phi);
49             vz = -sqrt(-2.0 * log(1.0 - rand(seed))) * cos(phi);
50
51             if(vx == 0.0 && vy == 0.0 && vz == 0.0) {
52                 vx = 0.001;
53                 vy = 0.001;
54                 vz = 0.001;
55             }
56
57             vel[i] = PS::F64vec(vx, vy, vz);
58
59         } else {
60             vx = sqrt(eng) * sin(theta) * cos(phi);
61             vy = sqrt(eng) * sin(theta) * sin(phi);
62             vz = sqrt(eng) * cos(theta);
63
64             if(vx == 0.0 && vy == 0.0 && vz == 0.0) {
65                 vx = 0.001;
66                 vy = 0.001;
67                 vz = 0.001;
68             }
69
70             vel[i] = PS::F64vec(vx, vy, vz);
71
72         }
73
74     }
75
76 }
```

# nbody.cpp

555 lines (320 SLOC) | 11.4 KB

```
1 #include<iostream>
2 #include<fstream>
3 #include<unistd.h>
4 #include<sys/stat.h>
5 #include<particle_simulator.hpp> FDPSのinclude
6 #ifdef ENABLE_PHANTOM_GRAPE_X86
7 #include <gp5util.h>
8 #endif
9 #ifdef ENABLE_CUDA
10 #define MULTI_WALK
11 #include"force_gpu_cuda.hpp"
12 #endif
13 #include "user-defined.hpp"
14
15 void makeColdUniformSphere(const PS::F64 mass_glb,
16                           const PS::S64 n_glb,
17                           const PS::S64 n_loc,
18                           PS::F64 *& mass,
19                           PS::F64vec *& pos,
20                           PS::F64vec *& vel,
21                           const PS::F64 eng = -0.25,
22                           const PS::S32 seed = 0) {
23
24     assert(n_glb > 0);
25
26     PS::F64 r = 1.0;
27     PS::F64 v = 0.0;
28
29     PS::F64 pi = 3.141592653589793238462643383279502884197169399375105820974944592307816406286208998628034825342117067982148086513282306647818915654848204587732991830484541326544634150390322016725886934157436394572489055895435499705938344695194953596774411071501056485337515420991895885455249353090115748334114732160704392333593344612484813829086938635662018553172011302918927829257125053759455349060688651629515359475985243750020359731732816096318505923213363177158934345941246835623519037143144295588174883754739056548945292389328125712268968748292092499377119494075895468116930686459953951258597823354524749460656318152959403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599244883418711093750515070597512436494034418527347343524321326537274894080893533515624869441574605085375388281194601565846730534351452707204127382364354924897968429493970933745245102989131503420562393377772156946034013629552251145434189047446730538352792591393457362705053759991592589975099604145472994115735759403599
```

```
78     delete [] mass;
79     delete [] pos;
80     delete [] vel;
81 }
82
83 template<class Tpsys>
84 void kick(Tpsys & system,
85           const PS::F64 dt) {
86     PS::S32 n = system.getNumberOfParticleLocal();
87     for(PS::S32 i = 0; i < n; i++) {
88         system[i].vel += system[i].acc * dt;
89     }
90 }
91
92 template<class Tpsys>
93 void drift(Tpsys & system,
94            const PS::F64 dt) {
95     PS::S32 n = system.getNumberOfParticleLocal();
96     for(PS::S32 i = 0; i < n; i++) {
97         system[i].pos += system[i].vel * dt;
98     }
99 }
100
101 template<class Tpsys>
102 void calcEnergy(const Tpsys & system,
103                  PS::F64 & etot,
104                  PS::F64 & ekin,
105                  PS::F64 & epot,
106                  const bool clear=true){
```

leap-frog法による  
時間積分

```
78     delete [] mass;
79     delete [] pos;
80     delete [] vel;
81 }
82
83 template<class Tpsys>
84 void kick(Tpsys & system,
85           const PS::F64 dt) {
86     PS::S32 n = system.getNumberOfParticleLocal();
87     for(PS::S32 i = 0; i < n; i++) {
88         system[i].vel += system[i].acc * dt;
89     }
90 }
91
92 template<class Tpsys>
93 void drift(Tpsys & system,
94            const PS::F64 dt) {
95     PS::S32 n = system.getNumberOfParticleLocal();
96     for(PS::S32 i = 0; i < n; i++) {
97         system[i].pos += system[i].vel * dt;
98     }
99 }
100
101 template<class Tpsys>
102 void calcEnergy(const Tpsys & system,
103                  PS::F64 & etot,
104                  PS::F64 & ekin,
105                  PS::F64 & epot,
106                  const bool clear=true){
```

getNumberOfParticleLocal()

で粒子数が取得できる

```
78     delete [] mass;
79     delete [] pos;
80     delete [] vel;
81 }
82
83 template<class Tpsys>
84 void kick(Tpsys & system,
85           const PS::F64 dt) {
86     PS::S32 n = system.getNumberOfParticleLocal();
87     for(PS::S32 i = 0; i < n; i++) {
88         system[i].vel += system[i].acc * dt;
89     } 粒子群クラスに[i]をつけると
90 } i粒子のデータが取得できる
91
92 template<class Tpsys>
93 void drift(Tpsys & system,
94            const PS::F64 dt) {
95     PS::S32 n = system.getNumberOfParticleLocal();
96     for(PS::S32 i = 0; i < n; i++) {
97         system[i].pos += system[i].vel * dt;
98     }
99 }
100
101 template<class Tpsys>
102 void calcEnergy(const Tpsys & system,
103                  PS::F64 & etot,
104                  PS::F64 & ekin,
105                  PS::F64 & epot,
106                  const bool clear=true){
```

```
163 PS::F64 FPGrav::eps = 1.0/32.0;
164
165 int main(int argc, char *argv[]) { メイン関数開始
166     std::cout<<std::setprecision(15);
167     std::cerr<<std::setprecision(15);
168
169     PS::Initialize(argc, argv);
170     PS::F32 theta = 0.5;
171     PS::S32 n_leaf_limit = 8;
172     PS::S32 n_group_limit = 64;
173     PS::F32 time_end = 10.0;
174     PS::F32 dt = 1.0 / 128.0;
175     PS::F32 dt_diag = 1.0 / 8.0;
176     PS::F32 dt_snap = 1.0;
177     char dir_name[1024];
178     PS::S64 n_tot = 1024;
179     PS::S32 c;
180     sprintf(dir_name,"./result");
181     opterr = 0;
182     while((c=getopt(argc,argv,"i:o:d:D:t:T:l:n:N:hs:")) != -1){
183         switch(c){
184             case 'o':
185                 sprintf(dir_name,optarg);
186                 break;
187             case 't':
188                 theta = atof(optarg);
189                 std::cerr << "theta =" << theta << std::endl;
190                 break;
191             case 'T':
```

```
163 PS::F64 FPGrav::eps = 1.0/32.0;
164
165 int main(int argc, char *argv[]) {
166     std::cout<<std::setprecision(15);
167     std::cerr<<std::setprecision(15);
168
169     PS::Initialize(argc, argv);      FDPS初期化
170     PS::F32 theta = 0.5;
171     PS::S32 n_leaf_limit = 8;
172     PS::S32 n_group_limit = 64;
173     PS::F32 time_end = 10.0;
174     PS::F32 dt = 1.0 / 128.0;
175     PS::F32 dt_diag = 1.0 / 8.0;
176     PS::F32 dt_snap = 1.0;
177     char dir_name[1024];
178     PS::S64 n_tot = 1024;
179     PS::S32 c;
180     sprintf(dir_name,"./result");
181     opterr = 0;
182     while((c=getopt(argc,argv,"i:o:d:D:t:T:l:n:N:hs:")) != -1){
183         switch(c){
184             case 'o':
185                 sprintf(dir_name,optarg);
186                 break;
187             case 't':
188                 theta = atof(optarg);
189                 std::cerr << "theta =" << theta << std::endl;
190                 break;
191             case 'T':
```

```
179 PS::S32 c;                                コマンドライン
180 sprintf(dir_name,"./result");              引数の解析
181 opterr = 0;
182 while((c=getopt(argc,argv,"i:o:d:D:t:T:l:n:N:hs:")) != -1){
183     switch(c){
184     case 'o':
185         sprintf(dir_name,optarg);
186         break;
187     case 't':
188         theta = atof(optarg);
189         std::cerr << "theta =" << theta << std::endl;
190         break;
191     case 'T':
192         time_end = atof(optarg);
193         std::cerr << "time_end = " << time_end << std::endl;
194         break;
195     case 's':
196         dt = atof(optarg);
197         std::cerr << "time_step = " << dt << std::endl;
198         break;
199     case 'd':
200         dt_diag = atof(optarg);
201         std::cerr << "dt_diag = " << dt_diag << std::endl;
202         break;
203     case 'D':
204         dt_snap = atof(optarg);
205         std::cerr << "dt_snap = " << dt_snap << std::endl;
206         break;
207     case 'l':
```

```
208     n_leaf_limit = atoi(optarg),
209     std::cerr << "n_leaf_limit = " << n_leaf_limit << std::endl;
210     break;
211 case 'l':
212     n_group_limit = atoi(optarg);
213     std::cerr << "n_group_limit = " << n_group_limit << std::endl;
214     break;
215 case 'N':
216     n_tot = atoi(optarg);
217     std::cerr << "n_tot = " << n_tot << std::endl;
218     break;
219 case 'h':
220     if(PS::Comm::getRank() == 0) {
221         printHelp();
222     }
223     PS::Finalize();
224     return 0;
225 default:
226     if(PS::Comm::getRank() == 0) {
227         std::cerr<<"No such option! Available options are here."<<std::endl;
228         printHelp();
229     }
230     PS::Abort();
231 }
232
233 makeOutputDirectory(dir_name);
234
235 std::ofstream fout_eng;
```

# 粒子群クラスの 生成・初期化

```
246
247     PS::ParticleSystem<FPGrav> system_grav;
248     system_grav.initialize();
249     PS::S32 n_loc      = 0;
250     PS::F32 time_sys = 0.0;
251     if(PS::Comm::getRank() == 0) {
252         setParticlesColdUniformSphere(system_grav, n_tot, n_loc);
253     } else {
254         system_grav.setNumberOfParticleLocal(n_loc);
255     }
256
257     const PS::F32 coef_ema = 0.3;
258     PS::DomainInfo dinfo;
259     dinfo.initialize(coef_ema);
260     dinfo.collectSampleParticle(system_grav);
261     dinfo.decomposeDomain();
262     system_grav.exchangeParticle(dinfo);
263     n_loc = system_grav.getNumberOfParticleLocal();
264
265 #ifdef ENABLE_PHANTOM_GRAPE_X86
266     g5_open();
267     g5_set_eps_to_all(FPGrav::eps);
268 #endif
269
270     PS::TreeForForceLong<FPGrav, FPGrav, FPGrav>::Monopole tree_grav;
271     tree_grav.initialize(n_tot, theta, n_leaf_limit, n_group_limit);
272 #ifdef MULTI_WALK
273     const PS::S32 n_walk_limit = 200;
274     const PS::S32 tag_max = 1;
```

## ドメイン情報の 生成・初期化 領域分割

```
246
247     PS::ParticleSystem<FPGrav> system_grav;
248     system_grav.initialize();
249     PS::S32 n_loc      = 0;
250     PS::F32 time_sys  = 0.0;
251     if(PS::Comm::getRank() == 0) {
252         setParticlesColdUniformSphere(system_grav, n_tot, n_loc);
253     } else {
254         system_grav.setNumberOfParticleLocal(n_loc);
255     }
256
257     const PS::F32 coef_ema = 0.3;
258     PS::DomainInfo dinfo;
259     dinfo.initialize(coef_ema);
260     dinfo.collectSampleParticle(system_grav);
261     dinfo.decomposeDomain();
262     system_grav.exchangeParticle(dinfo);
263     n_loc = system_grav.getNumberOfParticleLocal();
264
265 #ifdef ENABLE_PHANTOM_GRAPE_X86
266     g5_open();
267     g5_set_eps_to_all(FPGrav::eps);
268 #endif
269
270     PS::TreeForForceLong<FPGrav, FPGrav, FPGrav>::Monopole tree_grav;
271     tree_grav.initialize(n_tot, theta, n_leaf_limit, n_group_limit);
272 #ifdef MULTI_WALK
273     const PS::S32 n_walk_limit = 200;
274     const PS::S32 tag_max = 1;
```

```
268 #endif
269
270     PS::TreeForForceLong<FPGrav, FPGrav, FPGrav>::Monopole tree_grav;
271     tree_grav.initialize(n_tot, theta, n_leaf_limit, n_group_limit);
272 #ifdef MULTI_WALK 相互作用ツリークラスの
273     const PS::S32 n_walk_limit = 200;
274     const PS::S32 tag_max = 100;
275     tree_grav.calcForceAllAndWriteBackMultiWalk(DispatchKernelWithSP,
276                                                 RetrieveKernel,
277                                                 tag_max,
278                                                 system_grav,
279                                                 dinfo,
280                                                 n_walk_limit);
281 #else
282     tree_grav.calcForceAllAndWriteBack(CalcGravity<FPGrav>,
283                                         CalcGravity<PS::SPJMonopole>,
284                                         system_grav,
285                                         dinfo);
286 #endif
287     PS::F64 Epot0, Ekin0, Etot0, Epot1, Ekin1, Etot1;
288     calcEnergy(system_grav, Etot0, Ekin0, Epot0);
289     PS::F64 time_diag = 0.0;
290     PS::F64 time_snap = 0.0;
291     PS::S64 n_loop = 0;
292     PS::S32 id_snap = 0;
293     while(time_sys < time_end){
294         if( (time_sys >= time_snap) || ( (time_sys + dt) - time_snap ) > (time_snap - time_sys)
295             char filename[256];
```

```
268 #endif
269
270     PS::TreeForForceLong<FPGrav, FPGrav, FPGrav>::Monopole tree_grav;
271     tree_grav.initialize(n_tot, theta, n_leaf_limit, n_group_limit);
272 #ifdef MULTI_WALK
273     const PS::S32 n_walk_limit = 200;
274     const PS::S32 tag_max = 1;
275     tree_grav.calcForceAllAndWriteBackMultiWalk(DispatchKernelWithSP,
276                                                 RetrieveKernel,
277                                                 tag_max,
278                                                 system_grav,
279                                                 dinfo,
280                                                 n_walk_limit);

```

## 力の計算

```
281 #else
282     tree_grav.calcForceAllAndWriteBack(CalcGravity<FPGrav>,
283                                         CalcGravity<PS::SPJMonopole>,
284                                         system_grav,
285                                         dinfo);
286 #endif
287
288     PS::F64 Epot0, Ekin0, Etot0, Epot1, Ekin1, Etot1;
289     calcEnergy(system_grav, Etot0, Ekin0, Epot0);
290     PS::F64 time_diag = 0.0;
291     PS::F64 time_snap = 0.0;
292     PS::S64 n_loop = 0;
293     PS::S32 id_snap = 0;
294     while(time_sys < time_end){
295         if( (time_sys >= time_snap) || ( (time_sys + dt) - time_snap ) > (time_snap - time_sys)
```

```
        char filename[256];
```

```
289 PS::F64 time_diag = 0.0;
290 PS::F64 time_snap = 0.0;
291 PS::S64 n_loop = 0;
292 PS::S32 id_snap = 0;          時間積分
293 while(time_sys < time_end){
294     if( (time_sys >= time_snap) || ( (time_sys + dt) - time_snap ) > (time_snap - time_sys)
295         char filename[256];
296         sprintf(filename, "%s/%04d.dat", dir_name, id_snap++);
297         FileHeader header;
298         header.time    = time_sys;
299         header.n_body = system_grav.getNumberOfParticleGlobal();
300         system_grav.writeParticleAscii(filename, header);
301         time_snap += dt_snap;
302     }
303
304     calcEnergy(system_grav, Etot1, Ekin1, Epot1);
305
306     if(PS::Comm::getRank() == 0){
307         if( (time_sys >= time_diag) || ( (time_sys + dt) - time_diag ) > (time_diag - time_sys)
308             fout_eng << time_sys << " " << (Etot1 - Etot0) / Etot0 << std::endl;
309             fprintf(stderr, "time: %10.7f energy error: %+e\n",
310                     time_sys, (Etot1 - Etot0) / Etot0);
311             time_diag += dt_diag;
312         }
313     }
314
315     kick(system_grav, dt * 0.5);
```

```
316     kick(system_grav, dt * 0.5);
317
318     time_sys += dt;
319     drift(system_grav, dt);
320
321     if(n_loop % 4 == 0){
322         dinfo.decomposeDomainAll(system_grav);
323     }
324
325     system_grav.exchangeParticle(dinfo);
326 #ifdef MULTI_WALK
327     tree_grav.calcForceAllAndWriteBackMultiWalk(DispatchKernelWithSP,
328                                                 RetrieveKernel,
329                                                 tag_max,
330                                                 system_grav,
331                                                 dinfo,
332                                                 n_walk_limit,
333                                                 true);
334 #else
335     tree_grav.calcForceAllAndWriteBack(CalcGravity<FPGrav>,
336                                         CalcGravity<PS::SPJMonopole>,
337                                         system_grav,
338                                         dinfo);
339 #endif
340
341     kick(system_grav, dt * 0.5);
342
343     n_loop++;
```

```
325     system_grav.exchangeParticles(dinfo),
326 #ifdef MULTI_WALK
327     tree_grav.calcForceAllAndWriteBackMultiWalk(DispatchKernelWithSP,
328                                                 RetrieveKernel,
329                                                 tag_max,
330                                                 system_grav,
331                                                 dinfo,
332                                                 n_walk_limit,
333                                                 true);
334 #else
335     tree_grav.calcForceAllAndWriteBack(CalcGravity<FPGrav>,
336                                         CalcGravity<PS::SPJMonopole>,
337                                         system_grav,
338                                         dinfo);
339 #endif
340
341     kick(system_grav, dt * 0.5);
342
343     n_loop++;
344 }
345
346 #ifdef ENABLE_PHANTOM_GRAPE_X86
347     g5_close();
348 #endif
349
350     PS::Finalize();    FDPS終了
351     return 0;
352 }
```

```
325     system_grav.exchangeParticles(dinfo),
326 #ifdef MULTI_WALK
327     tree_grav.calcForceAllAndWriteBackMultiWalk(DispatchKernelWithSP,
328                                                 RetrieveKernel,
329                                                 tag_max,
330                                                 system_grav,
331                                                 dinfo,
332                                                 n_walk_limit,
333                                                 true);
334 #else
335     tree_grav.calcForceAllAndWriteBack(CalcGravity<FPGrav>,
336                                         CalcGravity<PS::SPJMonopole>,
337                                         system_grav,
338                                         dinfo);
339 #endif
340
341     kick(system_grav, dt * 0.5);
342
343     n_loop++;
344 }
345
346 #ifdef ENABLE_PHANTOM_GRAPE_X86
347     g5_close();
348 #endif
349
350     PS::Finalize();
351     return 0;
352
```

352行！

# 最後に

- ユーザーが書かなければならぬのは大体これくらい。  
→重力の場合は352+148行で終わる。
  - コード内に並列化を意識するようなところは無かった。  
→コンパイルの方法を切り替えるだけで、  
OpenMPやMPIを切り替えられる。



# 実習の流れ

- 詳しくはFDPS講習会の手引を御覧ください。  
(<http://www.jmlab.jp/?p=650>)

- 実習用のFOCUSスパコンにログインし、サンプルコードを  
(1)並列化無し (2)OpenMP (3)OpenMP + MPI  
の3パターンについてコンパイル・実行

## 【計算內容】重力

# cold collapse

# 流体 (Smoothed Particle Hydrodynamics法)

# adiabatic sphere collapse

## その後結果の解析

