FDPS: Framework for Developing Particle Simulator

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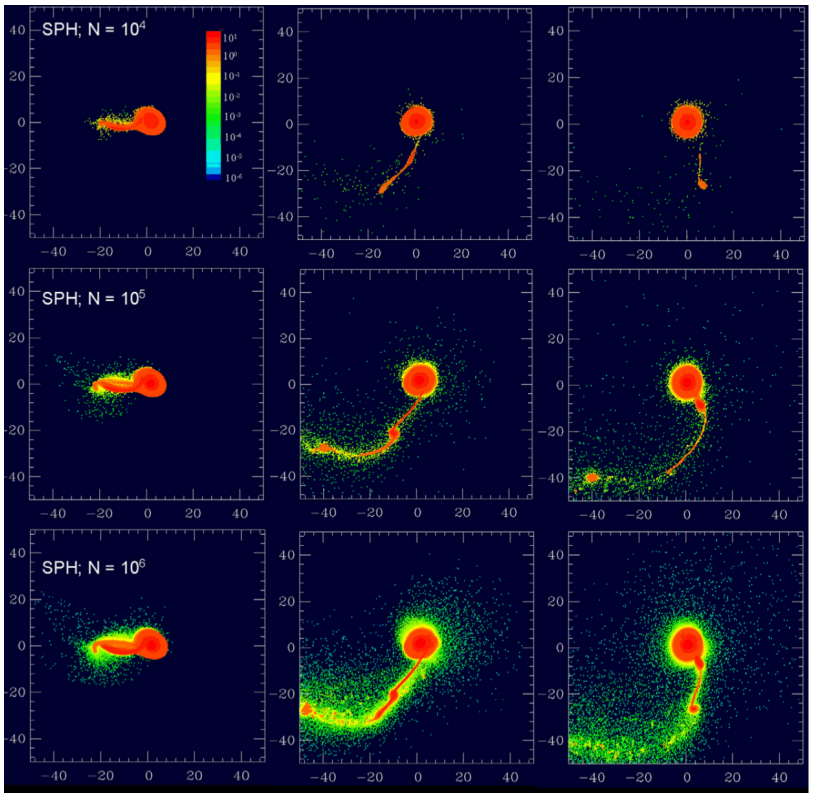
Talk plan

1. **What we (don't) want to do when writing particle-based simulation codes.**
2. **What should be done?**
3. **Design of FDPS**
4. **Current status**
5. **Issues on heterogeneous many-core systems**
6. **Performance of FDPS on TaihuLight (and PEZY-SC2)**

What we want to do

- We want to try large simulations.
- Computers (or the network of computers...) are fast enough to handle hundreds of millions of particles, for many problems.
- In many fields, largest simulations still employ 1M or less particles....



(example: Canup+ 2013)

What we want to do

More precisely, what we do not want to do

- **We do not want to write parallel programs using MPI.**
- **We do not want to modify data structure and loop structure to make use of data caches.**
- **We do not want to do complicated optimizations to hide interprocessor communications.**
- **We do not want to write tricky codes to let compilers make use of SIMD instruction sets.**
- **We do not want to do machine-specific optimizations or write codes using machine-specific languages (C*d*).**

But what we can do?

Traditional ideas:

- Hope that parallelizing compilers will solve all problems.
- Hope that big shared memory machines will solve all problems.
- Hope that parallel languages (with some help of compilers) will solve all problems.

But...

- These hopes have never been.....
- Reason: low performance. Only approaches which achieve the best performance on the most inexpensive systems have survived.

Then what can we really do?

1. **Accept the reality and write MPI programs and do optimization**
   Limitation: If you are an ordinary person the achieved performance will be low, and yet it will take more than infinite time to develop and debug programs. Your researcher life is likely to finish before you finish programming.
2. **Let someone else do the work**
   Limitation: If that someone else is an ordinary person the achieved performance will be low, and yet it will take more than infinite time and money.

- **Neither is ideal**
- **We do need "non-ordinary people".**

Products of "non-ordinary people"

Within Astrophysics

- **pkdgrav (Quinn et al. 1997)**
- **Gadget (Springel et al. 2001)**
- **GreeM (Ishiyama et al. 2009)**
- **REBOUND (Rein and Liu 2012)**

Problems with "non-ordinary people"

- If you can secure non-ordinary people there might be some hope.
- But they are very limited resource.

If we can apply "non-ordinary people" to many different problems, it will be the solution.

How can we apply "non-ordinary people" to many different problems?

Our approach:

- **Formulate an abstract description of the approach of "non-ordinary people", and apply it to many different problem.**
- **"Many different" means particle-based simulations in general.**
- **Achieve the above by "metaprogramming"**
- **DRY (Don't Repeat Yourself) principle.**

To be more specific:

Particle-based simulations includes:

- **Gravitational many-body simulations**
- **molecular-dynamics simulations**
- **CFD using particle methods(SPH, MPS, MLS etc)**
- **Meshless methods in structure analysis etc (EFGM etc)**

Almost all calculation cost is spent in the evaluation of interaction between particles and their neighbors (long-range force can be done using tree, FMM, PME etc)

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However, calculation time on accelerator-based or heterogenious systems show different behaviours. I'll come back to this issue later.

Our solution

If we can develop a program which can generate a highly optimized MPI program for

- domain decomposition (with load balance)
- particle migration
- interaction calculation (and necessary communication)

for a given particle-particle interaction, that will be the solution.

Design decisions

- API defined in C++
- Users provide
  - Particle data class
  - Function to calculate particle-particle interaction

  Our program generates necessary library functions. Interaction calculation is done using parallel Barnes-Hut tree algorithm
- Users write their program using these library functions.

Actual "generation" is done using C++ templates.

Status of the code

Iwasawa+2016 (PASJ 2016, 68, 54+arxive 1601.03138)

- **Publicly available**
- **A single user program can be compiled to single-core, OpenMP parallel or MPI parallel programs.**
- **Parallel efficiency is very high**
- **As of version 3.0 (released 2016) GPUs can be used and user programs can be in Fortran**

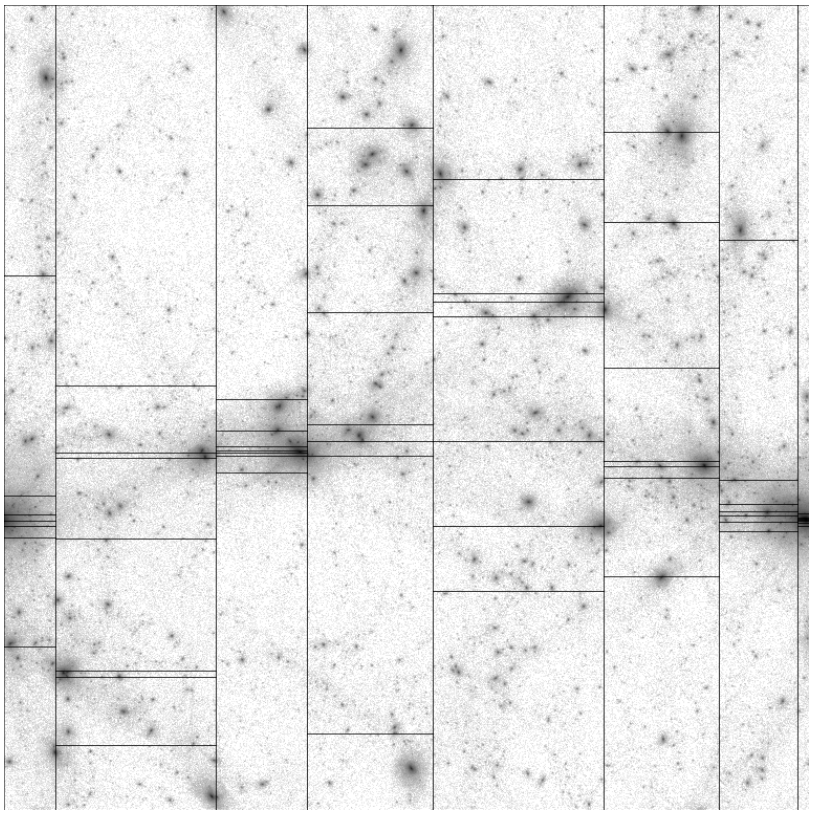
Tutorial
FDPS Github: https://github.com/FDPS/FDPS

Getting FDPS and run samples

```
> git clone git://github.com/FDPS/FDPS.git
> cd FDPS/sample/c++/nbody
> make
> ./nbody.out
```

To use OpenMP and/or MPI, change a few lines of Makefile

Domain decomposition



Each computing node (MPI process) takes care of one domain

Recursive Multisection (JM 2004)

Size of each domain are adjusted so that the calculation time will be balanced (Ishiyama et al. 2009, 2012)

Works reasonable well for up to 160k processes (so far the max number of processess we tried)

Sample code with FDPS

1. Particle Class

```
#include <particle_simulator.hpp> //required
using namespace PS;
class Nbody{                //arbitorary name
public:
    F64    mass, eps;   //arbitorary name
    F64vec pos, vel, acc; //arbitorary name
    F64vec getPos() const {return pos;} //required
    F64 getCharge() const {return mass;}//required
    void copyFromFP(const Nbody &in){   //required
        mass = in.mass;
        pos  = in.pos;
        eps  = in.eps;
    }
    void copyFromForce(const Nbody &out) { //required
        acc = out.acc;
    }
```

Particle class (2)

```
    void clear() { //required
        acc = 0.0;
    }
    void readAscii(FILE *fp) {//to use FDPS IO
        fscanf(fp,
               "%lf%lf%lf%lf%lf%lf%lf%lf",
               &mass, &eps, &pos.x, &pos.y, &pos.z,
               &vel.x, &vel.y, &vel.z);
    }
    void predict(F64 dt) { //used in user code
        vel += (0.5 * dt) * acc;
        pos += dt * vel;
    }
    void correct(F64 dt) { //used in user code
        vel += (0.5 * dt) * acc;
    }
};
```

Interaction function

```
template <class TParticleJ>
void CalcGravity(const FPGrav * ep_i,
                 const PS::S32 n_ip,
                 const TParticleJ * ep_j,
                 const PS::S32 n_jp,
                 FPGrav * force) {
    PS::F64 eps2 = FPGrav::eps * FPGrav::eps;
    for(PS::S32 i = 0; i < n_ip; i++){
        PS::F64vec xi = ep_i[i].getPos();
        PS::F64vec ai = 0.0;
        PS::F64 poti = 0.0;
```

Interaction function

```
        for(PS::S32 j = 0; j < n_jp; j++){
            PS::F64vec rij    = xi - ep_j[j].getPos();
            PS::F64    r3_inv = rij * rij + eps2;
            PS::F64    r_inv  = 1.0/sqrt(r3_inv);
            r3_inv  = r_inv * r_inv;
            r_inv  *= ep_j[j].getCharge();
            r3_inv *= r_inv;
            ai     -= r3_inv * rij;
            poti   -= r_inv;
        }
        force[i].acc += ai;
        force[i].pot += poti;
    }
}
```

Time integration (user code)

```
template<class Tpsys>
void predict(Tpsys &p,
             const F64 dt) {
    S32 n = p.getNumberOfParticleLocal();
    for(S32 i = 0; i < n; i++)
        p[i].predict(dt);
}

template<class Tpsys>
void correct(Tpsys &p,
             const F64 dt) {
    S32 n = p.getNumberOfParticleLocal();
    for(S32 i = 0; i < n; i++)
        p[i].correct(dt);
}
```

Calling interaction function through FDPS

```
template <class TDI, class TPS, class TTFF>
void calcGravAllAndWriteBack(TDI &dinfo,
                             TPS &ptcl,
                             TTFF &tree) {
    dinfo.decomposeDomainAll(ptcl);
    ptcl.exchangeParticle(dinfo);
    tree.calcForceAllAndWriteBack
        (CalcGravity<Nbody>(),
         CalcGravity<SPJMonopole>(),
         ptcl, dinfo);
}
```

Main function

```
int main(int argc, char *argv[]) {
    F32 time  = 0.0;
    const F32 tend  = 10.0;
    const F32 dtime = 1.0 / 128.0;
    // FDPS initialization
    PS::Initialize(argc, argv);
    PS::DomainInfo dinfo;
    dinfo.initialize();
    PS::ParticleSystem<Nbody> ptcl;
    ptcl.initialize();
    // pass initeraction function to FDPS
    PS::TreeForForceLong<Nbody, Nbody,
        Nbody>::Monopole grav;
    grav.initialize(0);
    // read snapshot
    ptcl.readParticleAscii(argv[1]);
```

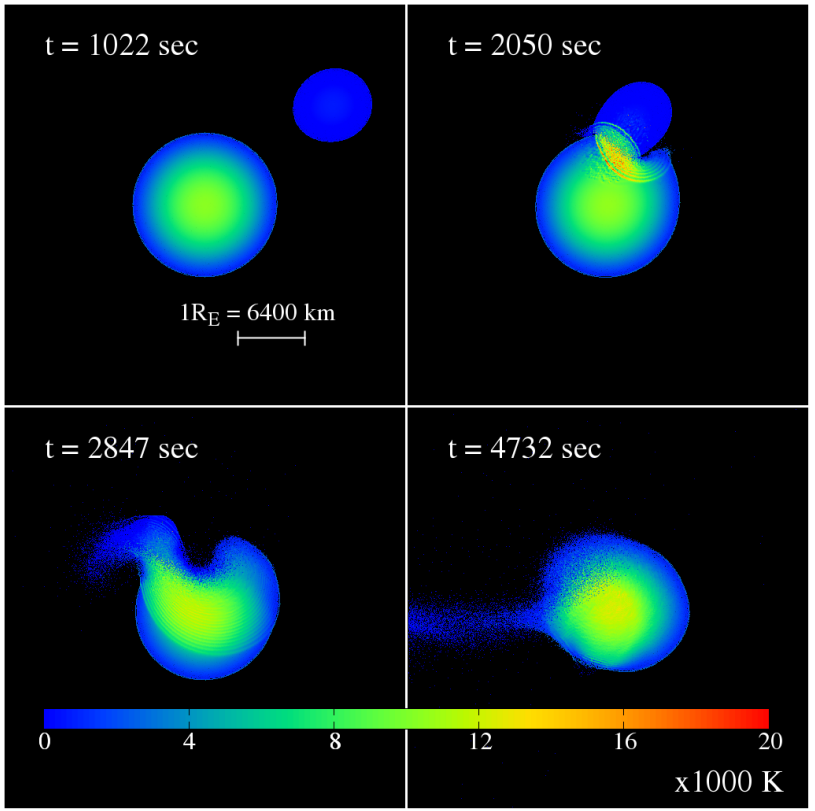
Main function

```
    // interaction calculation
    calcGravAllAndWriteBack(dinfo,
                            ptcl,
                            grav);
    while(time < tend) {
        predict(ptcl, dtime);
        calcGravAllAndWriteBack(dinfo,
                                ptcl,
                                grav);
        correct(ptcl, dtime);
        time += dtime;
    }
    PS::Finalize();
    return 0;
}
```

Remarks

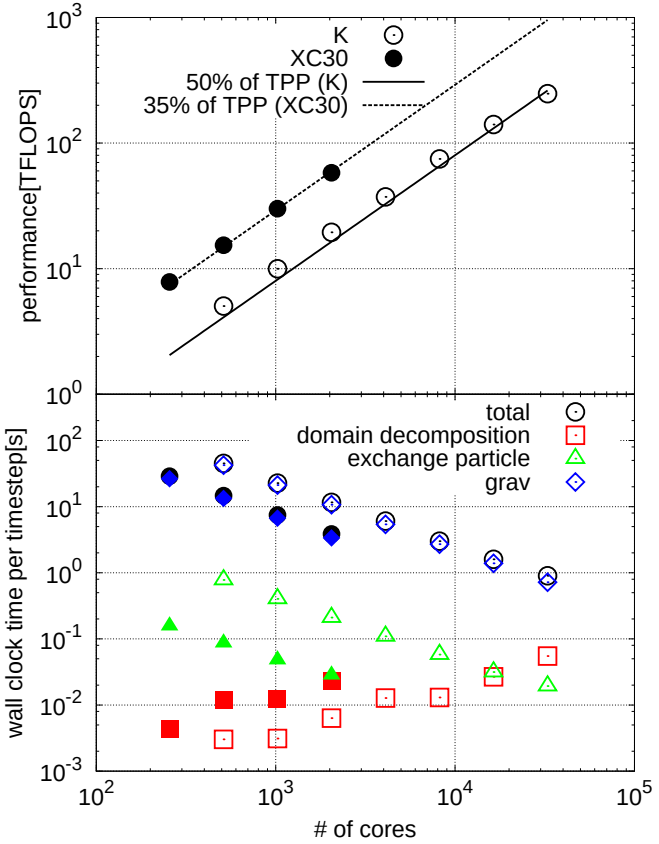
- **Multiple particles can be defined (such as dark matter + gas)**
- **User-defined interaction function should be optimized to the given architecture for the best performance (for now)**
- **This program runs fully parallelized with OpenMP + MPI.**

Example of calculation



Giant Impact calculation (Hosono et al. 2017, PASJ 69, 26+)
Figure: 9.9M particles
Up to 2.6B particles tried on K computer
We need more machine time to finish large calculation... Moving to PEZY systems.

Performance examples



Strong scaling with 550M particles

Measured on both K computer and Cray XC30 at NAOJ

Gravity only, isolated spiral galaxy

scales up to 100k cores

30-50% of the theoretical peak performance

Version 2.0

GPGPU and other accelerators

- FDPS Version 1.0: interaction function calculates forces from one group of particles to one group of particles (single "interaction list")
- Version 2.0: interaction function should handle multiple interaction lists in a single call (to hide large startup overhead of GPGPUs)

Version 3.0

API to user programs written in Fortran

- **"C++ is very difficult to learn/write"**
- **There are still many Fortran users**

Fortran API

- Particle data in Fortran structured data type
- Using Fortran iso_c_binding functions, make Fortran-defined class and functions visible from C++ library functions
- Generate C++ class and member functions from Fortran source and directives

Particle definition

```
module user_defined_types
   use, intrinsic :: iso_c_binding
   use fdps_vector
   use fdps_super_particle
   !**** Full particle type
   type, public, bind(c) :: full_particle !$fdps FP,EPI,EPJ,Force
      !$fdps copyFromForce full_particle (pot,pot) (acc,acc)
      !$fdps copyFromFP full_particle (id,id) (mass,mass) (eps,eps) (pos,pos)
      !$fdps clear id=keep, mass=keep, eps=keep, pos=keep, vel=keep
      integer(kind=c_long_long) :: id
      real(kind=c_double)  mass !$fdps charge
      real(kind=c_double) :: eps
      type(fdps_f64vec) :: pos !$fdps position
      type(fdps_f64vec) :: vel !$fdps velocity
      real(kind=c_double) :: pot
      type(fdps_f64vec) :: acc
   end type full_particle
```

Version 4.0

- Released on Nov 8, 2017
- Mainly performance enhancement from our experience on Sunway TaihuLight
- Barnes-Hut tree in cylindrical coordinates for narrow ring calculation
- Many other improvements on scalability and/or efficiency

Performance (and tuning) of FDPS on TaihuLight (and PEZY-SC2)

- **Why did we do that?**
- **TaihuLight and SC2 — view from the application side**
- **FDPS (or *N*-body simulation) on TaihuLight — New algorithms introduced**
- **Achieved performance**

Why did we do that?

- **Why not?**
- **TaihuLight and PEZY-SC2 have many things in common, and they are among the fastest machines. Their architecture might be tomorrow's standard.**
- **We can learn how we should improve FDPS so that it will be useful on future HPC platforms.**

TaihuLight and SC2 — view from the application side

Good news:

- **They are fast — the fastest in the world and in Japan**

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Not-so-good news:

- **Extreme performance ratio between general-purpose and "special-purpose" cores (effectively much more than a factor of 100)**
- **Extremely limited main memory bandwidth (BF $\sim$ 0.0x)**
- **Even more limited network bandwidth**

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Good for HPL, but...

Jack Dongarra et al. 2014
"HPCG: ONE YEAR LATER"

HPL has a Number of Problems

- HPL performance of computer systems are **no longer so strongly correlated to real application performance**, especially for the broad set of HPC applications governed by partial differential equations.

- **Designing a system for good HPL performance can actually lead to design choices that are wrong** for the real application mix, or add unnecessary components or complexity to the system.

Well, then, what's RIGHT?

Should HPC machines be designed to run "real application mix"?

What should be the goal of "hardware-software codesign"?

The ultimate goal

- **Both the hardware and software (or, their combination) must be "optimal"**
- **Probably the only meaningful "optimality" in the post-Moore era is of energy efficiency (energy-for-the-solution)**

Cost of DP mult and off-chip data move

- PEZY-SC2 achieve 17 Gflops/W. FMA operation itself would be around 50-60Gflops/W = 20pJ/flop
- Data move with HBM2 would be around 20 GB/s/W= 400pJ/word
- Even with HBM2, a machine with B/F=0.3 would spend equal power for computing and DRAM access (and similar or more for on-chip data move)
- Relative cost of data movement will be higher in the future

Implication on algorithm/software development

- We need to "minimize" data move
- In other words, we need to understand the theoretical lower limit of data movement necessary to solve a given problem with a given numerical scheme.
- However, at present we have no clue on it. We do not know what is the lower limit. We do not know how to get there either.

We can learn a lot by trying to use machines with low B/F and low network bandwidth

What we did on TaihuLigt

Standard Parallel Barnes-Hut tree algorithm on accelerator

- construct load-balanced domain decomposition
- move particles to new home
- construct local tree
- exchange "local essential tree"
- construct global tree
- traverse tree for a group of particles, construct an "interaction list" and let the accelelrator do the actual interaction calculation. Do this for all groups

Problem with the standard alogirithm

- On TaihuLight, all steps other than interaction calculation are slow
- They are extremely slown on MPE, but even when moved to CPEs, they are slow due to the limited memory bandwidth
- There aresy a number of other issues...

Our current implementation

- Use the "interaction list" for multiple timesteps (similar to "bookkeeping" or "neighbour list" method
- "semi-dynamic" load balance between CPEs
- manual tuning (in assembly language) of the interaction kernels
- Elimination of all-to-all communications through the introduction of multi-process "superdomains"
- Problem-specific optimizations for planetary ring calculations

Amount of memory access and calculation

Memory access:

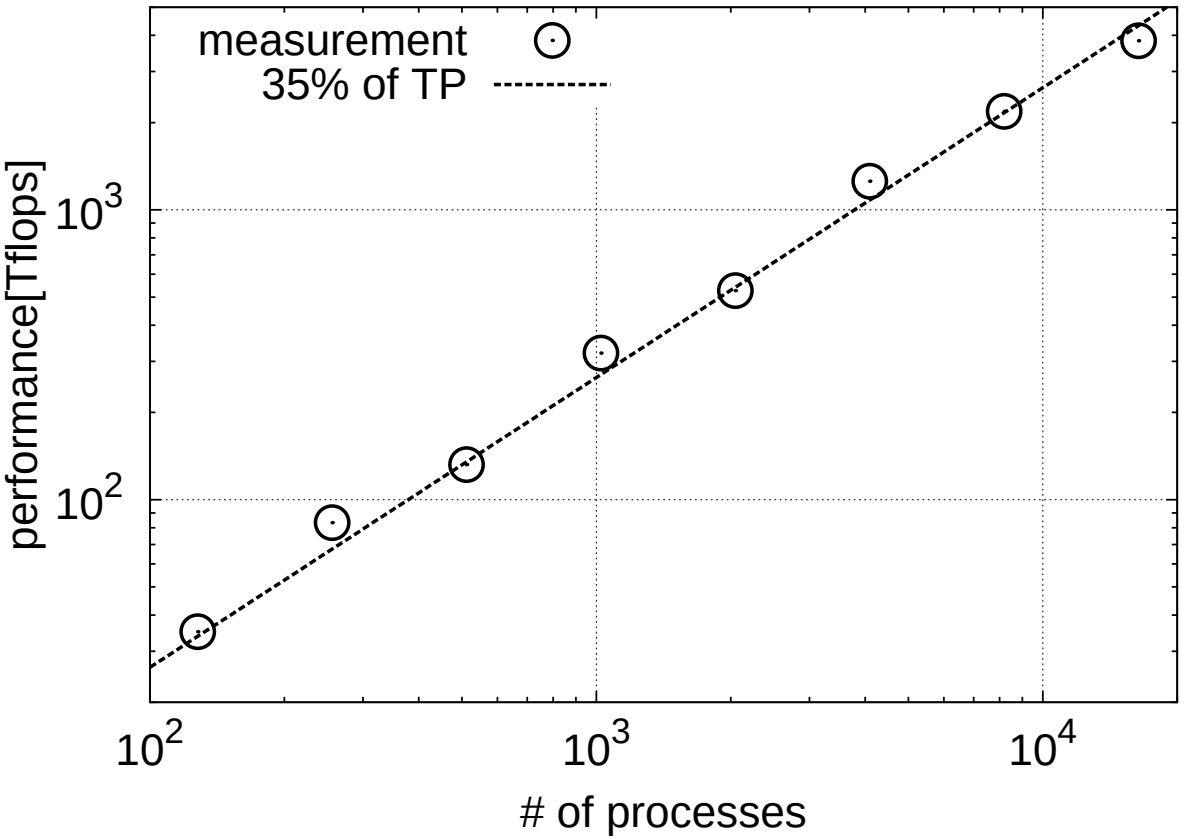
- Tree physical quantity update: $\sim N$
- Force calculation: $\sim 10N$
- Time integration (merged with force caculation)

around 300 bytes/particle/timestep

Force calculation:
around 3e4 operations/particle/timestep

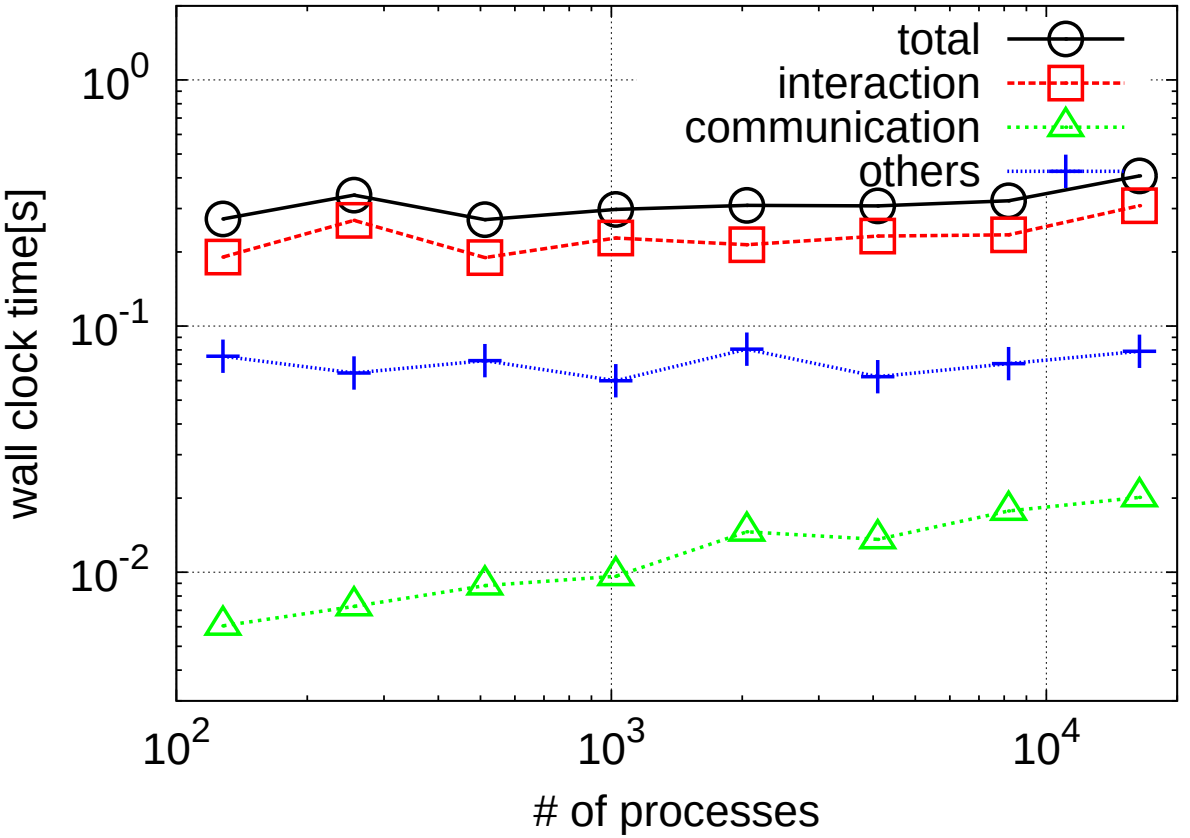
B/F 0.01 can be achieved. To use machines with B/F$<$ 0.01, we need new ideas.

Achieved performance



Nearly 4PF on 1/10 of TaihuLight

Calculation time breakdown



Summary

- **Please visit: https://github.com/FDPS/FDPS**
- **A Framework for Developing parallel Particle Simulation code**
- **FDPS offers library functions for domain decomposition, particle exchange, interaction calculation using tree.**
- **Can be used to implement pure Nbody, SPH, or any particle simulations with two-body interactions.**
- **Uses essentially the same algorithm as used in our treecode implementation on K computer (GreeM, Ishiyama, Nitadori and JM 2012).**
- **Improvements for heterogenious manycore systems are ready**
- **Good weak scaling and performance not far from theoretical limit on TaihuLight. Hopefully also on PEZY-SC2.**