Performance of FDPS on Sunway TaihuLight and Other Modern HPC Systems

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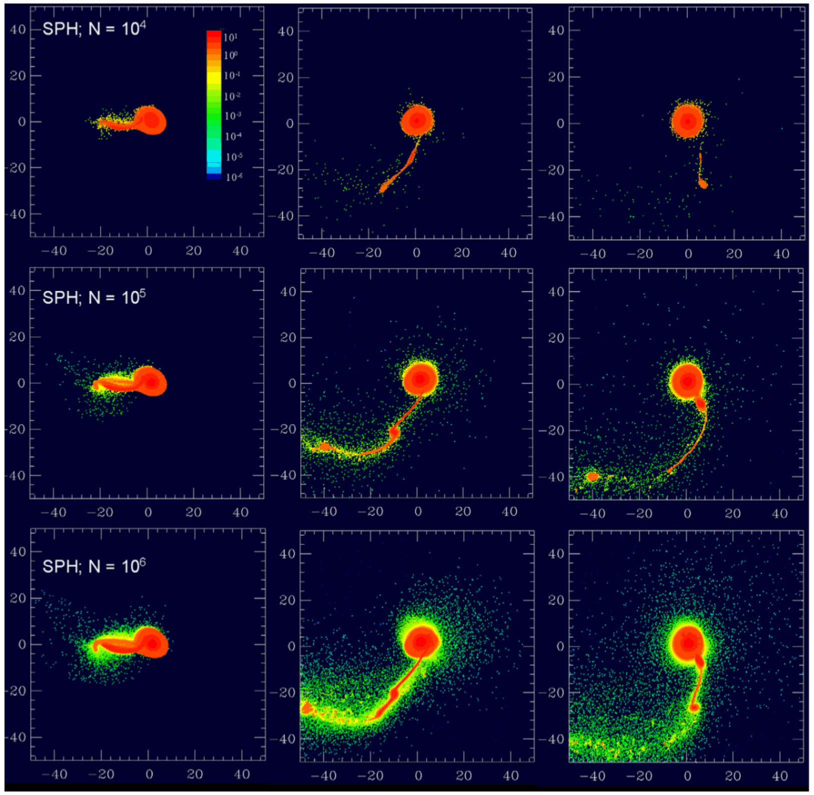
Talk plan

1. **What we want to do when writing particle-based simulation codes.**
2. **What should be done?**
3. **Design of FDPS**
4. **Performance**
5. **Performance on Sunway TaihuLight**

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

- Write a simple program expressing the numerical scheme used
- Run it on notebooks, desktops, clusters and large-scale HPC platform

What we are doing now

- rewrite the entire program using MPI to make use of multiple nodes.
- apply complicated optimizations to hide interprocessor communications.
- rewrite data structure and loop structure to make efficient use of data caches.
- rewrite inner loops and data structure to let compilers make use of SIMD instruction sets.
- apply machine-specific optimizations or write codes using machine-specific languages (C*d*, Open**).

What we hoped 30 years ago

- **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”

Astrophysics

- pkdgrav (Quinn et al. 1997)
- Gadget (Springel et al. 2001)
- GreeM (Ishiyama et al. 2009)

Molecular Dynamics
GROMACS, LAMMPS, NAMD, and several others

Other fields?

Problems with “non-ordinary people”

- If you can secure non-ordinary people there might be some hope.
- But they are very limited resources.
- Not enough non-ordinary people to meet the needs of many application areas.

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)

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
- Version 4.0 offers many performance improvements
- 30 — 100 users (estimated) worldwide

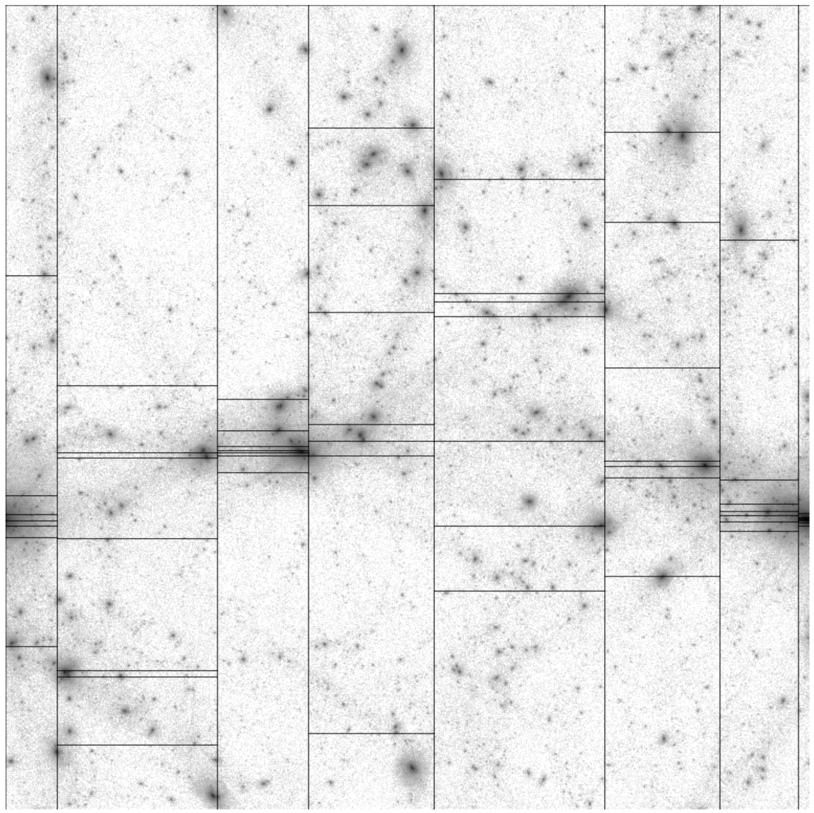
Tutorial
FDPS Github: https://github.com/FDPS/FDPS

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 processes 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]);
```

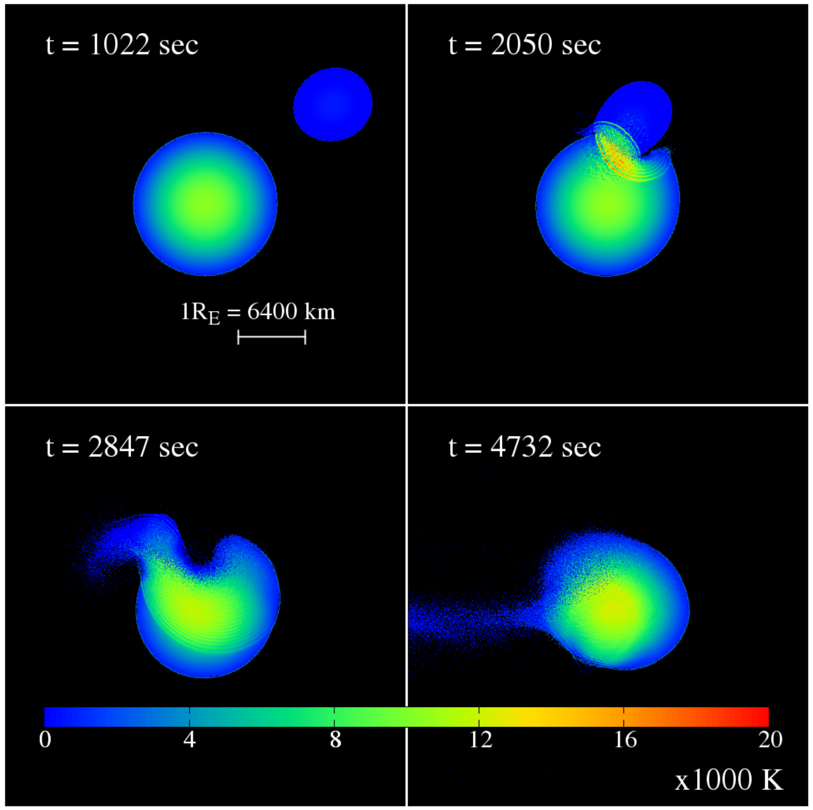
Main function

```
    // 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



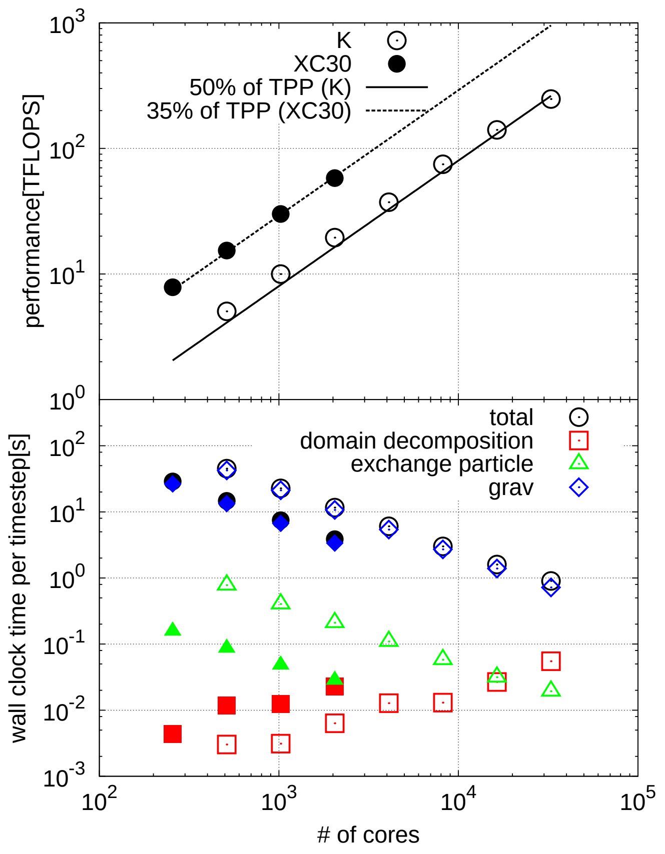
Giant Impact calculation (Hosono et al. 2017, PASJ 69, 26+)

Figure: 9.9M particles

Up to 2.6B particles tried on K computer

We need more machine time to finish large calculation... Currently PEZY systems are used. (Sasaki and Hosono, The Astrophysical Journal, in press)

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

Performance (and tuning) of FDPS on TaihuLight

- Overview of Sunway TaihuLight
- FDPS (or N-body simulation) on TaihuLight — New algorithms introduced
- Achieved performance

TaihuLight

- The fastest supercomputer in the world
- Extreme performance ratio between general-purpose and “special-purpose” cores (effectively much more than a factor of 100)
- Extremely limited main memory bandwidth (BF $\sim$ 0.03)
- Even more limited network bandwidth

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 TaihuLight

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 accelerator do the actual interaction calculation. Do this for all groups**

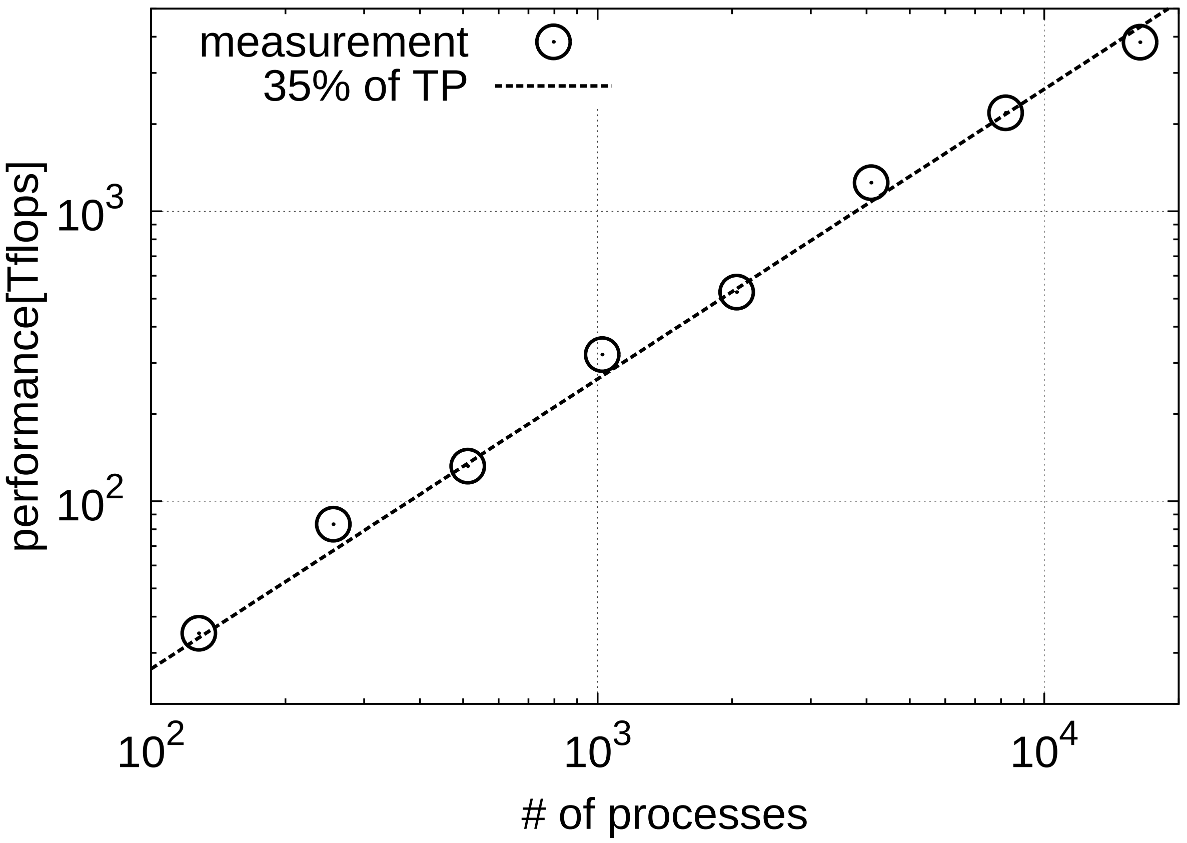
Problem with the standard algorithm

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

Our current implementation

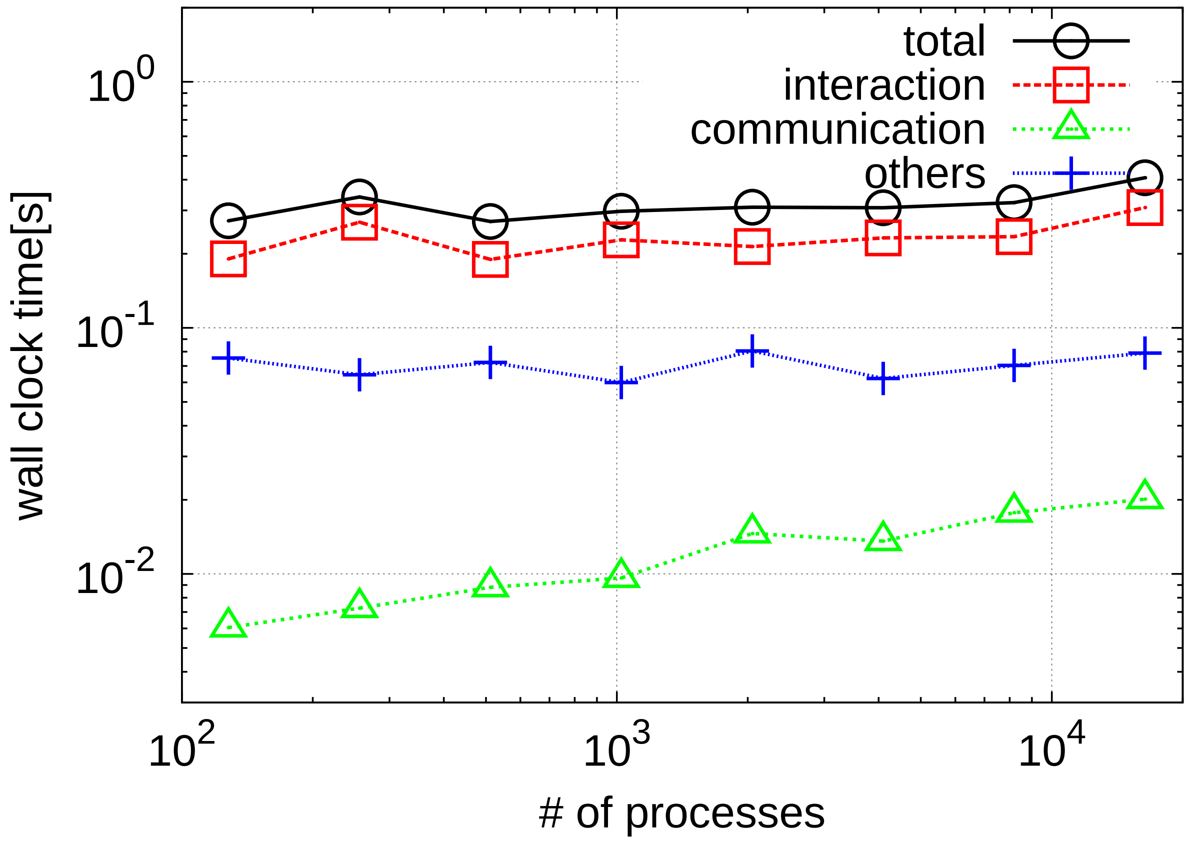
- Use the “interaction list” for multiple timesteps (similar to “bookkeeping” or “pairlist” method
- “semi-dynamic” load balance between CPEs
- manual tuning (in assembly language) of the interaction kernels
- Elimination of all-to-all communications through the introduction of multi-process “superdomains”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

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 heterogeneous manycore systems are ready
- Good weak scaling and performance not far from theoretical limit on TaihuLight.

Amount of memory access and calculation

Memory access:

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

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.