Current status of FDPS and Future plans

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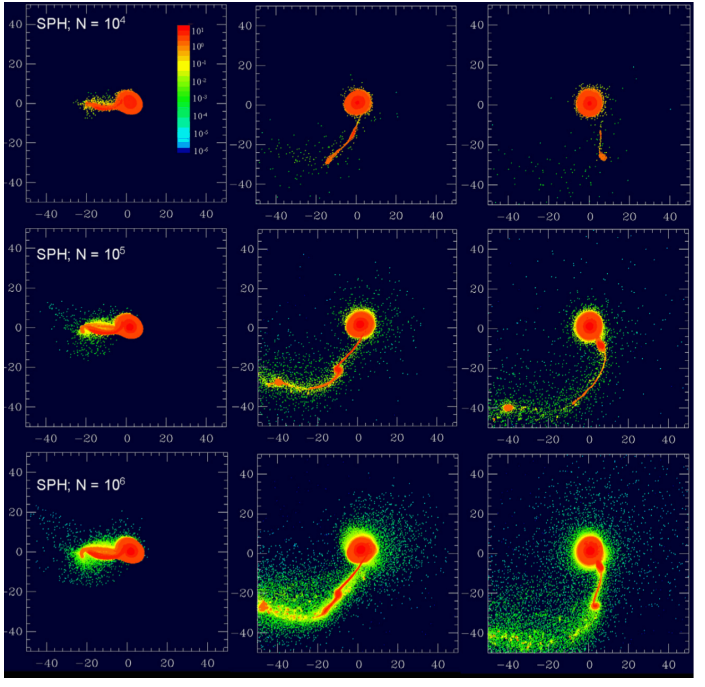
and many others

Talk plan

1. What we want to do when writing particle-based simulation codes. (or any other large-scale HPC code)
2. What should be done?
3. Design of FDPS
4. Performance
5. Future plan

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 (Cu**, Open**).

Existing efficient codes

Astrophysics

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

Molecular Dynamics
GENESIS, GROMACS, LAMMPS, Modylas, NAMD, and several others

Developers need to write codes for domain decomposition, particle move, and interaction calculation.

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 concept

- 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.

Initial release

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 (and now also pure C).**
- **Versions 4.0 and 5.0 offers many performance improvements.**

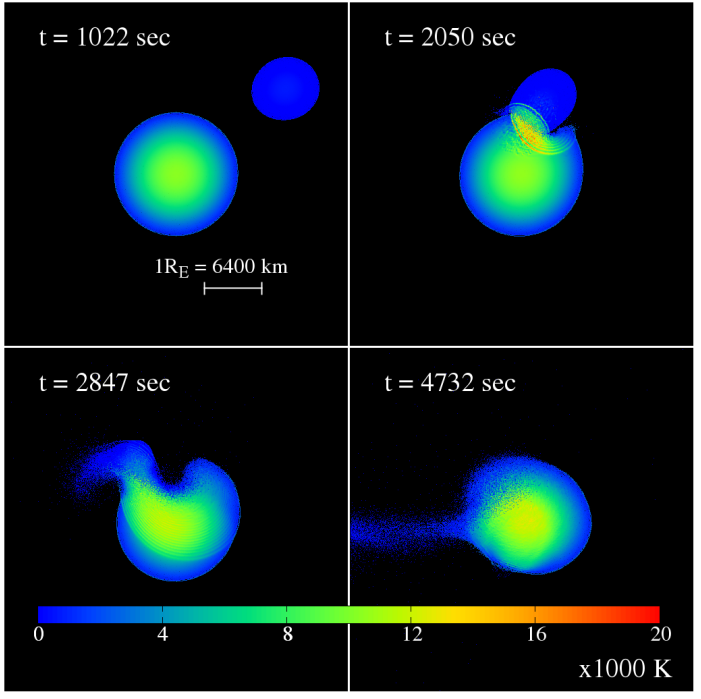
Tutorial
FDPS Github: https://github.com/FDPS/FDPS

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

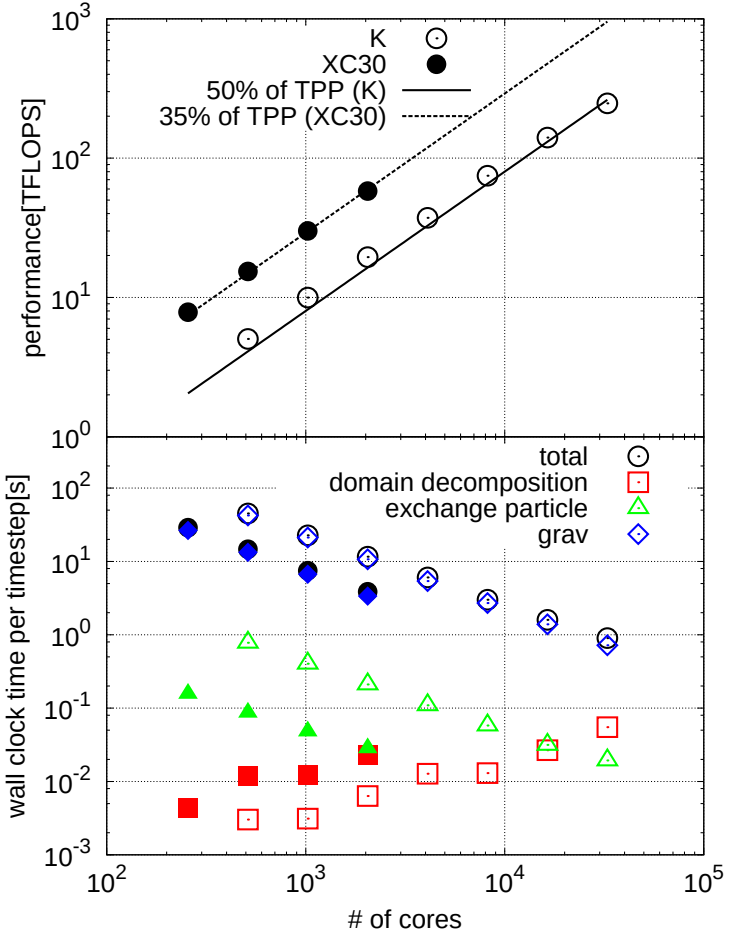
Example of calculation



Giant Impact calculation (Hosono et al. 2017, PASJ 69, 26+)
Figure: 9.9M particles
Up to 2.6B particles tried on K computer

animation Terrestrial magma ocean origin of the Moon, Hosono et al. Nature Geoscience volume 12, 418423(2019)

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

Preparation for Fugaku and next-generation platforms

Compared to K computer, future machines will have

- **Larger number of cores, more FPUs per core**
- **(relatively) weak main memory**
- **(relatively) weak network**

Our software should be ready for such machines to be useful.

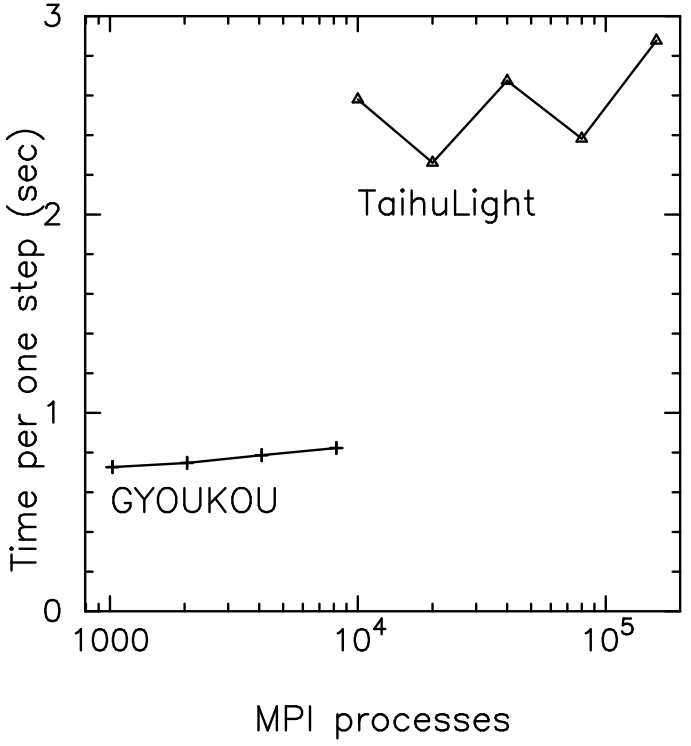
How to be “future-proof”?

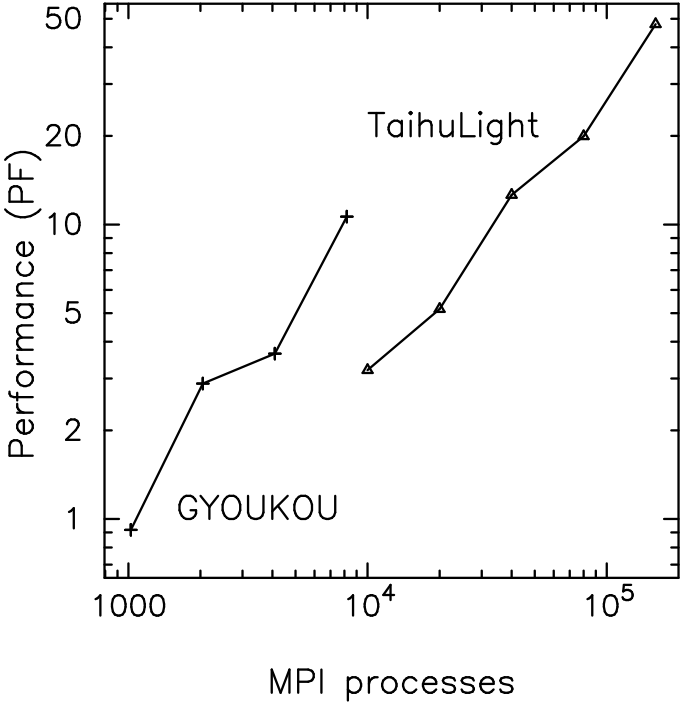
- **One possibility: try to use machines with weak main memory and weak network.**
- **Examples as of 2015-2020: Sunway Taihulight and PEZY-SC2(GYOUKOU)**

Our current implementation

- Elimination of all-to-all communications and other operations with the cost proportional to the number of nodes.
- Use the same “interaction list” for multiple timesteps (similar to “bookkeeping” or “pairlist” method
- Minimize the main memory access within FDPS (tree construction etc)
- Minimize internode communication
- manual tuning of interaction kernels

Achieved performance





30-40% of the theoretical peak on both machines.
10M particles/MPI process
Planetary ring simulation

Future plan

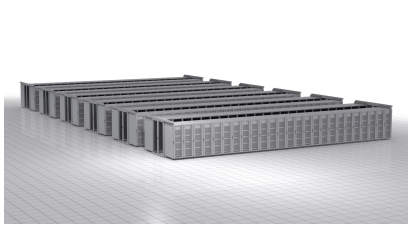
Current status of FDPS:

- **Users do not need to parallelize their codes by themselves. FDPS does it.**
- **Optimization of the interaction kernel should still be done by users.**

What should be done

User: writes high-level description of interaction kernel
FDPS: generates optimized code for supported architectures

- **Fugaku**
- **x86**
- **NVIDIA/AMD GPGPUs**
- **MN-Core**
- **(FPGA)**
- **...**

Example of high-level description

```
EPI F32vec xi:pos
EPI F32    eps2i:eps2
EPJ F32vec xj:pos
EPJ F32    mj:mass
EPJ F32    eps2j:eps2
FORCE F32vec f:acc
FORCE F32 phi:pot
rij = xi - xj
r2 = eps2i + eps2j + rij*rij
rinv = rsqrt(r2)
mrinv = mj*rinv
f -= mrinv*rinv*rinv*rij
phi -= mrinv
```

Example of high-level description (2)

```
EPI U32    ti:type
EPI F32vec ri:pos
EPI F32vec vi:vel
EPI F32    hi:h

EPJ U32    tj:type
EPJ F32vec rj:pos
EPJ F32vec vj:vel
EPJ F32    mj:mass
EPJ F32    uj:eng
FORCE F32 dens:dens
FORCE F32 pres:pres
FORCE F32 gradh:gradh
FORCE F32 divv:divv
FORCE F32 rotv:rotv
F32 gamma
function gradW(dr,h)
  r = sqrt(dr*dr)
  u = r*inv(h)
  p1u = 1.0f - u
  h2 = h*h
  h5 = h2*h2*h
  coeff = 1155.0f*inv(12.5663706144f*h5)
  p1u2 = p1u*p1u
  p1u5 = p1u2*p1u2*p1u
  return - coeff*p1u5*(1.0f + 5.0f*u)
end
```

```
function W(r,h)
  u = r*inv(h)
  p1u = max(0.0f, 1.0f - u)
  coeff = 495.0f*inv(100.530964915f*h*h*h)
  p1u2 = p1u*p1u
  p1u6 = p1u2*p1u2*p1u2
  return coeff*p1u6*(1.0f + u*(6.0f + 11.6666666667f*u))
end

function dwdh(r,h)
  u = r*inv(h)
  p1u = max(0.0f, 1.0f - u)
  h2 = h*h
  coeff = 165.0f*inv(100.530964915f*h2*h2)
  p1u2 = p1u*p1u
  p1u5 = p1u2*p1u2*p1u
  return -coeff*p1u5*(9.0f + u*(45.0f + u*(-5.0f - 385.0f*u)))
end
g1u = gamma - 1.0f
dr = ri - rj
dv = vi - vj
if tj > 0.0
  rij = sqrt(dr*dr)
else
  rij = 2.0f*hi
endif
```

```
wij = W(rij,hi)
dens += mj*wij
pres += g1u*mj*uj*wij
dwdh_ij = dwdh(rij,hi)
gradh += g1u*mj*uj*dwdh_ij
divv -= g1u*mj*uj*(dr*dv)*gradW(dr,hi)
tmp.x = dv.y*dr.z - dv.z*dr.y
tmp.y = dv.z*dr.x - dv.x*dr.z
tmp.z = dv.x*dr.y - dv.y*dr.z
rotv -= g1u*mj*uj*tmp
```

What need to be done

- (For CPUs) AoS/SoA conversion, use of SIMD intrinsics, loop fission, stripmining, unrolling, software pipelining...
- (For GPUs and other accelerators) generation of kernel code and codes for communication between CPU and GPU.

Current status:

- Automatic generation for Fugaku is working.
- The generated code is currently slightly (10-15%) slower than our best hand-optimized code.

Summary

- FDPS is a framework which helps the development of scalable high-performance particle-based simulation codes
- It can be used with arbitrary particle structure and particle-particle interaction function
- Efficiency of application written using FDPS is very high on large-scale machines including K and Sunway Taihulight. (30-50% of the peak)
- We are working on automatic generation of highly optimized kernel for particle-particle interactions, and that for Fugaku is almost ready
- FDPS will be used in various projects on Fugaku