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

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:pott
rij = xi - xj
r2 = eps2i + eps2j + rij*rij
rinv = rsqrt(r2)
mrinv = mj*rinv
f -= mrinv*rinv*rinv*rij
phi -= mrinv
function $W(r,h)$

$$u = r \times \text{inv}(h)$$
$$u1 = \max(0.0f, 1.0f - u)$$
$$\text{coeff} = 495.0f \times \text{inv}(100.530964915f \times h \times h)$$
$$u1u2 = u1u1u$$
$$u1u6 = u1u2u2u2u2$$
$$\text{return coeff} \times u1u6 \times (1.0f + u \times (6.0f + 11.6666666667f \times u))$$

end

function $dwdh(r,h)$

$$u = r \times \text{inv}(h)$$
$$u1 = \max(0.0f, 1.0f - u)$$
$$\text{coeff} = 495.0f \times \text{inv}(100.530964915f \times h \times h \times h)$$
$$u1u2 = u1u1u$$
$$u1u6 = u1u2u2u2u2$$
$$\text{return coeff} \times u1u6 \times (1.0f + u \times (6.0f + 11.6666666667f \times u))$$

end

function gradW(dr,h)

$$r = \sqrt{dr \times dr}$$
$$u = r \times \text{inv}(h)$$
$$u1 = \max(0.0f, 1.0f - u)$$
$$dr = r - r$$
$$dv = vi - vj$$
$$h2 = h \times h$$
$$h5 = h2 \times h2$$
$$\text{coeff} = 1155.0f \times \text{inv}(12.5663706144f \times h5)$$
$$u1u2 = u1u1u$$
$$u1u5 = u1u2u2u2u$$
$$\text{return} - \text{coeff} \times u1u5 \times (1.0f + 5.0f \times u)$$

end
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.