Particle Simulator Research Team

Team Leader
Junichiro Makino
imakino@riken.jp



We have developed **FDPS** (Framework for Developing Particle Simulator), a universal software application that can be used to write high-performance, particle-based simulations.

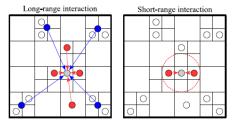
https://github.com/FDPS/FDPS

The Design of FDPS

FDPS is a C++ header library. A user of FDPS can develop the simulation code in the following three steps:

- 1. Define the data structure for the single particle, as a class in C++ language.
- 2. Define the interaction function f, that receives arrays of interacting particles, and calculates and accumulates the force on the particles.
- 3. Write the main program using the data class and functions provided by FDPS.

The Implementation of FDPS



FDPS handles long-range interactions by Burnes-Hut algorithm, and short-range interactions by tree-search based neighbor list. FDPS takes care of inter-node (MPI) and intra-node (OpenMP) communications, and load balancing. FDPS adopts three-dimensional multi-section domain decomposition, that is used in Gordon-Bell-prize-winning particle simulator GreeM.

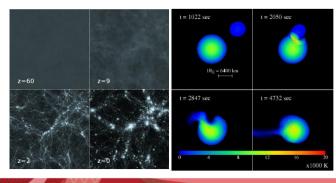
The user code are passed small subset of particles delivered by FDPS. The user still have to SIMD-ize their interaction code for performance.



Figure: An Example of 7x6 domain decomposition.

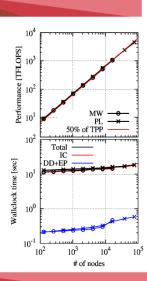
Applications

Simulations of cosmological structure formation with gravity code (left) and planet collision with smoothed-particle hydrodynamics code (right), both implemented using FDPS:



Performance

The left figure shows the performance of the gravity code, measured in the flops (top) and wall-clock time per timestep (bottom), as functions of the number of nodes. The code keeps 50% of the theoretical peak performance and scales up to 76,544 nodes, on the K computer.



Getting Started

FDPS is open-sourced under MIT license at https://github.com/FDPS/FDPS
Tutorials, specifications, and ready-to-run example programs are found in the above URL.

With FDPS, our dream of letting one-core programmers to utilize large-scale supercomputers had come true, for particle simulation applications.



Getting Started with FDPS

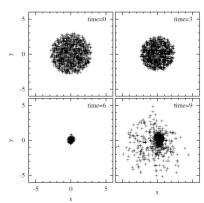
c.f. The FDPS tutorial available from https://github.com/FDPS/FDPS/blob/master/doc/doc_tutorial_e.pdf

Download FDPS via SVN

- \$ svn co --depth empty https://github.com/FDPS/FDPS
- \$ cd FDPS
- \$ svn up trunk
 - -- or --
- # Download FDPS via Git
- \$ git clone git://github.com/FDPS/FDPS.git

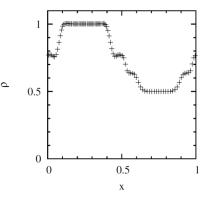
Build and Run the N-body example

- \$ cd \$(FDPS).sample/nbody/
- \$ make
- \$./nbody.out
- \$ gnuplot
- > plot "result/0009.dat" using 3:4



Build and Run the Smoothed Particle Hydro example

- \$ cd \$(FDPS).sample/sph/
- \$ make
- \$./sph.out
- \$ gnuplot
- > plot "result/0040.dat" using 3:9



N-body example with OpenMP & MPI

- Set the variable CC to your MPI C++ compiler
- Uncomment the line "CFLAGS += -DPARTICLE_SIMULATOR_THREAD_PARALLEL -fopenmp"
- Uncomment the line "CFLAGS += -DPARTICLE_SIMULATOR_MPI_PARALLEL"
 Then
- \$ make
- \$ MPIRUN -np NPROC ./nbody.out

Here, "MPIRUN" should be mpirun or mpiexec depending on your MPI conguration, and "NPROC" is the number of processes you will use.

