

## Particle Simulator Research Team

### 1. Team members

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### 2. Research Activities

We are developing particle-based simulation software that can be used to solve problems of vastly different scales.

Simulation schemes for hydrodynamics and structural analysis can be divided into grid-based and particle-based methods (see Figure 1). In grid-based methods, the computational region is mapped to regular or irregular grids. Continuous distributions of physical values are represented by discrete values at grid points, and the governing partial differential equation is approximated to a set of finite difference equations.

In the case of the particle-based methods, physical values are assigned to particles, while the partial differential equation is approximated by the interactions between particles.

Both methods are widely used, and they have their advantages and disadvantages. The computational cost of grid-based schemes is generally lower than that of particle-based methods with similar number of freedoms. Thus, if a near-uniform grid structure is appropriate for the problem to be solved, grid-based methods perform better.

The advantage of the particle-based methods comes from the fact that they use "Lagrangian" schemes, in which the particles move following the motion of the fluid in the case of the CFD calculation. In the case of grid-based methods, we generally use "Eulerian" schemes, in which the grid points do not move.

There are three points in which the Lagrangian schemes are better than Eulerian schemes.

One is that the Lagrangian schemes are, to some extent, adaptive to the requirement of the accuracy, since when a low-density region is compressed to become high density, Second one is that the timestep criteria are quite different. In the case of the Lagrangian schemes, the timestep is determined basically by local sound velocity, while in the Eulerian scheme by global velocity. Thus, if a relatively cold fluid is moving very fast, the timestep for the Eulerian schemes can be many orders of magnitude shorter than that for Lagrangian schemes. Finally, in the case of fast-moving low-temperature fluid, the required accuracy would be very high for Eulerian scheme, since the error comes from the high velocity, while that error would be transferred to internal energy of the fluid element which is much smaller than that of the kinetic motion.

Of course, there are disadvantages of Lagrangian schemes. The primary one is the difficulty of construction of such schemes in two or higher dimensions. In the case of one-dimensional calculation, it is easy to move grid points following the motion of the fluid, but in two or higher dimensions, the grid structure would severely deform if we let the grid points follow the flow. Thus, we have to reconstruct the grid structure every so often. This requirement causes the program to become complex. Moreover, reconstruction of the grid structure (so called remeshing) means we lose numerical accuracy.

Particle-based methods "solve" this difficulty by not requiring any mesh. In particle-based methods, particles interact with its neighboring particles, not through some connection through grid, but through distance-dependent kernel functions. Thus, there is no need of remeshing. As a result, particle-based schemes are simple to implement, and can give reasonable results even when the deformation is very large. Another important advantage is that it is relatively easy to achieve high efficiency with large-scale particle-based simulation.

In the case of grid-based schemes, in order achieve some adaptivity to the solution, we have to use either irregular grid or regular grid with adaptive mesh refinement. In both cases, adaptivity breaks the regularity of the mesh structure, resulting in non-contiguous access to the main memory. In the case of the particle-based schemes, it does require some irregular memory access, but it is relatively straightforward to make good use of spacial locality, and thereby achieving high efficiency. Similarly, very high parallel performance can be achieved.

However, it has its own problems. In the case of the SPH method, it has been known that the standard scheme cannot handle the contact discontinuity well. It also require rather strong artificial viscosity, which results in very low effective Reynolds number.

Thus, in many fields of computational sciences, many groups are working on implementation of high-performance particle-based simulation codes for their specific problem.

One serious problem here is that, high-performance, highly-parallel simulation codes for particle-based simulations are becoming more and more complex, in order to make full use of modern supercomputers. We need to distribute particles to many computing nodes in an appropriate way, so that the communication between nodes is minimized and at the same time near-optimal load balance is achieved. Within each nodes, we need to write an efficient code to find neighbor particles, rearrange data structure so that we can make good use of the locality, make good use of multiple cores and SIMD units within each core.

Even for the case of very simple particle-particle interaction such as the Lenard-Jones potential or Coulomb potential, the calculation code tends to be very large, and since the large fraction of the code is written to achieve a high efficiency on a specific architecture, it becomes very hard to port a code which is highly optimized to one architecture to another architecture.

Our goal is to develop a "universal" software that can be applied to a variety of problems whose scales are vastly different.

In designing such universal software, it is important to ensure that it runs efficiently on highly parallel computers such as the K computer. Achieving a good load balance with particle-based simulation is a difficult task, since using a regular spatial decomposition method causes severe load imbalance, though this works well for grid-based software. Consequently, we have developed an adaptive decomposition method that is designed to work in a way that the calculation time on each node is almost the same, resulting in near-optimal load balance.

The strategy to develop such a universal software is as follows.

We first construct an highly parallel and very efficient implementation of the TreePM algorithm for gravitational N-body problem. This is actually not a completely new implementation, but the GreeM code developed by researchers of the Strategic Program for Innovative Research (SPIRE) Field 5 "The origin of matter and the universe. In collaboration with the Field 5 researchers, we improve the efficiency of the code and study the issues of the data structure, domain decomposition, load balance strategy etc.

In the second stage, we will develop a prototype of the parallel particle simulation platform. We will design the platform so that it can be used for multiple physical systems. In practice, we consider the

following three applications as the initial targets.

1. Gravitational N-body simulation
2. Smoothed Particle Hydrodynamics
3. Molecular Dynamics

In the meantime, we will also investigate the way to improve the performance and accuracy of the current particle-based algorithms for hydrodynamics.

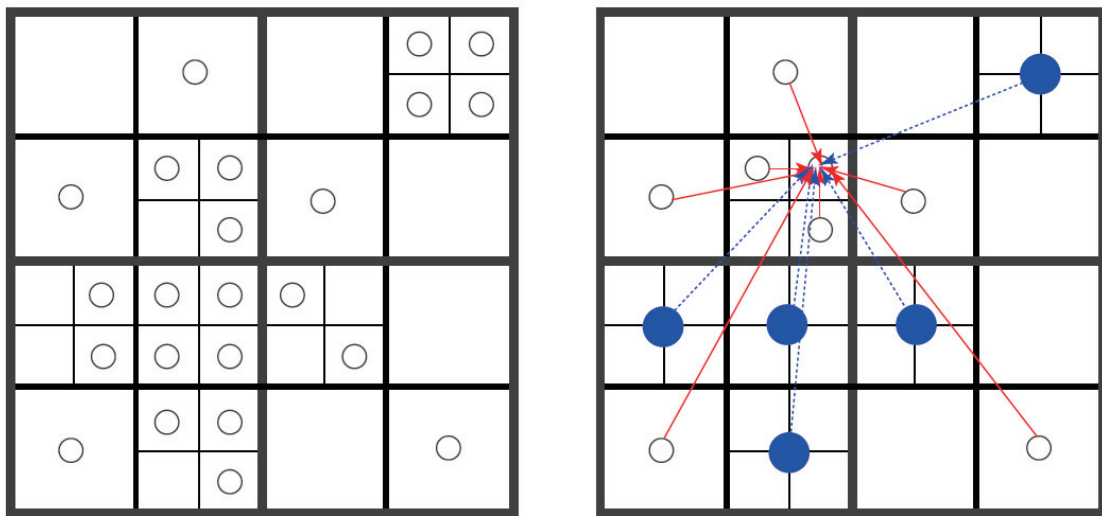
### 3. Research Results and Achievements

As we stated in section 2, we are working on the three major subtopics, in order to develop the universal platform for particle simulations.

In the following, we briefly describe the status of our research in each subtopic.

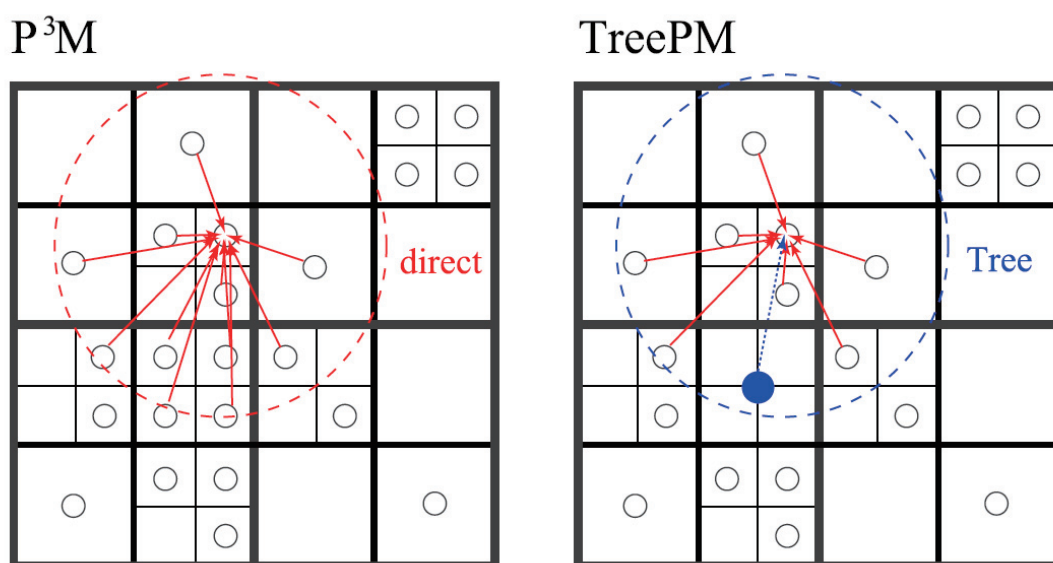
#### 3.1. High-performance gravitational N-body solver.

We use the TreePM algorithm as the basic method for the evaluation of gravitational interaction between particles. TreePM is a combination of the tree method and the P<sup>3</sup>M (particle-particle particle-mesh) scheme. Figure 1 shows the basic idea of the tree algorithm. The space is divided into a hierarchical octree structure (quadtree in the figure). Division is stopped when a cell contains one or no particle. When we calculate the force on a particle, we evaluate the force from a group of particles, with size larger for more distant particles. In this way, we can reduce the calculation cost from  $O(N^2)$  to  $O(N \log N)$ .



**Figure 1. Basic idea of the tree algorithm**

The tree algorithm is widely used, but when the periodic boundary condition is applied, we can actually use a more efficient efficient scheme, since we can calculate the long-range, periodic term using FFT. The  $P^3M$  scheme has been used for such problem, but it has the serious problem that when the density contrast becomes high, the calculation cost increases very quickly. The TreePM scheme solves this difficulty by using the tree algorithm to evaluate the forces from nearby particles. Even when there are very large number of neighbor particles, the calculation cost does not increase much, since the calculation cost of the neighbor force is proportional to the logarithm of the number of neighbors.



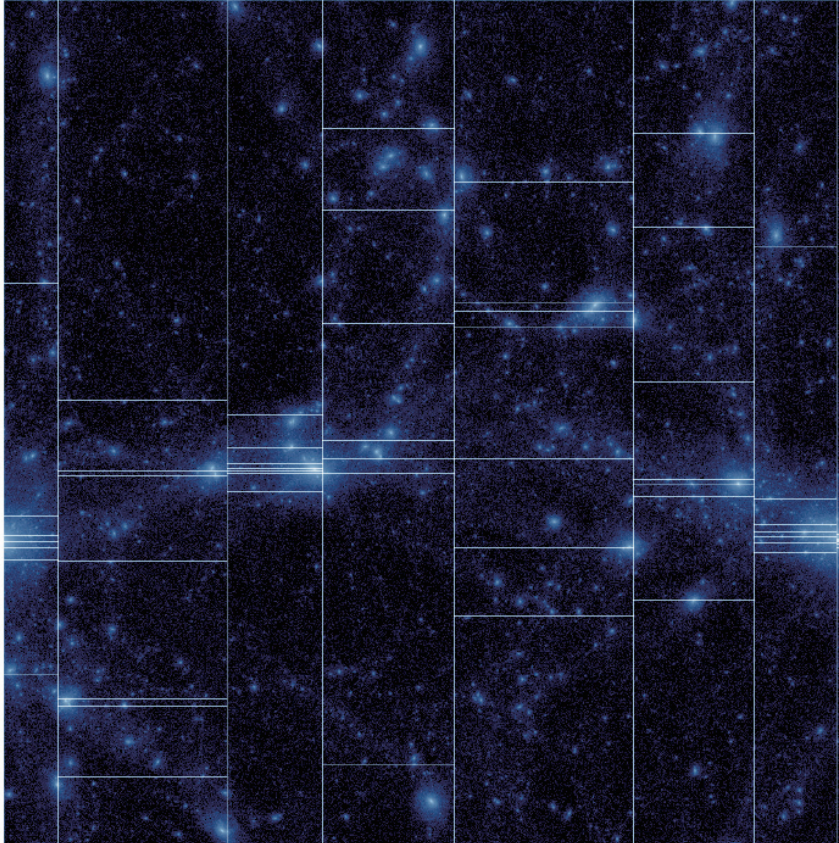
**Figure 2.  $P^3M$  and TreePM**

In order to map the problem to the distributed-memory parallel computer such as the K computer, we adopted the approach to divide the space into domains and assign particles in one domain to one calculation node. We used the orthogonal recursive multisection method developed by the team leader some years ago. It is the generalization of the orthogonal recursive bisection (ORB), which has been widely used in many parallel implementations of the tree algorithm.

With ORB, we recursively divide space into two halves, each with the same number of particles. An obvious disadvantage of the ORB approach is that it can utilize the computing nodes of integral powers of two. Thus, in the worst case we can use only half of the available nodes.

The difference between the multisection method and the ORB is that with the multisection method we allow the divisions to arbitrary number of domains, instead of bisection. This would allow too many possible divisions. In our current implementation, we limit the number of levels to three, and

make the numbers of divisions at all levels as close as possible. Thus, our domain decomposition is topologically a simple three-dimension grid. This fact makes the multisection method well suited to the machines with the 3D torus network like the K computer.



**Figure 3 Recursive multisection in two dimension**

We have developed a "reference code" for gravitational N-body simulation on the K computer. This code is fairly well optimized for the K computer, and shows quite good scalability for even for relatively small-size problems. The asymptotic speed per timestep for large number of nodes is around 7ms. This speed is comparable to that of highly optimized molecular dynamics codes on K, even though our code is designed to handle highly inhomogenous systems.

We used this code as the reference implementation for more generalized particle simulation platform which will be described in the next subsection.

### 3.2. Particle Simulation Platform.

We have completed and released Version 1.0 of the particle simulation platform, which we call FDPS (Framework for Developing Particle Simulator).

The basic idea of FDPS is that the application developer (or the user) specified the way the particles interact with each other, and the rest is taken care by FDPS. Here, "the rest" includes domain decomposition and re-distribution of particles, evaluation of interactions between particles, including those in different domains (different MPI processes, for example).

In practice, there are many additional details the user should give. Consider a relatively simple case of particles interacting with softened  $1/r$  potential. There are a number of small but important points one has to decide on. For example, what algorithm should be used for the interaction calculation? Even if we limit the possibilities to reasonably adaptive schemes for open boundary problems, we have the choice between Barnes-Hut tree and FMM. For both algorithms, there are many different ways to parallelize them on distributed-memory parallel computers. Also, there are infinitely many variations for the time integration schemes.

The base layer of FDPS offers the domain decomposition based on the recursive multi section algorithm (Makino 2004), with arbitrary weighting function for the load balancing (Ishiyama et al 2009). It also offers the parallel implementation of interaction calculation between particles.

The domain decomposition part takes the array of particles on each node as the main argument. It then generates an appropriate domain for each node, redistribute particles according to their locations, and returns.

The interaction calculation part takes the array of particles, the domain decomposition structure, and the specification of the interaction between particles as main arguments. The actual implementation of this part need to take into account a number of details. For example, the interaction can be of long-range nature, such as gravity, Coulomb force, and interaction between computational elements in the boundary element method (BEM). In this case, the user should also provide the way to construct approximations such as the multipole expansion and the way to estimate error. The interaction might be of short-range nature, with either particle-dependent or independent cutoff length. In these cases, the interaction calculation part should be reasonably efficient in finding neighbor particles.

We have successfully implemented all of these functionalities in FDPS version 1.0. (<https://github.com/FDPS/FDPS>). Using FDPS, a gravitational N-body simulation code can be written in 120 lines, and that code is actually fully scalable even to full-node runs on K computer. For SPH calculations, we have also achieved similar scaling.

FDPS is implemented as a class template library in C++ language. It receives the class definition of particles and a function (or multiple functions in the case of complex interactions) to evaluate the interaction between particles. When a user program is compiled with the FDPS library, the class template is instantiated with the user-specified definition of the particle class. Thus, even though the FDPS library functions are generic ones not specialized to a particular definition of particles, it behaves as if it is a specialized one.

The measured performance of applications developed using FDPS is quite good. Both for gravity-only calculation and SPH calculation, weak-scaling performance is practically perfect, up to the full-node configuration of K computer. Moreover, the measured efficiency, in terms of the fraction of the peak floating-point performance, is also very high. It is around 50% for gravity-only calculation. For SPH calculations, at the time of writing the performance is around 10%.

### 3.3. Improvements on SPH.

SPH (Smoothed Particle Hydrodynamics) has been used in many field, including astrophysics, mechanical engineering and civil engineering. Recently, however, it was pointed out that the standard formulation of SPH has numerical difficulty at the contact discontinuity. The reason is that the formulation of the standard SPH requires that the density is differentiable, which is by definition no the case at the contact discontinuity.

We have been working on the possible solution on this problem. One approach is to reformulate SPH so that it does not use the density in the right-hand side of the equation of motion. We one way to achieve the density independence. We constructed an SPH scheme which uses artificial density-like quantity as the base of the volume estimator. It evolves through usual continuity equation, but with additional diffusion term. Thus, we can guarantee the continuity and differentiability of this quantity, except at the initial condition or at the moment when two fluid elements contact with each other. This scheme seems to work extremely well, and we are currently working on the way to extend this scheme so that it can handle free surface accurately.

We are also working on a completely different approach, in which we replace the SPH formulation to evaluate the gradient to other schemes. SPH has a known problem that its kernel estimate contains  $O(1)$  error, since the summation of contributions from neighbor particles is not guaranteed to be unity. The reason why SPH uses this mathematically inconsistent formulation is to achieve symmetry and conservation. In SPH discretization, interaction between two particles is symmetric, which guarantees the conservation of linear and angular momenta. However, the use of SPH



approximation resulted in rather low accuracy, which limits the reliability of the results obtained using SPH. We are experimenting with several different schemes which can achieve much higher accuracy, while losing some of the nice features of SPH such as the symmetry of interaction.

#### 4. Schedule and Future Plan

We plan to improve the performance of FDPS further in FY 2015. In particular, we plan to extend the API so that the users of FDPS can easily use heterogeneous machines such as machines with GPGPUs or Intel MIC.

#### References

Ishiyama, T. Nitadori, K. and Makino, J., 2012, 4.45 Pflops astrophysical N-body simulation on K computer: the gravitational trillion-body problem, SC '12 Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis Article No. 5 IEEE Computer Society Press Los Alamitos, CA, USA ©2012 ISBN: 978-1-4673-0804-5

#### 5. Publication, Presentation and Deliverables

##### (1) Journal Papers

1. “Binary formation in planetesimal disks. II. Planetesimals with a mass spectrum”. Kominami, J. D., Makino, J., Publications of the Astronomical Society of Japan 66, 123. 2014
2. “Merger criteria of multiple massive black holes and the impact on the host galaxy”. Tanikawa, A., Umemura, M. Monthly Notices of the Royal Astronomical Society 440, 652-662. 2014

##### (2) Conference Papers

1. “Nanoblock Unroll: Towards the Automatic Generation of Stencil Codes with the Optimal Performance”, Takayuki Muranushi; Keigo Nitadori, Junichiro Makino, Proceedings of the Second Workshop on Optimizing Stencil Computations, 49-55
2. “Systems Demonstration: Writing NetBSD Sound Drivers in Haskell”, Takayuki Muranushi; Motomu Okabe, 2014 ACM SIGPLAN Symposium on Haskell, 77-78
3. “Experience Report: Type-checking Polymorphic Units for Astrophysics Research in Haskell”, Takayuki Muranushi; Richard A. Eisenberg, 2014 ACM SIGPLAN Symposium on Haskell, 31-38
4. “24.77 Pflops on a gravitational tree-code to simulate the Milky Way Galaxy with 18600 GPUs”, Jeroen Bédorf, Evghenii Gaburov, Michiko S. Fujii, Keigo Nitadori, Tomoaki Ishiyama, and Simon Portegies Zwart, In Proceedings of the International Conference for

## High Performance Computing, Networking, Storage and Analysis (SC '14), 54-65

## (3) Invited Talks

1. 谷川 衝「銀河中における巨大ブラックホールの合体と成長の研究」、谷川衝、「超巨大ブラックホール研究推進連絡会」第2回ワークショップ、2014/11/3-4、筑波大学
2. 谷川 衝「中間質量ブラックホール」、第13回DECIGOワークショップ、2014/10/26、京都大学
3. 谷川 衝「星団の力学進化と恒星進化」、第1回DTAシンポジウム「星形成領域および星団環境での惑星の形成と進化」、2014/9/29-30、国立天文台
4. Keigo Nitadori “A block-step version of KS regularization”, Steller N-body Dynamics, 2014/9/10, Sexten Center for Astrophysics, Italy
5. 牧野 淳一郎 エクサスケールコンピュータとその上での分子シミュレーション 第28回分子シミュレーション討論会 2014/11/13 仙台
6. 牧野 淳一郎 ゴードン・ベル賞ってどんなもの? --- 歴史と意義 理研東京事務所 記者勉強会 2014/11/11
7. 牧野 淳一郎 スーパーコンピュータの歴史 --- 「京」コンピュータまで、その先 PDF 北大での講義1コマ 2014/10/30
8. 牧野 淳一郎 HPC と省電力設計 Calypto Uses Forum 2014 2014/08/29
9. 粒子法の大規模並列化フレームワークとSPH法に関するいくつかの話題先駆的科学計算に関するフォーラム 2014/08/5-6

## (4) Posters and presentations

1. 細野 七月 “iSALE と粒子法コードの比較に向けて”、2014/10/11、日本惑星科学会
2. 細野 七月 “Terrestrial magma ocean origin of the moon”、2014/10/23-25、衝突研究会
3. 谷川 衝「連星白色矮星の合体とIa型超新星」、第27回理論懇シンポジウム「理論天文学・宇宙物理学と境界領域」、2014/12/24-26、国立天文台
4. 谷川 衝「連星白色矮星の合体とIa型超新星」、第2回DTAシンポジウム「コンパクト天体の活動性と磁氣的性質」、2014/10/27-29、国立天文台
5. 谷川 衝「連星白色矮星の合体に伴う星周物質の形成」、日本天文学会2014年秋季年会、2014/9/11-13、山形大学
6. 岩澤全規 “Particle-Particle Particle-Tree(P3T)法のGPUへの実装及び高密度星団系への応用”、2014/9/11、日本天文学会2014年秋季年会
7. anikawa, A. “Detection rate of binary black holes formed in globular clusters”, 3-7 Jun 2013, Yukawa Institute for Theoretical Physics Kyoto University, Yukawa International Seminar 2013 Gravitational Waves Revolution in Astronomy & Astrophysics

(5) Patents and Deliverables

1. FDPS <https://github.com/FDPS/FDPS>

(6) Awards