# Parallel TREE code for two-component ultracold plasma analysis

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**Abstract**

The TREE method has been widely used for long-range interaction $N$-body problems. We have developed a parallel TREE code for two-component classical plasmas with open boundary conditions and highly non-uniform charge distributions. The program efficiently handles millions of particles evolved over long relaxation times requiring millions of time steps. Appropriate domain decomposition and dynamic data management were employed, and large-scale parallel processing was achieved using an intermediate level of granularity of domain decomposition and ghost TREE communication. Even though the computational load is not fully distributed in fine grains, high parallel efficiency was achieved for ultracold plasma systems of charged particles. As an application, we performed simulations of an ultracold neutral plasma with a half million particles and a half million time steps. For the long temporal trajectories of relaxation between heavy ions and light electrons, large configurations of ultracold plasmas can now be investigated, which was not possible in past studies.

*Key words:* ultracold plasma, two-component plasma, TREE, domain decomposition, intermediate granularity, ghost TREE, dynamic memory management, hybrid parallel computing
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## 1 Introduction

For $N$-body problems in gravitational and electrostatic phenomena, significant computing resources are required due to the long range interactions. Despite advances in computing speed, it is still difficult to obtain sustainable results of realistically large configurations for many physical applications.

An ultracold plasma (UCP) is extensively studied in plasma physics, and is a typical example of long-range interactions for an open boundary. Experimentally, it is generated by photoionization of laser-cooled heavy atoms, and the system has a low temperature (T = $\mu$K to mK) compared to a conventional hot plasma (T = $10^3$ to $10^7$K) [1]. By the initial disorder of particles, ions are heated, and active momentum transfer occurs between electrons and ions. We shall study the behavior of charged particles and the physical properties of ultracold neutral plasmas.

Studying electron-ion coupling relaxation, it was found that several millions of time steps are required for ultracold plasma evolution. This is a huge computing load, and the required time frame restricts the size of problems that can be considered. We first implemented a molecular dynamics (MD) method with all pair-wise calculations of long-range interactions. However, such an approach, while accurate, scales with the square of the number ($N$) of charged particles. Thus, it allowed only simulations of $10^3$ to $10^4$ particles over sufficiently long time [2,3,4]. In experiments, common sizes of ultracold plasmas are reported as more than $10^6$ particles [1,5,6], and larger computing capacity is therefore imperative for realistic simulations.

Consequently, an approximate method for evaluating the electrostatic forces is necessary in order to accelerate computing speed and increase the simulation capacity. One of the candidates is the TREE method [7], which has been widely used in astrophysical problems due to its $N \log N$ scaling of the computing cost. The basic idea is that particle interactions are calculated explicitly at close range while effective, averaged properties are considered for far-field interactions. Gravitational problems have a potential of $1/r$, where $r$ is the distance between two points, and are similar to a Coulomb system. Therefore we will be able to apply all the methods, which have been developed for astrophysics, to electron and ion interactions.

In addition to the serial TREE method, a parallel version has been constructed in order to distribute the computing load and thereby accelerate computation. A specific shape of particle ensembles is considered from experimental data [5,6]: charged particles are distributed non-uniformly, but the overall shape is roughly symmetric. Particles are located inside of a certain spherical volume, and this confirms simple and balanced domain decompositions for parallel computing of ultracold neutral plasmas. With the help of dynamic memory management and effective TREE communication, a highly efficient parallel code has been built. Finally, we demonstrate that the program works well for ultracold plasma analysis. The following describes how the TREE method is implemented for a two-component plasma (TCP) simulation, and how it is parallelized. Basic applications are also presented.

## 2 TCP analysis

For a fully ionized plasma, we describe the interactions as Coulomb forces between well-defined charged particles. However, because the electron mass is small compared to the ion, electrons will move faster than ions. This results in much smaller numerical time steps and longer relaxation times when simulating electrons compared to that of an ionic one-component plasma (OCP).

Since the dominating potential is Coulombic, each charged particle will interact with all the other charged particles and the interaction between particles cannot be truncated at a characteristic distance. Using a TREE method, this extensive calculation can be achieved efficiently, and the computing load can be balanced. The force on each charged particle is calculated from the interaction with the TREE. Velocity and position of particles are updated using velocity Verlet [8] time integration once the force field has been evaluated.

### *2.1 Modified Coulomb potential*

The Coulomb pair potential between two point-charges, separated by the distance $r$, is given by

$$V_{ij} = \frac{C}{r}. \tag{1}$$

$$C = \frac{q_i q_j e^2}{4\pi\epsilon_0}, \tag{2}$$

where $q_i$ and $q_j$ are the fractional charges of particles $i$ and $j$. $e$ is the unit charge, and $\epsilon_0$ is the vacuum permittivity. For the same kind of particles (electron-electron and ion-ion), the forces are repulsive whereas attractive forces are present for electron-ion interactions. Consequently, the bare Coulomb potential will result in an attractive singularity for the electron-ion pair at close distance ($r \approx 0$). However, quantum diffraction between electrons and ions in physical systems prevents such point wise collisions, thus requiring a modification to the bare Coulomb potential. Several modified Coulomb interactions have been proposed [9,10,11]; we implemented the Kelbg potential:

$$V_{ei} = \frac{C}{r}\Big[1 - \exp\Big(-\frac{r}{\lambda_{ei}}\Big)\Big], \tag{3}$$

where $\lambda_{ei}$ is the thermal de Broglie wavelength

$$\lambda_{ei} = \sqrt{\frac{2\pi\hbar^2}{\mu_{ei}k_B T}}. \tag{4}$$

At close distances ($r < \lambda_{ei}$), the exponential term is dominant, and equation (3) asymptotes as $\frac{C}{\lambda_{ei}}\Big[1 - \frac{r}{2\lambda_{ei}}\Big]$. The exponential term is negligible in the far field ($r \gg \lambda_{ei}$) where the equation converges to $\frac{C}{r}$. The thermal de Broglie wavelength plays a key role for close encounters; however, the temperature is not a well-defined quantity for these types of systems. A better criterion results by setting $\lambda_{ei}$ to a fixed value $r_s$ based on an averaged closest-approach or the lowest Rydberg state allowed in recombination. Considering Rydberg states, $20 - 180$Å will be the range of the parameter, and we use $\lambda_{ei} = 100$Å [2] for our simulations. The basic properties of the TCP remain independent of this cut-off parameter; its effect is merely to prevent very close encounters that require very short time steps to resolve the dynamics accurately. For the electron-electron and ion-ion interactions, the bare Coulomb potential is applied.

## 3 TREE construction

Before explaining the parallel TREE method, we describe how to build a TREE data structure for given particle sets. First, we assume a large cube that encloses all particles. Then we evenly divide the cube into eight small boxes, and each particle is associated with a box. Further subdividing each of the small boxes into eight even smaller pieces, all of the particles are associated with the smaller boxes again. This refining is repeated until every box contains no more than one particle. This hierarchical procedure leads to the tree shaped data structure.

The finest state of a TREE is called a **leaf**. Above leaves, there exist large intermediate branches, referred to as **twig**s [12]. A pseudo-particle is an effectively-charged particle of a twig, and the charge corresponds to the sum of the charges of subordinate twigs and leaves. The position of the pseudo-particle is interpolated from the lower twig or leaf positions depending on the charge ratio.

When calculating the interactions between a particle and the TREE structure, the distance between the particle and the twig, and the size of the box enclosing the corresponding twig will be inspected. If the relation satisfies certain criteria, the effective charge of the twig will be employed for the Coulomb potential. If not, the twig is opened until the criterion is met. The opening criterion, due to Barnes as described in [13], reads

$$\frac{s}{\theta} + \delta < d, \tag{5}$$

where $s$ is the size of box, $d$ is the distance between a particle and a pseudo-particle, and $\delta$ is the distance between a pseudo-particle and the center of the box.

An opening criterion of $\theta < 1.0$ is commonly practiced. A high opening criterion approximates force fields with upper branches of the TREE - thus it accelerates simulations at the expense of accuracy. In contrast, a low opening criterion demands fine calculations and results in higher accuracy with more computing resources. Depending on the given problems and the required accuracy, an appropriate $\theta$ will be determined. As mentioned above, neighboring particles will interact with each other but the interactions of remote particles will be replaced by approximate pseudo-particles. Finally, the algorithm results in $N \log N$ scaling of computing cost, instead of $N^2$ scaling of all pair-wise calculations. More detailed explanations about TREE construction can be found elsewhere [7,12].

## 4 Parallelization

Even though the TREE method is computationally more efficient than direct evaluations of all pair-wise interactions for large configurations, a single processor calculation still remains inadequate for the task at hand. Therefore, we parallelized the TREE method onto multiple processors in order to distribute the computational load and accelerate computing speed. There have been several parallel schemes for TREE methods like hashed oct-tree [14], FLY [15], and dynamic and adaptive domain decomposition [16]. We have developed a simple domain decomposing parallel method using a ghost TREE communication. The problem domain is decomposed into coarse grains, rather than fine segments, that still allows for large scale parallel processing. Details are given below. The parallel routine was developed with the conventional message passing interface (MPI) library [17], allowing applications across most contemporary parallel computing platforms.

## *4.1 Domain decomposition*

The basic configuration of the particles of ultracold plasmas maintains over time a generally spherical and roughly symmetrical distribution having though a highly non-uniform radial component as shown in Figure 1. The center of the sphere can be placed at the origin, and we can assume that particles are distributed randomly within the sphere. Using Cartesian coordinates, an eight processor parallelization and domain decomposition can be defined as shown in Figure 2. Each segment of geometrical space will be designated to each processor, and they will communicate with each other. For more than eight processors, a finer domain decomposition might be performed, but we still keep the eight segment domain decompositions. We discuss the large-scale parallel computing below.

## *4.2 Particle management*

Due to the temporal evolution of particle positions during a simulation, some particles will move between the spatial regions of the processors, and each processor will have to manage the migrations. For effective memory management, a dynamic memory allocation scheme has been implemented. After a Verlet time integration step, new positions of all the particles are determined. Investigating the new positions, the particles which exceed the spatial range of their processor will be identified. Their information will be stored in a buffer, and each processor will remove these particles from memory. Then each processor sends and receives migrating particle data. For newly imported particles, their information is attached at the end of the memory block.

## *4.3 TREE communication*

At the core of the parallel TREE algorithm is the communication between processors, namely what and how to communicate. If we share the whole TREE structure of all processors, communication will be operationally easy. This scheme, though, requires huge data communication and management resources. Hence, we need to be selective with communicating only necessary information among processors.

Considering the basics of the TREE method, we need leaf information at close range but only twig (pseudo-particle) information for larger distances. This rule is also applied for parallel computing, and we employ pre-pruning before communication [18,13]. If two processors are neighbors, a large fraction of the TREE will be necessary whereas a small fraction will be enough if the processors are remote.

After copying the local TREE into a buffer, each processor begins to communicate with the other processors. Asynchronously, each processor sends its buffer and receives the TREE information of other processors, called the ghost TREE [19]. Using ghost TREEs, the interactions with other particles of other processors will be evaluated.

With a given opening criterion, a certain amount of the local TREE will be sent to other processors, but we still need another step to convert the data. The TREE data are managed by FORTRAN pointers, but they are not supported by a common MPI library to send/receive. Therefore, we need to convert them into combinations of MPI_INTEGER and MPI_REAL variables. Not only the data component of each leaf and twig, but also the order and branch of the TREE should be communicated, and we have developed a simple data array to keep the order of the TREE structure.

As shown in Figure 3, the TREE structure and order can be represented by an architecture series. Each natural number indicates the node array of a pseudo-particle, which contains position and effective charge. A negative number (= -1) means a back step, and all of the branches and orders of the TREE structure can be represented by the architecture series. Conversely, received ghost TREE data can be decoded into pointer forms using the received architecture series. Corresponding pseudo code is shown below:

```
RECURSIVE SUBROUTINE REBUILD(POINTER, N)
    N = N + 1
    ALLOCATE POINTER
    POINTER = NODE(ARCH(N))
    IF  ARCH(N+1)>0 THEN
       CALL  REBUILD(POINTER_Child_1, N)
       N = N + 1
       IF  ARCH(N+1)>0 THEN
           CALL  REBUILD(POINTER_Child_2, N)
           N = N + 1
       END IF
       ......

       IF  ARCH(N+1)>0 THEN
           CALL  REBUILD(POINTER_Child_8, N)
           N = N + 1
       END IF
    END IF
END SUBROUTINE
```

## *4.4 Large scale parallel processing*

As mentioned earlier, the simulations of ultracold plasma evolution demand a large number of time steps, typically of the order of $10^5 - 10^6$. This time frame and the available computing power mediate the largest configuration which we can handle as around a million particles. The fine granularity of $N$ domain decompositions of $N$ processors will reduce the size of the local TREE to a system of less than $10^4$ particles for which the TREE efficiency becomes poor [12], for large scale parallel computing. But the intermediate granular parallelism, which employs an intermediate granularity by administrating local TREEs as a unit of a single segment of Figure 2, still keeps the local TREE as $10^5$ particles or more than that, providing higher efficiency. Also we can expect easy book-keeping and simple data handling.

We maintain eight piece domain decompositions, as shown above, and apply processors of multiples of eight. Then each segment of Figure 2 will have the same number of local processors. All particles of each segment are distributed evenly for each local processor for load balance. When the local TREE of each segment is built, all local processors of each segment swap and share the position of particles of the segment. Then the local TREE is built at every local processor, without parallelism. However, particle interactions with the local TREE, which consume most of the computing resources, are calculated in parallel.

For the communication between segments, one of the local processors will be assigned as the **head processor**. After calculating particle interactions with the local TREE, the head processor of each segment will copy and send the local TREE to other segments while receiving ghost TREEs from the corresponding segments. This communication is performed only by the head processor, and the communication burden can thereby be reduced. After communication between head processors, the received ghost TREEs are distributed again on the local processors inside the segment. Ghost TREEs are handled as the same way of local TREEs. The decoding is done in serial but particle interactions are done in parallel.

The schematic flow of each segment is shown in Figure 4. Using this method, multiples of eight processors can participate in the parallel computing. Even though this method does not fully distribute the computing load with fine granularity, it allows for easy book-keeping and reduces the communication load. Although the experimental charge distributions of ultracold plasmas are non-uniform, they retain an overall spherical and roughly symmetrical appearance. Therefore eight-segment domain decomposition will divide the problem domain quite evenly, and we can expect good load balance from the beginning. Also divided particles are distributed uniformly for the local processors of each segment. During simulations, some of particles will move between segments as discussed above, and new particles are sent to a local processor, which has the least particles in the segment. These procedures maintain good load balance for each processor.

In addition to the message passing interface, OpenMP [20] has been implemented in order to utilize shared memory processing. Basic operation of the code is executed in a single thread, but particle interactions with the TREE are forked along multiple threads and computation is thereby accelerated.

## 5 Computational experiments

As an example to illustrate the developed method, we investigate the dynamics of electrons and ions with initial conditions of previous work [2]. The configuration has same electron/ion density ($\rho_i = 4.32 \times 10^9$/cc), and particles are distributed inside a sphere. The initial temperature is 3 K for electrons and $1 \times 10^{-6}$ K for ions. A reduced ion mass simulation [2], which artificially reduces the ion mass from 131 to 0.01 amu, is employed in order to expedite momentum transfer between electrons and ions. A time step of 20 fs and $5 \times 10^5$ time steps are employed for the plasma evolutions.

With these configurations, a UCP system of $5 \times 10^3$ electrons ($q = -1$) and $5 \times 10^3$ ions ($q = +1$) has been tested with all pair-wise and TREE methods in order to evaluate the developed parallel TREE code. The test machine is grendel, a linux cluster at Los Alamos National Laboratory, which is composed of 126 nodes of dual 2.4GHz Xeon processors with Myrinet interconnections. 2Gb of memory is equipped for each node. Los Alamos MPI (LAMPI) library and OpenMP API of intel fortran compiler 9.1.036 were employed to compile the code. As shown in Figure 5, the average kinetic energy ($= 3k_BT/2$) of the electrons ($\mathrm{T_e}$) and ions ($\mathrm{T_i}$) approach the same asymptote. Therefore, we conclude that the developed TREE code reproduces the energy transfer well. As for computing cost, the all pair-wise method took 62 hours with 16 processors while the TREE code ($\theta = 0.4$) used 26 hours with 64 processors. Even though the TREE code efficiency is less than the all pair-wise calculations for this small set of particles, the TREE code scales as $N \log N$, while the all pair-wise method scales as $N^2$ as discussed above. Consequently, the TREE code is imperative for larger systems involving millions of particles. For a one-million particle set, the all pair-wise method requires $10^4$ times more computing resources than above, and this is not practical.

To determine parallel performance, larger sets of particles were tested. Also several opening criteria have been tested, and the corresponding errors were found. Finally, simple applications of large ultracold plasmas are given below.

## *5.1 Parallel performance*

Parallel performance was tested with $10^5$ particles ($5 \times 10^4$ electrons and $5 \times 10^4$ ions). Two kinds of opening criteria were tested, $\theta = 0.4$ and 0.6. The results below were achieved on flash, a linux cluster at Los Alamos National Laboratory, which is composed of 300 nodes per segment, with dual Opteron processors of 2.0-2.4GHz and Myrinet interconnections. 8-16Gb of memory is equipped for each node. Los Alamos MPI (LAMPI) library and OpenMP API of intel fortran compiler 9.1.037 were employed to compile the code.

The results are summarized in Figure 6. Scalability is the ratio between wall-clock time of a parallel execution and the time of the corresponding serial code. With a dual processor machine, 16, 32, and 64 nodes were used while the number of processors are 32, 64, and 128 respectively. For 128 processors, better than 80% parallel efficiency was achieved for both opening criteria.

Also a $10^6$ particle set ($5 \times 10^5$ electrons and $5 \times 10^5$ ions) was tested to study parallel efficiency. Because the size is 10 times larger than above, we simulated with up to 256 processors; the results are summarized in Figure 7. Compared to a small system, the effect of the opening criteria is clear. A low opening criterion imposes larger computing loads, showing efficient parallel computing, and more wall clock time is consumed. A high opening criterion shows less parallel efficiency, but completes a calculation faster. With current computing resources and $\theta = 0.6$, one million particle system with one million time steps takes approximately 700 hours with 256 processors.

The effect of configuration size was tested. Systems with 0.1, 1.0, and 10 millions of particles (half electrons and half ions) have been tested with different number of nodes. 100 time steps were tested and wall-clock times were examined per each section as shown in Table 1. First, using 8 nodes of 16 processors, basic domain decomposition was tested. Even though 2 processors of a single node share the same segment, parallel computing is done by OpenMP only. Consequently, a single segment is taken care of by a single node only, and the result will serve as a reference for the bare eight segment domain decomposition, without the intermediate parallelism. Most of the computing resource is devoted to particle interactions and updates. By pre-pruning, the load of communication and ghost TREE management is affected by the opening criterion. The relative cost of each section is quite consistent for the size variations of systems. 64 nodes of 128 processors were also applied, employing intermediate parallelism. Because 8 nodes share a single segment, the cost of communication and TREE management is relatively high compared to 8 node calculations. But it decreases as the number of employed particles increases, providing better efficiency. For the 64 node results, wall-clock times and speed ratios, calculated relative to the 1 million particle results, are shown in Figure

8. For the change of problem sizes, speed ratios show $N \log N$ scaling.

### *5.2 Opening criterion study*

TREE code performance and accuracy depend on the opening criterion. $5 \times 10^4$ electrons and $5 \times 10^4$ ions were tested with several opening criteria in order to determine accuracy and efficiency differences under same computing conditions. 1,000 time steps were employed with 64 nodes of 128 processors on flash cluster. Figure 9 provides the results where the error of total energy was measured against the all pair-wise results, and scaling ratio is relative wall-clock time for $\theta = 0.1$. For $\theta \leq 0.6$, energy errors are quite small ($< 0.01\%$) and converge to the result of all pair-wise calculations for smaller $\theta$, accompanying fluctuations. However, computing cost increases quite quickly as $\theta$ decreases; $\theta = 0.1$ demands three times the computing time of $\theta = 0.2$, and $\theta = 0.2$ costs three times that of $\theta = 0.4$. Therefore a balance between accuracy and efficiency needs to be determined. Also the energy error increases during the long temporal relaxation of charged particles, and $\theta \leq 0.7$ will be required for plasma relaxation simulations of our study.

### *5.3 Evolution of two-component ultracold plasmas*

Using the above mentioned initial conditions and reduced ion masses, electron and ion temperatures were investigated up to 10 ns with $2.5 \times 10^5$ electrons and $2.5 \times 10^5$ ions, along $5 \times 10^5$ time steps. Figure 10 provides the results, which are consistent with previous work [2]. We can see that the average ion temperature increases rapidly for early times and saturates after 2 ns. Compared to the previous work (500 electrons and 500 ions), we employed much more particles, resulting in higher initial potential energy and more heating of the ions. We found periodic oscillations in the electron temperature evolution, which might be the effect of an electron plasma wave. This will be studied extensively in future work [21].

## 6 Concluding remarks

To analyze the relaxation behavior of ultracold plasmas, a TREE code has been developed. Also, a parallel implementation has been conducted in order to allow for simulations of sufficiently large systems over sufficiently long time. Dynamic data management was implemented for efficient memory allocation of data communication, and eight-segment domain decomposition was applied with a ghost TREE method. A parallelism of an intermediate granularity was developed for large scale parallel processing, and optimized for systems with millions of charged particles. Finally, the developed code has been found to work well with the given ultracold plasma systems and efficient parallel performance has been demonstrated for various configurations.

As discussed above, a simulation of two-component ultracold plasmas requires significant computing resources. Previously, only $10^3$ to $10^4$ particles could be employed because of the long temporal trajectories of ultracold plasma relaxation. Here, with the developed parallel TREE code, we have increased the computing capacity up to $10^6$ interacting particles. This is a crucial achievement in the study of ultracold plasma dynamics. Much larger and realistic configurations of ultracold plasmas can now be investigated.

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## References

[1] T. C. Killian, S. Kulin, S. D. Bergeson, L. A. Orozco, C. Orzel, S. L. Rolston, Creation of an ultracold neutral plasma, Physical Review Letters 83 (23) (1999) 4776–4779.

[2] S. Mazevet, L. A. Collins, J. D. Kress, Evolution of ultracold neutral plasmas, Physical Review Letters 88 (5) (2002) 055001.

[3] S. G. Kuzmin, T. M. O'Neil, Numerical simulation of ultracold plasmas: How rapid intrinsic heating limits the development of correlation, Phys. Rev. Lett. 88 (6) (2002) 065003.

[4] S. G. Kuzmin, T. M. O'Neil, Numerical simulation of ultracold plasmas, Physics of Plasmas 9 (2002) 3743–3751.

[5] C. E. Simien, Y. C. Chen, P. Gupta, S. Laha, Y. N. Martinez, P. G. Mickelson, S. B. Nagel, T. C. Killian, Using absorption imaging to study ion dynamics in an ultracold neutral plasma, Physical Review Letters 92 (14) (2004) 143001.

[6] Y. C. Chen, C. E. Simien, S. Laha, P. Gupta, Y. N. Martinez, P. G. Mickelson, S. B. Nagel, T. C. Killian, Electron screening and kinetic-energy oscillations in a strongly coupled plasma, Physical Review Letters 93 (26) (2004) 265003.

[7] J. Barnes, P. Hut, A hierarchical $o(n \log n)$ force calculation algorithm, Nature 324 (1986) 446–449.

[8] M. P. Allen, D. J. Tildesley, Computer simulation of liquids, Oxford Science Publications, 1987.

[9] V. G. Kelbg, Theorie des Quanten-Plasmas, Annalen der Physik 12 (1963) 219–224; Quantenstatistik der Gase mit Coulomb-Wechselwirkung, Annalen der Physik 12 (1964) 354–360; Klassische statistische Mechanik der Teilchen-Mischungen mit sortenabhängigen weitreichenden zwischenmolekularen W echselwirkungen, Annalen der Physik 14 (1964) 394–403.

[10] C. Deutsch, Nodal expansion in a real matter plasma, Physics letters 60A (4) (1977) 404–441.

[11] T. Pschiwul, G. Zwicknagel, MD-simulations of the dynamic properties of a nonideal two-component plasma, Contribution to plasma physics 41 (2-3) (2001) 271–274.

[12] S. Pfalzner, P. Gibbon, Many-body tree methods in physics, Cambridge university press, 1996.

[13] J. Dubinski, A parallel tree code, New Astronomy 1 (1996) 133–147.

[14] M. S. Warren, J. K. Salmon, A parallel hashed oct-tree n-body algorithm, in: Supercomputing, 1993, pp. 12–21.

[15] U. Becciani, V. Antonuccio-Delogu, Are you ready to FLY in the universe? a multi-platform $n$-body tree code for parallel supercomputers, Computer Physics Communications 136 (2001) 54–63.

[16] P. Miocchi, R. Capuzzo-Dolcetta, An efficent parallel tree-code for the simulation of self-gravitating systems, Astronomy and Astrophysics 382 (2002) 758–767.

[17] W. Gropp, E. Lusk, A. Skjellum, Using MPI, The MIT press, 1999.

[18] J. K. Salmon, Parallel hierarchical n-body methods, Ph.D. thesis, California Institute of Technology (1991).

[19] Z. Wang, N. Ghoniem, S. Swaminarayan, R. LeSar, A parallel algorithm for 3d dislocation dynamics, Journal of computational physics 219 (2006) 608–621.

[20] `http://www.openmp.org/drupal/`.

[21] B. Jeon, J. D. Kress, L. A. Collins, N. Grønbech-Jensen, Evolution of ultracold plasmas: two-component plasma analysis, in preparation.

Table 1
Computing resource (in seconds) for parallel TREE simulations in terms of employed particles and opening criterion. $N$ is the number of particles. $\theta$ is the opening criterion. $n$ is the number of computing nodes.

| | | | section | | | |
|---|---|---|---|---|---|---|
| $n$ | $N$ | $\theta$ | particle interactions and updates | local TREE management | ghost TREE management | commu-nication |
| 8 | 0.1 million | 0.4 | 314.0 | 1.5 | 17.8 | 2.5 |
| | | 0.6 | 139.2 | 1.5 | 8.0 | 1.7 |
| | 1 million | 0.4 | $6.6 \times 10^3$ | 20.4 | 346.9 | 9.9 |
| | | 0.6 | $2.4 \times 10^3$ | 20.4 | 141.0 | 6.3 |
| | 10 million | 0.4 | $9.1 \times 10^4$ | 255.3 | $2.1 \times 10^3$ | 42.1 |
| | | 0.6 | $3.1 \times 10^4$ | 254.6 | 909.2 | 26.9 |
| 64 | 0.1 million | 0.4 | 40.1 | 1.9 | 7.5 | 7.2 |
| | | 0.6 | 18.2 | 2.5 | 3.4 | 4.7 |
| | 1 million | 0.4 | 826.2 | 22.9 | 71.9 | 29.7 |
| | | 0.6 | 305.0 | 21.9 | 33.3 | 19.5 |
| | 10 million | 0.4 | $1.1 \times 10^4$ | 270.6 | 469.5 | 130.0 |
| | | 0.6 | $4.0 \times 10^3$ | 272.3 | 205.7 | 85.1 |

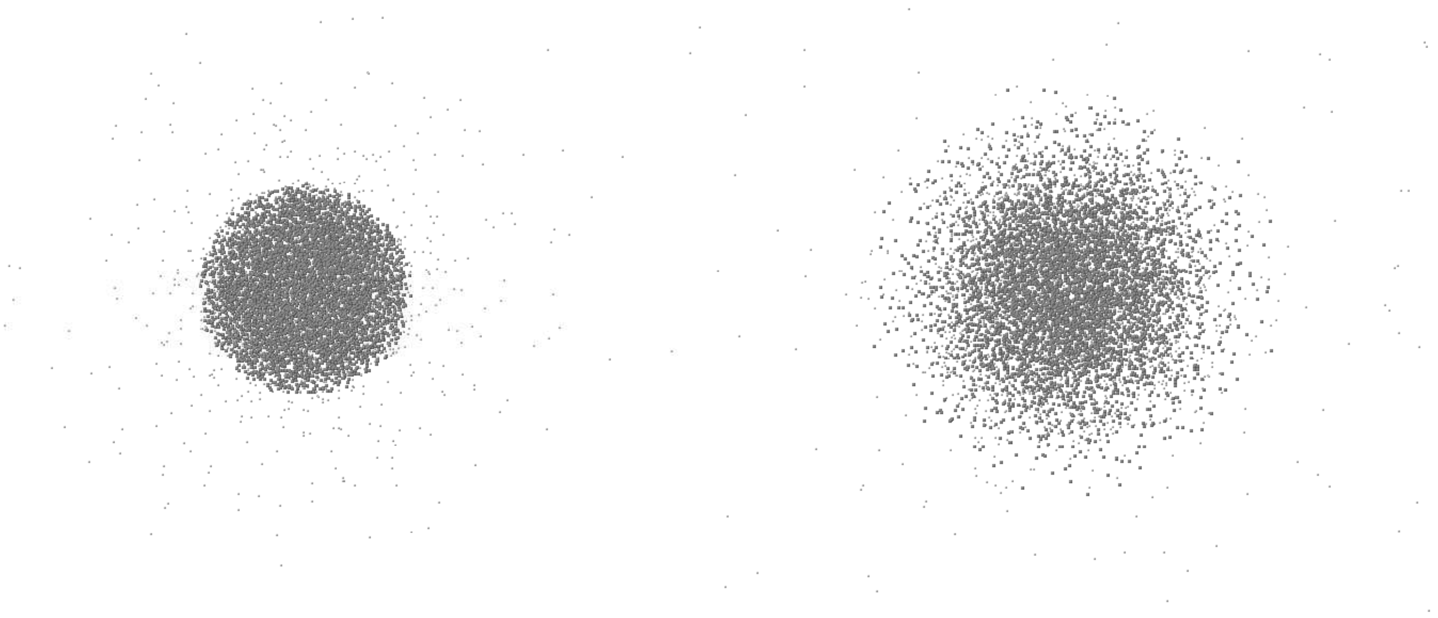

Fig. 1. Electron($5 \times 10^3$)/ion($5 \times 10^3$) distribution - 0 ns (left) and 10ns (right) with reduced ion mass scheme.

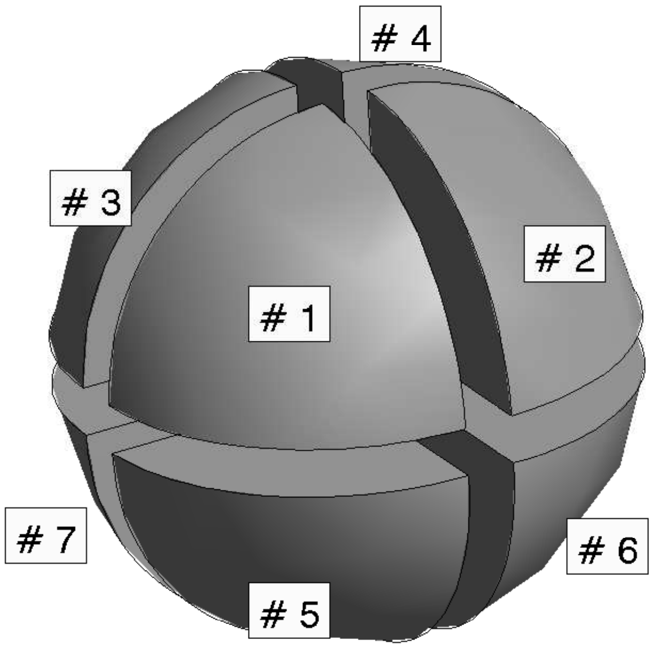

Fig. 2. Schematic view of eight-segment domain decomposition.

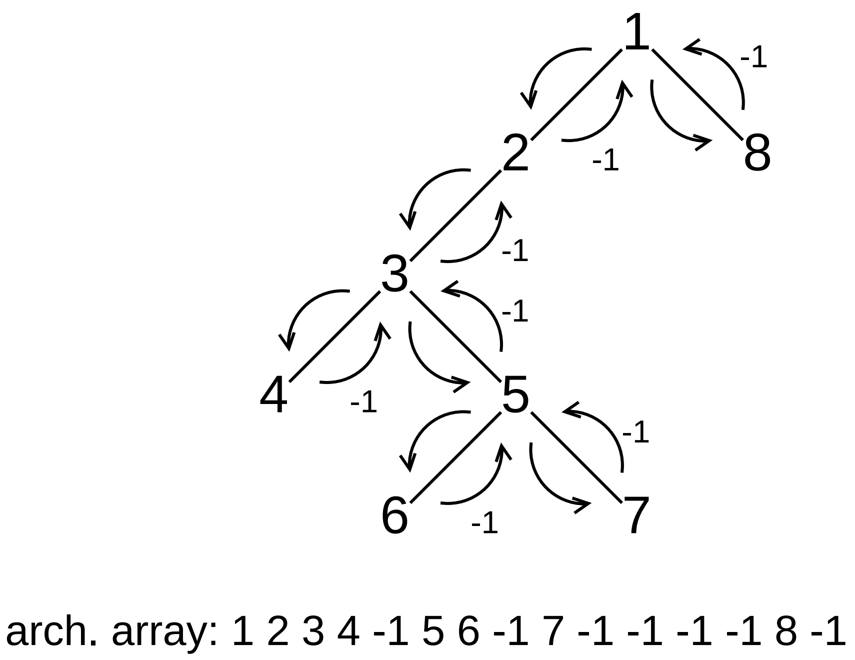

Fig. 3. Architecture array for a sample TREE.

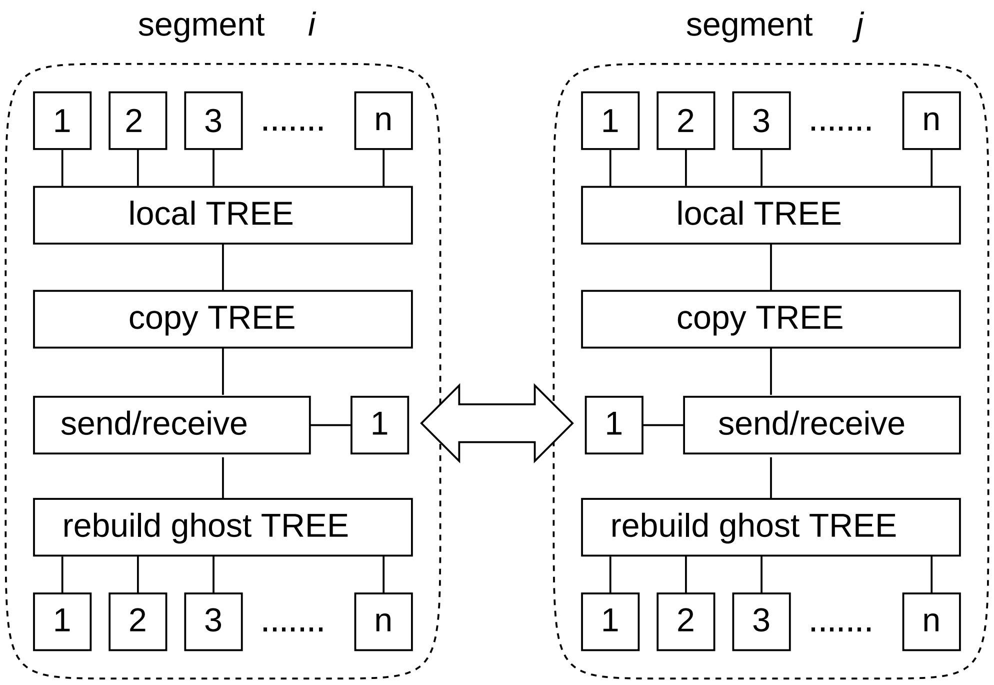

Fig. 4. Calculation and communication flow of each segment.

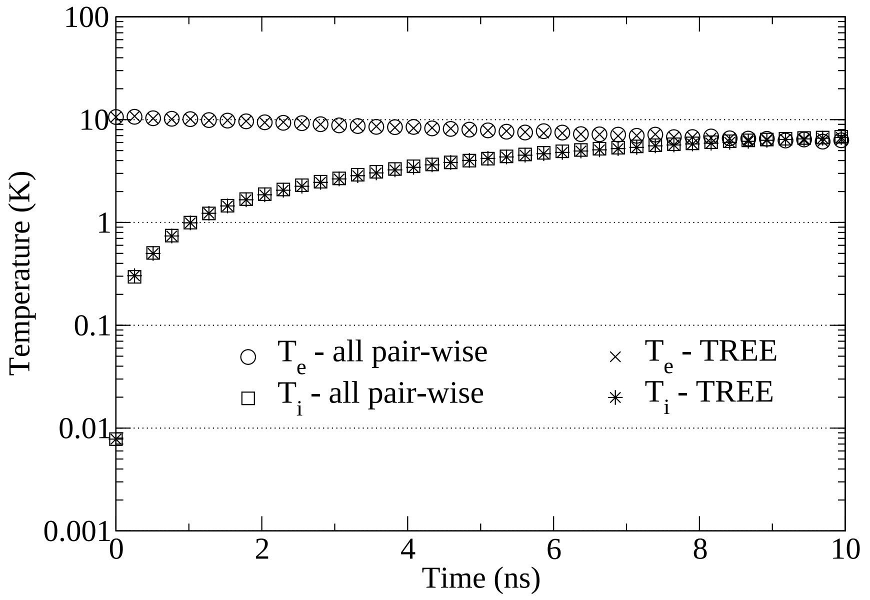

Fig. 5. Electron ($T_e$) and ion ($T_i$) temperature by the all pair-wise evaluation and the TREE method ($5 \times 10^3$ electrons and $5 \times 10^3$ ions).

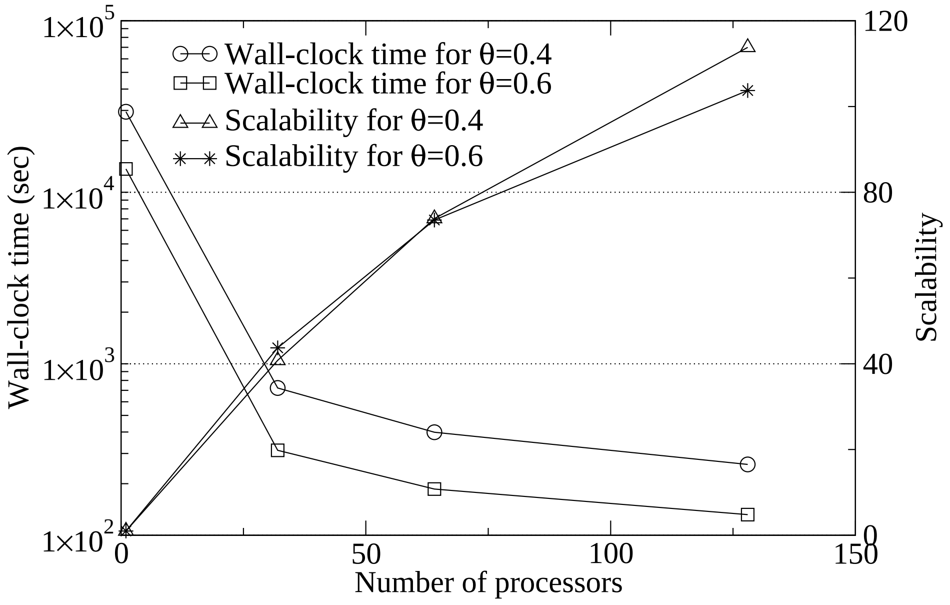

Fig. 6. Performance using MPI and OpenMP hybrid parallel computing for $5 \times 10^4$ electrons and $5 \times 10^4$ ions. Based on the result of a single processor calculation, scalabilities were determined.

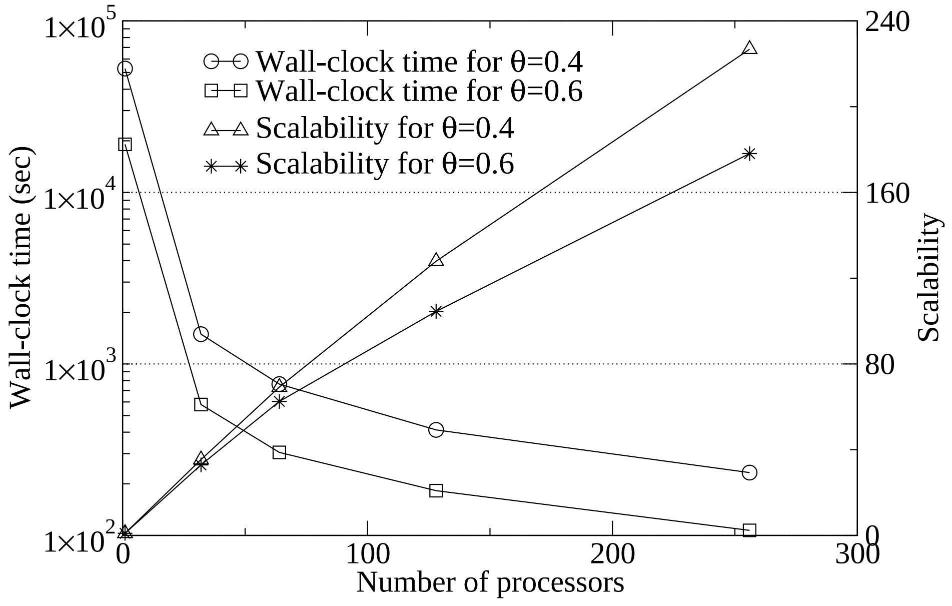

Fig. 7. Performance using MPI and OpenMP hybrid parallel computing for $5 \times 10^5$ electrons and $5 \times 10^5$ ions. Based on the result of a single processor calculation, scalabilities were determined.

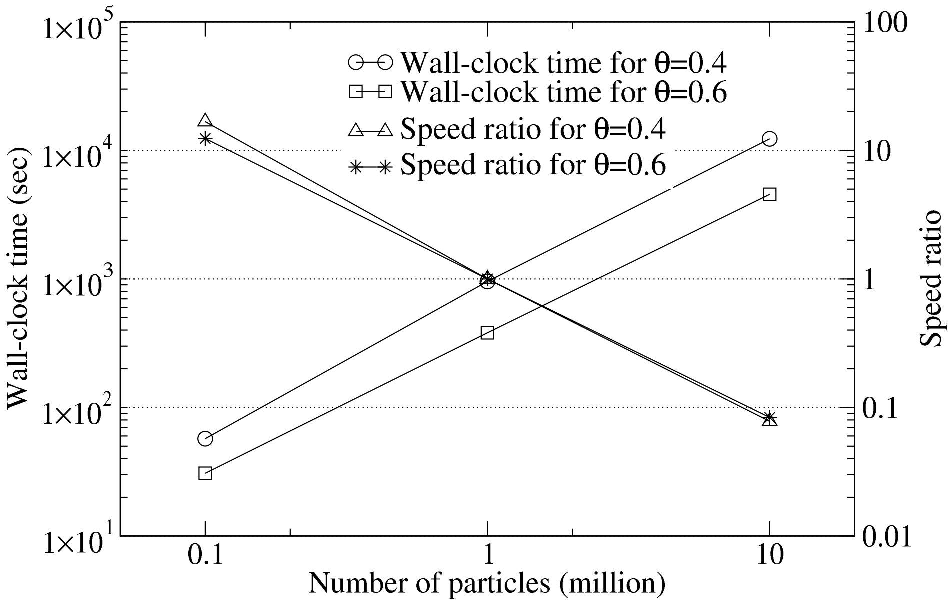

Fig. 8. Performance curves of the parallel TREE code for different sizes. Speed ratio is the wall-clock time ratio for the 1.0 million particle results.

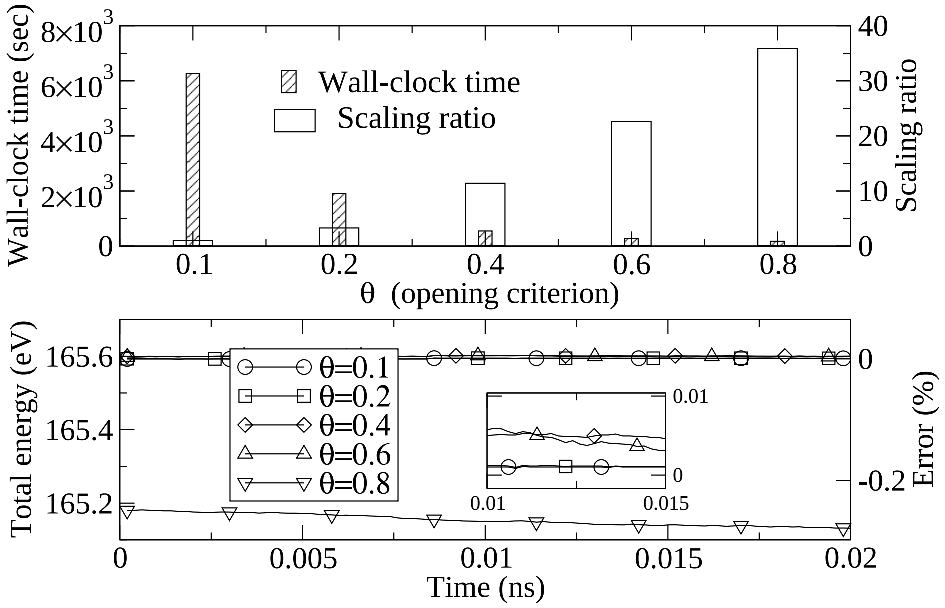

Fig. 9. Performance and energy curves in terms of opening criteria. Scaling ratios are the wall-clock time ratios with respect to $\theta = 0.1$, whereas the reference of error estimations was from all pair-wise calculations. The inset shows fine differences for $\theta = 0.1 - 0.6$, where x-axis is time (ns) and y-axis is error(%).

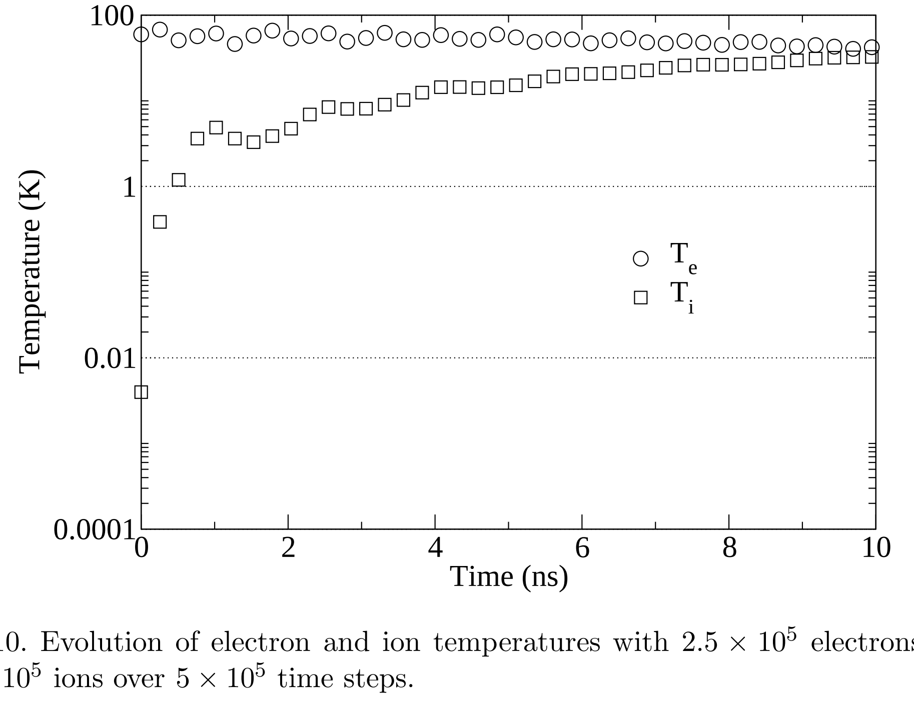

Fig. 10. Evolution of electron and ion temperatures with $2.5 \times 10^5$ electrons and $2.5 \times 10^5$ ions over $5 \times 10^5$ time steps.