DIRECT PARALLEL POISSON SOLVER WITH THE MULTIPLY GRID SPACING SUPPORT FOR PLASMA SIMULATION VIA PIC METHOD

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Problem of the plasma simulation area decomposition for Poisson equation solution via PIC method using parallel computing is treated. Modification of the existing method moving to reduction of the computational complexity is discussed. The approach to use different grid spacing for subdomains is proposed. Method of approximate solution that results in the substantial decrease of the data transmitted is brought forward.
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INTRODUCTION

Computer simulation via PIC method demonstrates the high accuracy of the plasma behavior description [1]. For the wide class of problems (e.g., for beam-plasma discharge – see [2]) the characteristic length of the system is of the order of 10^3 Debye radii and the simulation time is of the order of 10^3 Langmuir periods. But PIC method needs the large RAM capacity and high computing performance. Consequently such problems need the clusters which are often based on single program, multiple data (SPMD) with the distributed memory architecture [3]. Algorithms used for these clusters must satisfy such important conditions as minimal volume of data transferred between the mesh nodes and uniform nodes' loading.

The integration of the field equations (Poisson equation in electrostatic case) remains a difficult task, because significant data non-locality is present. Besides, there is a problem of dynamic balancing for the inhomogeneous plasma case (for the beam-plasma discharge, for example) that is not considered in the existing literature. For inhomogeneous plasma the Debye length can vary in space, but for correct simulation we need to use the computation grid spacing less than Debye length [1]. On the other hand, small grid spacing usage is not optimal for regions with large Debye length. Consequently it is necessary to decompose the problem into subdomains with different spacing. In this paper the domain decomposition method which supports this requirement is proposed. Besides, it is shown how to obtain maximal computation productivity and to reduce the transmitted data number by using approximate solving.

1. EXISTING DOMAIN DECOMPOSITION METHOD AND ITS EXTENSION FOR NON-UNIFORM GRIDS

Poisson equation solving method based on decomposition of the main problem into subdomains with zero Dirichlet boundary conditions and calculating of the screen charges at the subdomains' interfaces was proposed in [5]. For subdomains' joining the author suggests to add the Laplace equation solution with the boundary potentials determined by interfaces' screen charges to the Poisson equation solution for subdomains. Recursive domain joining method is proposed.

But the above mentioned method is not valid for subdomains with different spacing. Besides, this method requires the multiply Laplace equation solving (4 times in 2D case).

The following formula is used for computation of the screen charges $\rho_{scr,i}$ on the vertical interface:

$$\rho_{scr,i} = \frac{\Phi_{left,i} - 2\times 0 + \Phi_{right,i}}{h_x^2} = \frac{\Phi_{left,i} + \Phi_{right,i}}{h_x^2}, \quad (1)$$

where $\Phi_{left,i}$ and $\Phi_{right,i}$ are pre-boundary potentials of left and right subdomains, respectively, and $i = 0...L_y$.
This formula can't be used if subdomains have different spacing along the interface, so arrays $\Phi_{left,i1}$ and $\Phi_{right,i2}$ have different sizes $i_1 = 0...L_{y1}$, $i_2 = 0...L_{y2}$.
We propose to use the spectral representation of the preboundary potentials and screen charges, so

$$\rho_{scr,k}^{SP} = \frac{\Phi_{left,k}^{SP} + \Phi_{right,k}^{SP}}{h_x^2}, \quad (2)$$

where $k = 0...max(L_{y1}, L_{y2})$. This formula is independent on the grids' step and it is correct for any $\Phi_{left,k}$ and $\Phi_{right,k}$ size. The missing high frequency components of spectrum for coarse grid are vanished. For computing of the interface potentials we use eigenvalues of the problem with height $max(L_{y1}, L_{y2})$ and width $L_{x1}+L_{x2}+1$. It will be shown that calculation of the spectral representations can be obtained directly without additional 1D fast Fourier transforms (FFTs).

Formula (2) isn't correct in the case of subdomains with different spacing in the direction perpendicular to the interface, because h_x is not uniform. In this case it is necessary to modify the interface potentials' computation algorithm. The following approach is proposed: the joining problem with non-uniform grid spacing can be considered as a sum of two joining problems with the uniform spacing assuming that one of the subdomains is vanished. So one can compute two interface charges' distribution:

$$\rho_{scr1,k}^{SP} = \frac{\Phi_{left,k}^{SP}}{h_{x1}^2}, \qquad \rho_{scr2,k}^{SP} = \frac{\Phi_{right2,k}^{SP}}{h_{x2}^2}. \quad (3)$$

Then for each screen charges' layer $\rho_{scr1,i}$ and $\rho_{scr2,i}$ we can compute potentials via formulas from [5]. Sum of the computed potentials gives the desired interface potential.

Note that subdomains grid spacing can't be arbitrary; the length of combined domain must be divisible by h_{x1} and h_{x2}.

2. MODIFICATION OF THE POISSON EQUATION SOLVING

As it was shown in [5], joining of domains requires two actions: solving of Poisson equation with zero Dirichlet boundary conditions for finding the pre-boundary potentials and solving the Laplace equation with interfaces' potentials. The sum of these solutions gives the correct solution for subdomain potential. We can improve this performance by combining Poisson and Laplace solving. Let us consider the Poisson solving for 2D Fourier expansion method. Using this method we need to compute 2D spectrum of the input charges' density

$$\rho_{k,l}^{SP} = \sum_{i=0}^{L_x-1}\sum_{j=0}^{L_y-1} \rho_{i,j} \sin\frac{\pi(k+1)(i+1)}{L_x+1}\sin\frac{\pi(l+1)(j+1)}{L_y+1} \quad (4)$$

by FFT (DST-I for this case), to divide the spectrum by eigenvalues

$$\Phi_{k,l}^{SP} = \frac{\rho_{k,l}^{SP}}{4}\left[\sin^2\frac{\pi(k+1)}{L_x+1}+\sin^2\frac{\pi(l+1)}{L_y+1}\right]^{-1}, \quad (5)$$

and then to compute the potential distribution from the spectrum by inverse FFT

$$\Phi_{i,j} = \sum_{k=0}^{L_x-1}\sum_{l=0}^{L_y-1} \rho_{k,l}^{SP} \sin\frac{\pi(k+1)(i+1)}{L_x+1}\sin\frac{\pi(l+1)(j+1)}{L_y+1} \quad (6)$$

(the normalizing coefficient is missed). But one can compute the pre-boundary potentials without full 2D FFT by computing only one sum of (6) for $i=0$, $i=L_x-1$ and $j=0$, $j=L_y-1$. For adding the Laplace equation solution to the Poisson equation solution it is possible to add the Laplace boundary conditions to the pre-boundary charges of the Poisson equation [6] or to add the spectrum of this pre-boundary charges to the Poisson equation spectrum by using (4) for $i=0$, $i=L_x-1$ and $j=0$, $j=L_y-1$. So only two full 2D FFTs and $O(L_yL_x)$ additional steps can be used instead of four FFTs. It is also important that we propose to use the spectral representation of the interface potentials. Consequently we don't need any additional 1D FFTs for finding the pre-boundary and interfaces' potentials, we can use the spectra directly.

3. OPTIMIZATION OF COMPUTATIONS FOR THE DECOMPOSITION IN TWO DIRECTIONS

As it was shown above, we don't need to solve Poisson equation and Laplace equation separately. But in the case of decomposition in two directions we need to compute the pre-boundary potentials when the perpendicular interfaces' potentials are found. We can use the Laplace equation solving with $O(L_xL_ylog(L_x))$ complexity [5]. But the better way can be proposed. Consider computation of the bottom pre-boundary subdomain potentials $\Phi_{bottom,l}$ when left interface potentials $\Phi_{left,k}$ are found. By adding interface potentials as the pre-boundary charges of the Poisson equation and expanding 1D charges' spectrum into 2D Poisson spectrum we can obtain the following formulas:

$$\Phi_{bottom,l}^{SP} = \sum_{n=0}^{L_y-1} \frac{\rho_{left,n}^{SP}}{EV_{k,n}}\sin\frac{\pi(n+1)}{L_y+1}\sin\frac{\pi(l+1)}{L_x+1}, \quad (7)$$

$$EV(k,n) = 4\left[\sin^2\frac{\pi(k+1)}{L_x+1}+\sin^2\frac{\pi(l+1)}{L_y+1}\right], \quad (8)$$

where $l=0, ..., L_x-1$, $k=0, ..., L_y-1$.
So, we can compute $\Phi_{bottom,l}$ by $O(L_yL_x)$ additional steps.

## 4. APPROXIMATE INTERFACE POTENTIAL FINDING TO REDUCE AMOUNT OF THE TRANSMITTED DATA

When decomposition in two directions is used the interface and pre-boundaries points are distributed into several nodes. There are no effective methods for the parallel FFT computation using the distributed memory systems, therefore it is necessary to send all the pre-boundary points into one main node for interface potentials' computing and then to send the obtained potentials to each node (Figure). The amount of data transmitted to the main node may be too large. Besides, each node can use the different grid spacing, so we need to compute FFT for the non-uniform grid. It's inconvenient to use formulas from [5] in this case. Another way can be proposed. Finding of the interface potentials ϕ_{scr} by the Fourier method can be replaced by sum of solutions of 1D screened Poisson equations:

$$\phi_{scr} = \sum_{l=0}^{L_y-1} \phi_l, \quad (9)$$

$$\Delta\phi_l - \alpha_l^2\phi_l = \rho_{scr}\sin^2\frac{\pi(i_0+1)(l+1)}{L_y+1}, \quad (10)$$

$$\alpha_l^2 = \frac{4}{h_y^2}\sin^2\frac{\pi(l+1)}{2(L_y+1)}, \quad (11)$$

where $l=0,...,L_y$ is the number of spatial harmonic, i_0 is the interface position. This result can be obtained via expanding of the Poisson solution in the single series (see [6], p. 194).
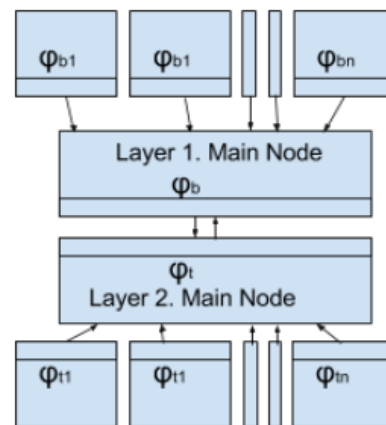
Data transmission for layers' joining

For high spatial harmonics with $l>>1$ parameter α_l depends weakly on l, so we can use the piecewise approximation α for (11) and reduce the number of screened equations in the set (10).

In practice, we need only 6 pieces for approximation of the harmonics' solution in the range $n=L_x/8, ..., L_x-1$

with the computer double type precision (10^{-15}). For solving of each screened Poisson equation as the tridiagonal problem we need to send only two values between nodes. We use the bisection algorithm [7] for minimizing the successive data exchange up to the value $O(log(N))$, where N is the number of nodes in the layer. In the low frequency range $n=0, ..., L_x/8$ we use FFT method, so the full data transmitted number is $C'=2(L_x/8+6)$ (for the same number of approximation terms) instead of $C=2L_x$. Note that if we do not perform the high frequency filtration for input ρ_{scr}, the approximate solution (9) with the reduced number of terms will contain incorrect low frequency components. Since we know the piecewise approximation for α_l, we can find the low frequency dispersion of solution (9) and subtract it from FFT low frequency solution dispersion.

For recursive domain only joining of the low frequency components is used. So full algorithm of the method contains the following steps (for horizontal layers):

1. Finding of the interfaces' screen charges by sending, e.g., the bottom layer pre-boundary potential to the top layer. The node pre-boundary potentials are sent only to the nodes with the common borders.

2. For each interface the high frequency solution of the potentials for main problem is found.

3. For each interface the low frequency spectrum of charges is computed.

4. The low frequency solution for the interface potentials is found using the recursive domain joining method.

5. The low frequency solutions obtained at the step 4 are added to the high frequency solutions obtained at the step 2.

CONCLUSIONS

1. Existing packages for PIC simulation do not contain effective methods of parallel Poisson equation solving.

2. Inhomogeneous plasma simulation needs the dividing of the simulation area into subdomains with different grid spacing.

3. Domain decomposition method for subdomains with different spacing is proposed.

4. The scheme of calculating for minimizing the number of computations is proposed. The proposed calculation needs the number of steps close to the method of expansion into the double Fourier series.

5. The transmitted data minimization method using approximate solving is proposed.

REFERENCES

1. C.K. Birdsall, A.B. Langdon / *Plasma Physics via Computer Simulation.* McGraw: "Hill book company", 1985.

2. D.I. Dadyka, I.O. Anisimov. 2D simulation of the initial stage of the beam-plasma discharge // *Problems of Atomic Science and Technology. Series "Plasma Physics" (21).* 2015, № 1 (95), p. 149-151.

3. D.A. Patterson, J.L. Hennessy. *Computer Organization and Design, Fourth Edition: The Hardware/Software Interface.* Morgan Kaufmann. 2011, p. 635-645.

4. F. Wolfheimer, E. Gjonaj, T. Weiland. Parallel particle-in-cell (PIC) codes //*Proceedings of International Computational Accelerator Physics Conference, Chamonix, France. 2006,* p. 290-295.

5. N.V. Snytnikov. A parallel algorithm for solving 2D Poisson's equation in the context of no stationary problems // *Computational Methods and Programming.* 2015, v. 16, p. 39-51.

6. A.A. Samarsky, E.S. Nikolaev. *Methods for solving grid equations.* M.: "Nauka", "Fizmatlit". 1978 (in Russian).

7. A.V. Terekhov. Parallel Dichotomy Algorithm for Solving Tridiagonal System of Linear Equation with Multiple Right-Hand Sides // *Parallel Computing.* 2010, v. 36, p. 423-438.

ПРЯМОЙ ПАРАЛЛЕЛЬНЫЙ МЕТОД РЕШЕНИЯ УРАВНЕНИЯ ПУАССОНА С ИСПОЛЬЗОВАНИЕМ РАЗЛИЧНОГО ШАГА СЕТОК ДЛЯ МОДЕЛИРОВАНИЯ МЕТОДОМ КРУПНЫХ ЧАСТИЦ В ЯЧЕЙКАХ

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Рассмотрена проблема декомпозиции области моделирования для уравнения Пуассона методом крупных частиц в ячейках. Предложены пути минимизации вычислительных затрат. Продемонстрирована возможность использования различного шага сеток для подобластей. Предложен метод значительного снижения объёма передаваемых между вычислительными узлами данных.

ПРЯМИЙ ПАРАЛЕЛЬНИЙ МЕТОД РОЗВ'ЯЗАННЯ РІВНЯННЯ ПУАССОНА З ВИКОРИСТАННЯМ РІЗНОГО КРОКУ СІТОК ДЛЯ МОДЕЛЮВАННЯ МЕТОДОМ КРУПНИХ ЧАСТИНОК У КОМІРКАХ

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Розглянуто проблему декомпозиції області моделювання для рівняння Пуассона методом крупних частинок у комірках. Запропоновано шляхи мінімізації обчислювальних витрат. Продемонстровано можливість використання різного кроку сіток для підобластей. Запропоновано метод значного зниження об'єму даних, що передаються між обчислювальними вузлами.