Numerical solution of the Vlasov-Poisson equations using a semi-Lagrangian WENO scheme implemented on GPU

E A Malkov\textsuperscript{1,2}, S O Poleshkin\textsuperscript{1}, A A Shershnev\textsuperscript{1} and A N Kudryavtsev\textsuperscript{1,3}

\textsuperscript{1} Khristianovich Institute of Theoretical and Applied Mechanics, Russian Academy of Sciences, Siberian Division, 630090 Novosibirsk, Russia
\textsuperscript{2} Siberian State University of Telecommunications and Information Sciences, 630102 Novosibirsk, Russia
\textsuperscript{3} Novosibirsk State University, 630090 Novosibirsk, Russia

E-mail: malkov@itam.nsc.ru, poleshkin@itam.nsc.ru, antony@itam.nsc.ru, alex@itam.nsc.ru

Abstract. A numerical method for solving the Vlasov–Poisson equations using a high-order semi-Lagrange conservative WENO scheme is developed. The Vlasov–Poisson equations govern evolution of the collisionless self-interacting medium and are widely used in plasma physics and astrophysics, in particular for modeling dynamics of galactic systems. The method is implemented for computations on Graphical Processing Units (GPUs). The GPU code is validated using an exact unsteady analytical solution describing nonlinear oscillations of a plane self-gravitating layer. The comparison with numerical results obtained with the serial CPU code show a significant, up to 50 times, speed-up of the computations.

1. Introduction

Rarefied gas flows in the field of a body force are governed by the kinetic equation

$$
\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f + \frac{\mathbf{F}}{m} \cdot \nabla u = \frac{1}{\text{Kn}} \left( \frac{\partial f}{\partial t} \right)_{\text{coll}}.
$$

(1)

Here $f(t, r, u)$ is the one-particle distribution function, i.e. the density, in a six-dimensional phase space, of some additive quantity such as the mass, the number of molecules, or the probability that characterizes the measure of the gas at the time moment $t$ located at the point $r$ of the physical space and having a corresponding velocity $u$. The function $\mathbf{F}(t, r, u)$ defines a body force field that, in general, is coordinated with the phase density, and $\text{Kn}$ is the Knudsen number equal to the ratio of the molecular free-path length and the characteristic length scale of the problem.

In numerical simulations of processes in plasmas, stellar systems, and neutral gas flows in the gravitational field, when the mean free path of molecules is comparable with the relative variation of this field, and also in computations of unsteady flows in noninertial frames of reference, the question arises whether the calculation of the convective transport represented by the left-hand side of the kinetic equation (1) is correct. In the case of moderate Knudsen numbers, the excessive dissipation introduced by a numerical scheme during calculation of the convective transport
terms can be “disguised” by the distribution function variation due to collisions. The situation is different for high Knudsen numbers (tending to infinity in the limit). Computer simulations of the dynamics of collisionless systems are particularly sensitive to the choice of the numerical scheme. Code validation is usually performed through comparisons of results obtained with different numerical schemes. For example, the results on the dynamic evolution of a gravitating system obtained using the conservative semi-Lagrange scheme are compared with the results of N-body simulations [1, 2, 3].

In the present study, it is proposed to use the exact unsteady solutions of the Vlasov–Poisson equations [4, 5, 6, 7] for testing codes for simulating the collisionless dynamics of gravitating systems. The proposed approach is illustrated using a one-parameter family of unsteady solutions of the Vlasov–Poisson equations constructed by means of the group analysis [7] and describing nonlinear oscillations of a plane self-gravitating layer. The computations of the plane layer evolution are computationally inexpensive but demonstrate the main problems of numerical simulation of the Vlasov–Poisson equations. Moreover, the results of these computations are fairly universal for considering fundamental problems of the evolution of gravitating systems.

2. Model of unsteady plane layer

A gravitating layer can be presented as a set of parallel planes with a homogeneous surface density interacting under the action of gravity. A continuum of such particles-planes is described by the kinetic equation in a two-dimensional phase space coupled with the Poisson equation:

\[
\frac{\partial f(t, z, u)}{\partial t} + u \frac{\partial f(t, z, u)}{\partial z} - \frac{\partial \Phi(t, z)}{\partial z} \frac{\partial f(t, u, z)}{\partial u} = 0, \tag{2}
\]

\[
\frac{\partial^2 \Phi(t, z)}{\partial z^2} = 4\pi G \int f(t, u, z) \, du. \tag{3}
\]

In the case of a homogeneous spatial density and, correspondingly, a quadratic potential, there exists an exact analytical solution of system (2-3) [8].

Using the group analysis, one can obtain a family of unsteady solutions that describe finite-amplitude oscillations of a gravitating layer with the same total energy [7]. The distribution functions from this family parametrized with the parameter \(\alpha\) are

\[
f(t, z, u) = \frac{\rho_0}{\pi} \left[ \alpha^2 \left( z_0^2 - \frac{z^2}{a^2} \right) - a^2 (u - \dot{a} z)^2 \right]^{-1/2}, \quad a = a(t). \tag{4}
\]

The homogeneous spatial density depends on time as

\[
\rho(t) = \frac{\rho_0}{a(t)}. \tag{5}
\]

Correspondingly, the potential is

\[
\Phi(t, z) = \frac{2\pi G \rho_0}{a(t)} z^2. \tag{6}
\]

The boundary of the plane layer changes as \(z(t) = a(t) z_0\). Without loss of generality, it is further assumed that \(4\pi G \rho_0 = 1\), \(\rho_0 = 1\) and \(z_0 = 1\). The function \(a(t)\) satisfies the equation

\[
\ddot{a} = \frac{\alpha^2}{a^3} - 1. \tag{7}
\]

The value \(h\) of the first integral of this equation
\[ h = \frac{a^2}{2} + \frac{\alpha^2}{2a^2} + a \]  

(8)

is taken equal to 3/2. This value corresponds to the steady layer with \( a(t) = 1 \) and \( \alpha = 1 \). The distribution function with the parameter \( \alpha \neq 1 \) and \( h = 3/2 \) are unsteady, but have the same total energy. The degree of unsteadiness is determined by the so-called virial ratio, i.e. the ratio of the doubled kinetic energy to the absolute value of the potential energy

\[ V_{rel} = \frac{2E_{kin}}{|W|} = \frac{\alpha^2}{a^3} \]  

(9)

3. Numerical simulations of oscillations of a homogeneous gravitating layer

The distribution function (4) is singular at the layer boundaries. As a result, numerical simulations of the plane self-gravitating layer oscillating in accordance with this solution require some caution when specifying the initial conditions for the computations. In the present paper, the initial data are taken as the values of the exact distribution function averaged over rectangular grid cells in the 2D phase space. In this case, the initial density of layer in coordinate space is perfectly homogeneous.

The layer oscillations are simulated numerically with the semi-Lagrange conservative WENO scheme [9, 10]. In semi-Lagrange methods, the solution of the 1D advection equation on the new time level is calculated by tracing characteristics (Lagrange trajectories) backward in time from the nodes of Euler (fixed) grid to determine the origins of the characteristics on the previous time level. The function values transported along the characteristics are obtained using a high-order WENO reconstruction via the primitive function. In our case, the fifth-order reconstruction is employed to prevent spurious numerical oscillations when the solution is discontinuous. The 2D computations are performed with the second-order direction splitting scheme [11] calculating successively the Lagrange advection first in the coordinate and then in the velocity space.

The most time-consuming parts of the code are parallelized to be executed on GPUs. At the splitting stage, a separate CUDA block of threads is assigned to each of the one-dimensional transport equations with its own constant transport velocity corresponding to a grid node, and the numerical scheme is parallelized over the threads of this block. An example of implementation can be found in Appendix.

In order to change the direction of the calculations, the matrix containing the phase density values is transposed. This technique enables us to achieve 50-fold acceleration on a NVIDIA GeForce GTX 1050 GPU as compared to serial calculations on one core of the Intel Core i5 processor with a frequency of 3.3GHz.

Numerical simulations were performed with the initial conditions for the distribution function (4) specified as \( a(0) = 1.2 \) and \( \dot{a}(0) = 0 \) and, correspondingly, \( \alpha^2 = 0.864 \) and \( V_{rel}(0) = 0.500 \). The computational domain in the phase space \( R_{space} \times R_{vel} \) was 7.20 × 4.65. The mesh in the phase space consisted of 384 × 384 nodes.

The time step was \( \tau = 0.1 \), which corresponds to \( CFL = F_{max} \tau h_u = 6.4 > 1.0 \). Here \( F_{max} \) is the maximum value of the force predicted by Eq. (3) and \( h_u \) is the grid step in velocity space.

Figure 1 shows the density profiles at different time moments and the values of density at the center of the layer as a function of time, the latter ones compared with theoretical predictions.

The evolution of the phase space distribution is shown in Fig. 2. It is seen that the distribution changes its shape from circular to elliptic and then returns to the original form.
Figure 1. Evolution of density profiles of a homogeneous layer over a period of oscillations (a) and comparison of the density values at the layer center with the exact solution (b) ($V_{rel}(0) = 0.5$).

Figure 2. Phase space evolution.

4. Conclusion
A numerical code based on the semi-Lagrange conservative WENO scheme is developed for solving the Vlasov-Poisson equations which govern the evolution of a collisionless medium with long-range forces. The code is implemented on GPU using the CUDA parallel computing platform. Numerical simulations of nonlinear oscillations of a plane layer of a self-gravitating gas are performed and the results of computations are compared with the exact analytical solutions that can be constructed using the group analysis. A high accuracy and efficiency of the numerical solver is demonstrated. The 50-fold speedup of the parallel GPU code in comparison with a serial code executed on CPU is observed. It is supposed to extend the present numerical approach for solving multidimensional problems of nonlinear dynamics of self-gravitating media, in particular for studying the stability of some non-stationary analytical solutions of the Vlasov–Poisson system [4, 5, 6, 7].

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Appendix. Program implementation

Listing 1 below shows a C++ implementation of the fifth-order WENO reconstruction used in a semi-Lagrangian numerical scheme for solving the transport equation. Calculation of the distribution function at the next time layer is based on the following instructions:

\[
Df[i] = (\text{flag}) \cdot Df[i - \text{shift}] + Df[i + \text{shift}];
\]

\[
Df[i] = dPhi(fP, N, i + 1, x_i, \text{flag}) - dPhi(fP, N, i, x_i, \text{flag});
\]

where \(Df\) is the array of the distribution function values at the grid nodes, \(fP\) is the array for storage of the primitive of the distribution function, \(N\) is the dimension of the distribution function array, \(i\) is the index of the distribution function array, \(h\) is the grid step, \(\text{shift}\) and \(x_i\) are the integer and fractional parts of the Courant number, and \(\text{flag}\) indicates the upstream direction. Iterations can be performed either consecutively or parallel by asynchronously calling the corresponding kernel function, which is executed on the GPU.

Listing 1.

```cpp
#if SINGLE
#define REAL float
#else
#define REAL double
#endif

__host__ __device__ REAL dPhi(REAL* fP, int N, int i, REAL x_i, int flag) {
    REAL U1, U2, U3, U4, U5, U6;
    if (flag) {
        U1 = fP[i - 3];
        U2 = fP[i - 2];
        U3 = fP[i - 1];
        U4 = fP[i];
        U5 = fP[i + 1];
        U6 = fP[i + 2];
    } else {
        U6 = fP[i - 2];
        U5 = fP[i - 1];
        U4 = fP[i];
        U3 = fP[i + 1];
        U2 = fP[i + 2];
        U1 = fP[i + 3];
    }

    REAL S1 = U4 + x_i * x_i * x_i * (-U1 / 6. + U2 / 2. - U3 / 2. + U4 / 6.) +
              x_i * x_i * (-U1 / 2. + 2. * U2 - 5. * U3 / 2. + U4) +
              x_i * (-U1 / 3. + 3. * U2 / 2. - 3. * U3 + 11. * U4 / 6.);

    REAL S2 = U4 + x_i * x_i * x_i * (-U2 / 6. + U3 / 2. - U4 / 2. + U5 / 6.) +
              x_i * x_i * (U3 / 2. - U4 + U5 / 2.) +
              x_i * (U2 / 6. - U3 + U4 / 2. + U5 / 3.);

    REAL S3 = U4 + x_i * x_i * x_i * (-U3 / 6. + U4 / 2. - U5 / 2. + U6 / 6.) +
```

\[
\text{xi}^2 (U_3 / 2. - U_4 + U_5 / 2.) + \\
\text{xi} (-U_3 / 3. - U_4 / 2. + U_5 - U_6 / 6.);
\]

REAL \(C_1 = (\text{xi} - 1.)*(\text{xi} - 2.) / 20.;\)
REAL \(C_2 = -(\text{xi} + 3.)*(\text{xi} - 2.) / 10.;\)
REAL \(C_3 = (\text{xi} + 3.)*(\text{xi} + 2.) / 20.;\)

REAL \(\beta_1 = 4.*U_1*U_1 / 3. - 9.*U_1*U_2 + 10.*U_1*U_3 - \\
11.*U_1*U_4 / 3. + 16.*U_2*U_2 - \\
37.*U_2*U_3 + 14.*U_2*U_4 + 22.*U_3*U_3 - \\
17.*U_3*U_4 + 10.*U_4*U_4 / 3.;\)

REAL \(\beta_2 = 4.*U_2*U_2 / 3. - 7.*U_2*U_3 + 6.*U_2*U_4 - \\
5.*U_2*U_5 / 3. + 10.*U_3*U_3 - 19.*U_3*U_4 + \\
6.*U_3*U_5 + 10.*U_4*U_4 - 7.*U_4*U_5 + 4.*U_5*U_5 / 3.;\)

REAL \(\beta_3 = 10.*U_3*U_3 / 3. - 17.*U_3*U_4 + 14.*U_3*U_5 - \\
11.*U_3*U_6 / 3. + 22.*U_4*U_4 - \\
37.*U_4*U_5 + 10.*U_4*U_6 + 16.*U_5*U_5 - \\
9.*U_5*U_6 + 4.*U_6*U_6 / 3.;\)

REAL \(\varepsilon = 1.0E-10;\)
REAL \(w_1 = C_1 / (\varepsilon + \beta_1) / (\varepsilon + \beta_1);\)
REAL \(w_2 = C_2 / (\varepsilon + \beta_2) / (\varepsilon + \beta_2);\)
REAL \(w_3 = C_3 / (\varepsilon + \beta_3) / (\varepsilon + \beta_3);\)

return \(w_1*S_1 + w_2*S_2 + w_3*S_3;\)

\}

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