A new MPI/OpenMP code for numerical modeling of relativistic hydrodynamics by means adaptive nested meshes

Igor Kulikov¹, Igor Chernykh¹, Anna Sapetina¹, Vladimir Prigarin¹

¹ Institute of Computational Mathematics and Mathematical Geophysics SB RAS, 6-th Lavrentyev avenue, Novosibirsk, Russian Federation
E-mail: kulikov@ssd.sscc.ru

Abstract. Many astrophysical phenomena are associated with gas motion at relativistic velocities. The source of such currents are active galactic nuclei, microquasars, pulsars, gamma bursts, black holes, neutron stars, and gravitational waves. To study such phenomena, it is necessary to perform simulation within the scope of special relativistic hydrodynamics. One of the difficulties of modeling relativistic flows is the different scale of processes, which requires the use of both parallel computing and adaptive meshes.

1. Introduction
Many astrophysical phenomena are associated with gas motion at relativistic velocities. The source of such currents are active galactic nuclei, microquasars, pulsars, gamma bursts, black holes, neutron stars and gravitational waves. One of the difficulties of modeling relativistic flows is the different scale of processes, which requires the use of both parallel computing and adaptive meshes. Today, many numbers of program codes were developed for simulation of relativistic astrophysical flows. Of particular interest is framework The Einstein Toolkit.

Einstein Toolkit [1] is a framework designed to solve the equations of special and general relativistic hydrodynamics with and without a magnetic field and other factors. The framework consists of several blocks. These are a parallel computing infrastructure for meta-calculations called Cactus [2], a parallel transformation to HDF5 format, a web-interface, and visualization tools. There are two methods of organizing calculations on adaptive nested grids: One is an approach called PUGH, which is based on a local refinement of a regular grid with a scalability of up to 130,000 processors. The other is an approach of multi-level grid nesting called Carpet [3, 4]. Both approaches meet modern requirements for accuracy and stability [5]). To implement the framework, a concept called "simulation factory" [6] with a set of abstractions to organize supercomputer simulations is used. These are remote access, configuration, assembly, shipment, and simulation management. Such abstractions may conceal some low-level constructions, allowing one to focus on solving applied problems. To translate the tensor systems of partial differential equations written in the computer algebra package Mathematica into a code for the C or Fortran languages, a package called Kranc is used [7]. The numerical methods employ a reconstruction of the primitive variables by total variation diminishing (TVD) of the solution,
the piecewise-parabolic method (PPM), and essentially non-oscillatory (ENO) methods. The HLL, Roe, and Marquina methods are used as solvers for the Riemann problem [8].

**GENESIS** [9] code was developed for the simulation of relativistic jets. The code has been adapted for an arbitrary equation of state [10], which allows simulating chemical kinetics of gas reactions and stellar equations of state [10]. The code includes a detailed description of a parallel implementation of the calculations, a data distribution scheme, and memory use. A procedure for restoring the primitive (physical) variables is described separately. A problem of the breakdown of a discontinuity with different values of the Lorentz factor has been solved as a test one. The available detailed description of the code allows the readers to create their own implementations on its basis.

This paper describes the author’s approach to solving the problems of relativistic hydrodynamics and its application to the jet modeling. In the second section, the equations of special relativistic hydrodynamics are written down and the numerical solution scheme is briefly described. The description of the HydroBox3D code architecture and the study of acceleration on the IBM Power 9 processor are provided in the third section. The fourth section deals with modeling a relativistic jet. The conclusion is given in the fifth section.

2. The Numerical Model

In the paper the light speed is taken $c \equiv 1$. The equations of relativistic hydrodynamics in the form of conservation laws are written in the form:

\[
\frac{\partial D}{\partial t} + \frac{\partial (D v_k)}{\partial x_k} = 0, \\
\frac{\partial M_j}{\partial t} + \frac{\partial (M_j v_k + p \delta_{jk})}{\partial x_k} = 0, \\
\frac{\partial E}{\partial t} + \frac{\partial (E + p) v_k}{\partial x_k} = 0,
\]

where

\[
D = \Gamma \rho, \quad M_j = \Gamma^2 \rho h v_j, \quad E = \Gamma^2 \rho h - p,
\]

where $\rho$ is the density, $v_k$ are the components of the velocity vector, $\delta_{jk}$ is the Kronecker symbol, $p$ is the pressure and $h$ is the special enthalpy:

\[
h = 1 + \frac{\gamma - 1}{\gamma - 1} \frac{p}{\rho}
\]

$\gamma$ is the adiabatic index. The Lorentz factor $\Gamma$ is determined by the formula:

\[
\Gamma = \frac{1}{\sqrt{1 - v^2}}
\]

the speed of sound is determined by the formula:

\[
c_s^2 = \gamma \frac{p}{\rho h}
\]

It shall be noted that in the numerical method, calculations are carried out in conservative variables $D, M_j, E$.

With respect to nonlinear relationship between conservative variables and primitive $\rho, v, p$, a special procedure for their recovery is required. To recovery of primitive variables, we use the Newton method to determine the root of the equation:

\[
f(p) = \Gamma^2 \rho h - p - E = 0
\]
according to the classical iterative scheme:

\[ p_{m+1} = p_m - \frac{f(p_m)}{f'(p_m)} \]  \hspace{1cm} (9)

where

\[ f'(p) = \frac{\gamma}{\gamma - 1} \Gamma^2 - \frac{M^2 \Gamma^3}{(E + p)^2} \left( D + 2 - \frac{\gamma}{\gamma - 1} p \Gamma \right) - 1 \]  \hspace{1cm} (10)

3. The Architecture of HydroBox3D Code

The principal architecture of HydroBox3D code (see Figure 1). To simulate the hydrodynamic evolution of astrophysical objects, the technology of nested meshes is used, which is described in detail in [11]. The implementation is adapted for the use on distributed memory architectures. To synchronize the overlap regions, the MPI technology is used. An important component of the code is the load balancing procedure for distributed nested meshes. For this, a one-dimensional domain decomposition and an estimate of the number of nested meshes cells in each slice of the root grid are used. This quantity is uniformly distributed among the processes. In each MPI-process, calculations are performed for each nested mesh using a two-level mechanism for distributing calculations among threads based on the "task loop" and "parallel for" pragmas of the OpenMP library. To solve the hydrodynamics equations, the piecewise-parabolic method on a local stencil [12, 13] or its modification based on the piecewise linear function is used. A modification of the HLLEM / HLLI method [14, 15] has also been implemented, whose study we intend to do separately. To solve the Poisson equation, a method based on a combination of the fast Fourier transform and successive over-relaxation is used. When the trigger snaps into action, the subgrid modeling starts with a new process initiation using SSH. The subgrid modeling uses a regular grid and a large set of subgrid processes.

For computational experiments we use 2 \times 12-core Typical 2.7 to 3.8 GHz (max) IBM Power 9 Processor, 32 \times 32 GB DDR4 Memory, and one 300GB 15K RPM SAS SFF-3 Disk Drive (OS Linux). In all configurations, the root mesh size of 128^3 was chosen as the base mesh. Three configurations of nested grids were considered:
Figure 2. Density isolines and flow structure in equatorial plane of galactic jet.

(i) All nested grids are size of $4^3$ (uniform grid with an effective resolution of $512^3$).
(ii) 75% of nested grids are size of $2^3$ and 25% are size of $8^3$ (effective resolution is $1024^3$).
(iii) 75% nested grids are size of $2^3$, 15% are size of $8^3$ and 10% are size of $32^3$ (effective resolution is $4096^3$).

When using a regular grid with an effective resolution of $512^3$, a 60-fold acceleration was obtained using 196 streams of IBM Power 9. A 42-fold acceleration was obtained using 64 streams of IBM Power 9 using a nested grid with an effective resolution of $1024^3$. When using a nested grid with an effective resolution of $4096^3$, a 34-fold acceleration was obtained using 48 streams of IBM Power 9. As can be seen from the results, the hyper-threading system works quite effectively with uniform loading of cores. In case of non-uniform loading the system has local optimum of number of used cores that is several times less than the total number of streams.

4. The Numerical Simulation of Relativistic Jet

Let us simulate a galactic jet of density $\rho_J = 10^{-3}$ cm$^{-3}$ and radius $R_J = 200$ parsec. The jet moves at Lorenz factor $\Gamma = 5$, relativistic Mach number $\mathcal{M} = 8$, the temperature of the galactic atmosphere $T_A = 10^7$ K, and the density $\rho_A = 10^{-2}$ cm$^{-2}$. The adiabatic index $\gamma$ is taken to be equal to $5/3$. Figures (2) show the results of a simulation of galactic jet evolution. The results of the simulation show that a shock wave is moving ahead with a propagation speed that corresponds to the speed of light. Behind the shock front there is a shell region. It separates the shock front and the hotspot where a maximum temperature is reached. The inner part of the cocoon flow is bounded by a contact surface, and the cocoon, in turn, contains a jet. On the outside of the cocoon, closer to the base, there propagate backflows which, in turn, interact with the jet flow.

5. Conclusion

In the paper, a new code for modeling special relativistic hydrodynamic flows on supercomputer architectures with distributed memory using the technology of nested grids was described. A 60-fold acceleration was obtained using 196 streams of IBM Power 9 using a regular grid with an effective resolution of $512^3$. 42-fold acceleration was obtained using 64 streams of IBM Power 9 using a nested grid with an effective resolution of $1024^3$. A 34-fold acceleration was
obtained using 48 streams using a nested grid with an effective resolution of 4096^3 IBM Power 9. In terms of computational experiments, the results of mathematical modeling of relativistic hydrodynamics of galactic jets are presented.

Acknowledgments
This work was supported by Russian Science Foundation (project no. 18-11-00044).

References
[1] Löffler F, et al 2012 Classical and Quantum Gravity 29 (11) 115001
[2] Goodale T, et al 2003 Lecture Notes in Computer Science 2565 197-227
[3] Schnetter E, Hawley S, and Hawke I 2004 Classical and Quantum Gravity 21 (6) 1465-1488
[4] Schnetter E, Diener P, Dorband E, and Tiglio M 2006 Classical and Quantum Gravity 23 (16) S553-S578
[5] Lehner L, Liebling S, and Reula O 2006 Classical and Quantum Gravity 23 (16) S421-S446
[6] Thomas M, and Schnetter E 2010 11th IEEE/ACM International Conference on Grid Computing 369-378
[7] Husa S, Hinder I, and Schnetter C 2006 Computer Physics Communications 174 (12) 983-1004
[8] Donat R, Font J A, Ibanez J M, and Marquina A 1998 Journal of Computational Physics 146 58-81
[9] Aloy M, Ibanez J M, Marti J, and Muller E 1999 The Astrophysical Journal Supplement Series 122 122-151
[10] Timmes F X, and Arnett D 1999 The Astrophysical Journal Supplement Series 125 277-294
[11] Kulikov I 2018 Journal of Physics: Conference Series 1103 012011
[12] Kulikov I, and Vorobyov E 2016 The Journal of Computational Physics 317 318-346
[13] Kulikov I, Chernykh I, and Tutukov A 2019 The Astrophysical Journal Supplement Series 243 4
[14] Balsara D, Li J, and Montecino G 2018 Journal of Computational Physics 375 1238-1269
[15] Deng X, Boivin P, and Xiao F 2019 Physics of Fluids 31 046102