A semi-implicit operator-difference scheme for three-dimensional self-gravitating flows

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CHALLENGES AND INNOVATIONS IN COMPUTATIONAL ASTROPHYSICS – III
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Outline

1. Introduction
2. Difference analogs of differential operators in three dimensions
3. Application of the operator-difference approach for constructing a semi-implicit scheme for gravitational gas dynamics equations on unstructured grids
4. Test computations
1. Stability condition for explicit numerical schemes (Courant-Friedrichs-Lewy condition)

\[ \text{CFL}_{\text{hydro}} = \max \left( \frac{|u| + c_s}{\Delta x} \right) \Delta t \]
\[ \text{CFL}_{\text{heat}} = \max \left( \frac{\chi}{\Delta x^2} \right) \Delta t \]
\[ \text{CFL}_{\text{adv}} = \max \left( \frac{|u|}{\Delta x} \right) \Delta t \]

- \( c_s \) - acoustic speed (sound, magnetic sound and so on)
- \( |u| \) - velocity value
- \( \chi \) – dissipation coefficient (viscosity, thermal conductivity)
- \( \Delta x, \Delta t \) – local mesh resolution and time-step
- Restriction for the time-step: \( \text{CFL} < 1 \)
1. In some cases (semi-)implicit schemes can outperform the explicit ones

- Heat transfer

- Gas dynamics with dissipation, multi-phase flows

- Stellar evolution (see e.g. Viallet et al. (2011))

- Flows with a wide range of local Mach numbers from $M \ll 1$ (presence of dense objects with high sound speed, at least incompressible regime) to $M \gg 1$ (highly compressible regime, strong shocks) $\leftarrow$ very common in astrophysics!

- Presence of sufficiently different characteristic times (e.g. rotation period vs. acoustic time, magnetic field evolution time)
1. Typical astrophysical examples

- Collapse of rotating protostellar clouds
- Core-collapse of a massive star
- Magnetorotational supernovae
- Neutron star mergers

- fig. – 3D simulation of magnetorotational supernova explosion by Moesta et al.

2. Support operators method

- Difference analogues of differential operators satisfy the same identities as the continuous ones
- Unstructured meshes (no allocated directions), we use tetrahedral meshes
- (Static) mesh refinement is included automatically
- Laplace operator transforms to a symmetric and sign-definite matrix

- It was used to construct a completely conservative operator-difference scheme in Lagrange variables for 2D MHD flows (Ardeljan N.V., Bisnovatyi-Kogan G.S., Moiseenko S.G. (2000))
2. Support operators method

• All functions are defined in linear mesh spaces (nodal, cell-nodal and so on)
• Operators are built in pairs
• First operator (e.g. GRAD) is obtained using any numerical differencing technique
• The second one (e.g. DIV) is evaluated from the difference analogue of the Green formula (for infinite space), written in terms of mesh scalar product

\[
(p, \nabla \cdot \vec{v}) + (\nabla p, \vec{v}) = 0
\]

\[
\sum_{l=1}^{N_n} \nabla \times p_l \vec{v}_l W_l + \sum_{k=1}^{N_n} p_k \nabla \times \vec{v}_k W_k = 0
\]

• Resulting DIV operator is, thus, conjugated to initial GRAD operator
• Same technique can be used to whole set of vector calculus operators in any geometry

2. Boundary operator

• Analogue for derivative in the boundary nodes
• Allows to include the boundary conditions of $2^{\text{nd}}$ and $3^{\text{rd}}$ types in operator-difference form
• Satisfies the Green formula with a boundary
• The approach was developed by Ardelyan et al.

\[
(p, \nabla \cdot \vec{v}) + (\nabla p, \vec{v}) = \oint p\vec{v}d\vec{S},
\]

\[
\sum_{l=1}^{N_n} \nabla \times p_l \vec{v} W_l + \sum_{k=1}^{N_n} p_k \nabla \times \cdot \vec{v}_k W_k = \sum_{q=1}^{N_{n\gamma}} \Phi \cdot \vec{v}_q p_q W_q
\]

2. Nodal difference operators

- piecewise-linear finite-element basis functions on a triangular\(\times\)tetrahedral Delaunne mesh (for 2D geometry see e.g. N.V. Ardelyan, M.N. Sablin (2002))
- piecewise-constant finite-volume approach on a median-dual mesh (e.g. T. Barth (1995))
- Summation is over the cells, adjoint to the sought-for node

\[
\nabla \times p_j = \frac{1}{12W_j} \sum_{i \in G_j} (\mathbf{n}_1 S_1 p_1 + \mathbf{n}_2 S_2 p_2 + \mathbf{n}_3 S_3 p_3 + \mathbf{n}_j S_j p_j)
\]

\[
\nabla \cdot \mathbf{v}_j = \frac{1}{12W_j} \sum_{i \in G_j} (\mathbf{n}_1 \cdot \mathbf{v}_1 S_1 + \mathbf{n}_2 \cdot \mathbf{v}_2 S_2 + \mathbf{n}_3 \cdot \mathbf{v}_3 S_3 + \mathbf{n}_j \cdot \mathbf{v}_j S_j)
\]

\[
(\Phi \cdot \mathbf{v})_\gamma = \frac{1}{12W_\gamma} \left( \sum_{q=1}^{K_\gamma} (\mathbf{v}_1 + \mathbf{v}_2 + \mathbf{v}_\gamma)_q \cdot \mathbf{n}_q S_q + \mathbf{v}_\gamma \cdot \sum_{q=1}^{K_\gamma} \mathbf{n}_q S_q \right).
\]
2. Cell-node difference operators

- Cell-node approximation
- GRAD operator (from nodes to cells, derived with the mean theorem):
  \[
  (\nabla_\triangle p)_i = \frac{1}{V_i} \sum_{k=1}^{4} (\bar{p}_k S_k \bar{n}_k)_i
  \]

- Green formula and its analogue
  \[
  \int p \nabla \cdot \bar{v} dV + \int \bar{v} \cdot \nabla p dV = 0
  \]
  \[
  \sum_{l=1}^{N_i} \nabla_{\times} \cdot \bar{v}_l p_l W_l = - \sum_{k=1}^{K_j} \bar{v}_k \nabla p_k V_k
  \]

- DIV operators (from cells to nodes):
  \[
  (\nabla_{\times} \cdot \bar{v})_j = -\frac{1}{3W_j} \sum_{k=1}^{K_j} \bar{v}_k \cdot (\bar{n}_1 S_1 + \bar{n}_2 S_2 + \bar{n}_3 S_3)_k
  \]

Kondratyev I.A., Moiseenko S.G. 2019, JPCS, 1163 012069

W – median-dual cell volume
V – cell volume
2. Example of cell-nodal operators application in 3D

- Heat transfer equation with anisotropic thermal conductivity in outer layers of a magnetized neutron star

\[(I - \delta_1) \nabla_x^0 \cdot \kappa \cdot \nabla_\Delta (I - \delta_1) T + (I - \delta_1) \nabla_x \cdot \kappa \cdot \nabla_\Delta T_{\text{core}} - \delta_2 \Phi \cdot \vec{n} \sigma T_s^4 = 0\]

\[\nabla \cdot \kappa(B, \rho, T) \cdot \nabla T = 0\]

\[T|_{\text{in}} = T_{\text{core}}, \quad \kappa(B, \rho, T) \nabla r T + F_s|_{\text{out}} = 0\]

\[T_{\text{core}} = 2 \cdot 10^8 K\]
\[\Theta_b = 45^\circ\]
\[\beta = 0.5\]
\[T_{\text{eff}} = 1.4 \cdot 10^6 K\]

Kondratyev et al., 2020, Mon. Not. R. Astron. Soc, 497, 2883
3. Gas dynamics with self-gravity

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 ,
\]

\[
\frac{\partial}{\partial t} (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla P - \rho \nabla \phi ,
\]

\[
\frac{\partial}{\partial t} (\rho E) + \nabla \cdot [(\rho E + P) \mathbf{v}] = \rho \mathbf{v} \cdot \nabla \phi ,
\]

\[
\nabla^2 \phi = 4\pi G \rho .
\]

• \( E = e + \frac{v^2}{2} \) – total energy density

• \( P = P(\rho, T) \); \( e = e(\rho, T) \) – general case

• \( P = (\gamma - 1) \rho e \) – ideal gas
3. A semi-implicit operator-difference approximation of gas dynamical equations

• Methods for low-Mach Navier-Stokes equations can be used to build so-called “All-Mach number solvers”, which treat only acoustic waves implicitly

• It was shown, that only pressure in the momentum equation as well as momentum in the energy equation should be treated implicitly (Casulli V, Greenspan D. Int J Numer Methods Fluids. 1984;4(11):1001-1012; W. Boscheri et al. / Journal of Computational Physics 415 (2020) 109486)

• Staggered meshes are widely used to obtain monotonic solution in $M \to 0$ limit, but we have built the scheme on a collocated mesh and found no oscillations as well (see also F.Cordier et al. / Journal of Computational Physics 231 (2012) 5685–5704)
3. A semi-implicit operator-difference approximation of gas dynamical equations

\[
\frac{\rho^{n+1} - \rho^n}{\tau} + \tilde{\nabla}_x \cdot (\rho^n v^n) = 0
\]

\[
\frac{\rho^{n+1} v^{n+1} - \rho^n v^n}{\tau} + \tilde{\nabla}_x \cdot (\rho^n v^n \otimes v^n) + \nabla_x P^{n+1} = 0
\]

\[
\frac{\rho^{n+1}(e + \frac{v^2}{2})^{n+1} - \rho^n E^n}{\tau} + \tilde{\nabla}_x \cdot \left( \rho^n v^n \left( \frac{v^2}{2} \right)^n \right) + \nabla_x \cdot \left( e^{n+1} + \frac{P^{n+1}}{\rho^{n+1}} \right) \rho^{n+1} v^{n+1} = 0
\]

- To approach to a second order in space, we use a linear reconstruction of conservative variables in advection fluxes (Barth, T.J., Jespersen, D.C., 1989, AIAA Paper, 89-0366) with Venkatakrishnan slope limiters (Venkatakrishnan, V., 1993, Technical Report AIAA-93-0880)
3. A semi-implicit operator-difference approximation of gas dynamical equations

• To obtain monotone profiles, we use a Rusanov-type dissipation, which only depends on the flow velocity

\[ \tilde{\nabla}_x \cdot F = \nabla_x \cdot F - \frac{1}{12W_j} \sum_{i \in G_j} \left( \left| \frac{\partial F}{\partial u} \right| (u_i - u_j) |n_{ij}S_{ij}| \right) \]

\[ u = (\rho, \rho v, \rho E) \]
\[ F = (\rho v, \rho v \otimes v, \rho v E) \]

• We have developed 2D and 3D cartesian versions of the hydro code
3. A semi-implicit operator-difference approximation of gas dynamical equations

- By substituting \((\rho v)^{n+1}\) in the energy equation, the nonlinear elliptic equation for a pressure can be obtained.

- It can be solved iteratively by Newton-type methods (r-iterations (Picard) + linear solver, see e.g. Dumbser, Casulli (2016))

\[
\rho^{n+1} e^{n+1,r+1} - \tau^2 \nabla_x \cdot \left( h^{n+1,r} \nabla_x P^{n+1,r+1} \right) = \rho^n E^n - \tau \tilde{\nabla}_x \cdot \left( \rho^n v^n \frac{(v^2)^n}{2} \right) - \tau \nabla_x \cdot \left( h^{n+1,r} \left( \rho^n v^n - \tau \tilde{\nabla}_x \cdot (\rho^n v^n \otimes v^n) \right) \right)
\]

**Stability condition**

\[ \tau < \min \frac{\Delta x}{|v|} \]

Usage of support operator approach allows to construct a matrix with good properties.
4. Test calculations – Riemann problem

- Sod shock tube (150 nodes, $t = 0.44$, $0 < x < 2$), comparison to 1D HLL scheme with good resolution

The method is about 2-3 times slower, than the explicit scheme for the shock tube calculations

Hereafter we consider an ideal gas with $\gamma = 1.4$
4. Test calculations – Sedov-Taylor blast wave

2D: $t = 0.067; \tau = 0.5\tau_{adv} \sim 3 - 4\tau_{cfl}$

For 3D case at larger times $\tau = 0.5\tau_{adv} \sim 10 - 20\tau_{cfl}$
4. Test calculations – slowly moving contact discontinuity

- The semi-implicit scheme is about 50 times faster, than the explicit solver.
- Flow profile has a better quality due to lower numerical dissipation (compared to second-order LLF scheme with linear reconstruction of primitive variables).


\[ N=150 \text{ nodes, } t = 139, \]
\[ V_x = 0.01, x_0 = 0.1 \]

500 time-steps with the semi-implicit scheme correspond to 40000 time-steps of an implicit Godunov-type scheme.
4. Test problems with self-gravity – Poisson solver

- Poisson equation with r.h.s.
  \[ \rho = \frac{z}{4\pi \sqrt{x^2 + y^2 + z^2}} \]

- Dirichlet boundary conditions, \( G = 1 \)

\[
(I - \delta) \nabla_x \cdot \nabla_x (I - \delta) \psi^n + (I - \delta) \nabla_x \cdot \nabla_x \delta \psi_\gamma = 4\pi G (I - \delta) \rho^n
\]
4. Test computations for the dust cloud collapse \((P = 0)\)

- At not very large times \((r(t)/r_0 > 10)\) a solution on a low-resolution mesh fits well with analytics (Colgate S.A., White R.H., Astrophys J, 143, 626 (1966))
Conclusion and future plans

• A three-dimensional semi-implicit operator-difference gas dynamical solver on an unstructured tetrahedral mesh is developed for astrophysical flows with self-gravity

• We plan to extend the scheme to the second order in time and to provide more tests on large meshes

• It is also planned to develop a massively-parallel MHD version of this code for studying magnetorotational processes in rotating protostellar clouds and core-collapse supernovae

Thank you for attention!