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

I.A. Kondratyev, S.G. Moiseenko

Space Research Institute RAS (Moscow, Russia)

CHALLENGES AND INNOVATIONS IN COMPUTATIONAL ASTROPHYSICS – III

17 June 2021

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)

$$CFL_{hydro} = \max(\frac{|u| + c_s}{\Delta x})\Delta t$$

$$CFL_{heat} = \max(\frac{\chi}{\Delta x^2})\Delta t$$

$$CFL_{adv} = \max(\frac{|u|}{\Delta x})\Delta t$$

- c_s- acoustic speed (sound, magnetic sound and so on)
- $|u|$ - velocity value
- χ – dissipation coefficient (viscosity, thermal conductivity)
- Δx, Δt – local mesh resolution and time-step
- Restriction for the time-step: **CFL<1**

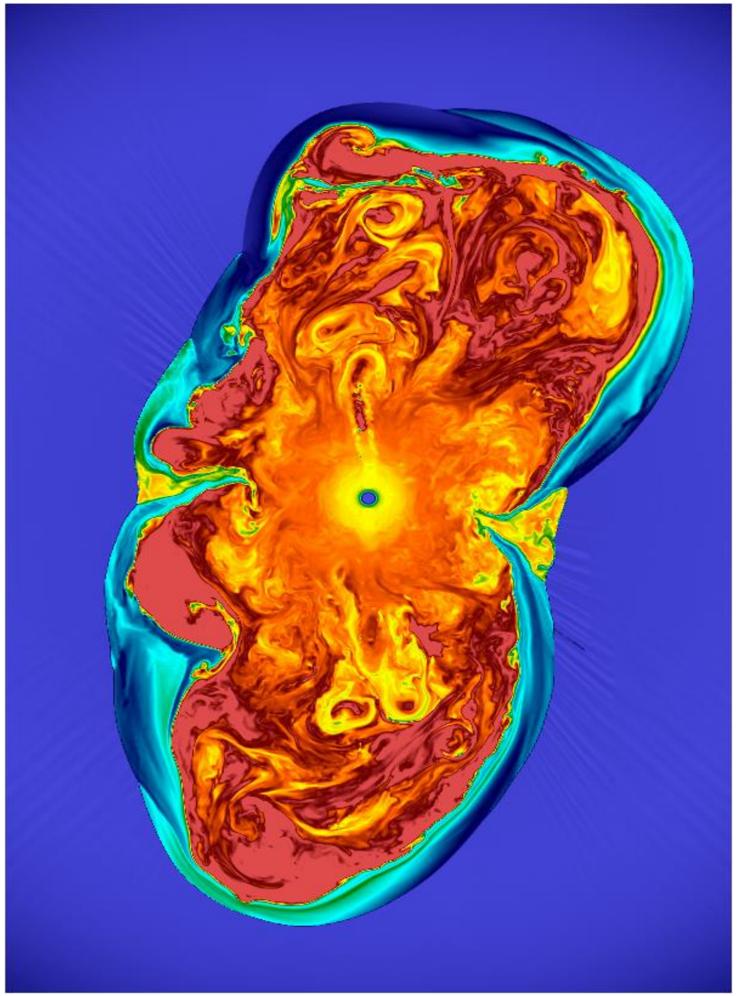
1. In some cases (semi-)implicit schemes can outperform the explicit ones

- 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 $\boldsymbol{M} \ll \mathbf{1}$ (presence of dense objects with high sound speed, at least incompressible regime) to $\boldsymbol{M} \gg \mathbf{1}$ (highly compressible regime, strong shocks) ← **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.



Moesta P. et al, Astrophys. J. Lett. 785, L29 (2014)

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

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

$$\sum_{l=1}^{N_n} \nabla_\times p_l \vec{v} W_l + \sum_{k=1}^{N_n} p_k \nabla_\times \cdot \vec{v}_k W_k = 0$$

Ardelyan N.V., Kosmachevskii K.V., Chernigovskii S.V. (1987)

- 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 2nd and 3rd types in operator-difference form
- Satisfies the Green formula with a boundary
- The approach was developed by Ardelyan et al.

Ardelyan N.V., Kosmachevskii K.V., Chernigovskii S.V. (1987)

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

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

2. Nodal difference operators

- piecewise-linear finite-element basis functions on a triangular\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

gradient

$$\nabla_{\times} p_j = \frac{1}{12W_j} \sum_{i \in G_j} \left(\vec{n}_1 S_1 p_1 + \vec{n}_2 S_2 p_2 + \vec{n}_3 S_3 p_3 + \vec{n}_j S_j p_j \right)$$

divergence

$$\nabla_{\times} \cdot \vec{v}_j = \frac{1}{12W_j} \sum_{i \in G_j} \left(\vec{n}_1 \cdot \vec{v}_1 S_1 + \vec{n}_2 \cdot \vec{v}_2 S_2 + \vec{n}_3 \cdot \vec{v}_3 S_3 + \vec{n}_j \cdot \vec{v}_j S_j \right)$$

boundary operator

$$(\Phi \cdot \vec{v})_{\gamma} = \frac{1}{12W_{\gamma}} \left(\sum_{q=1}^{K_{\gamma}} (\vec{v}_1 + \vec{v}_2 + \vec{v}_{\gamma})_q \cdot \vec{n}_q S_q + \vec{v}_{\gamma} \cdot \sum_{q=1}^{K_{\gamma}} \vec{n}_q S_q \right) .$$

2. Cell-node difference operators

- Cell-node approximation
- GRAD operator (from nodes to cells, derived with the mean theorem):

$$(\nabla_{\triangle} p)_i = \frac{1}{V_i} \sum_{k=1}^{4} (\bar{p}_k S_k \vec{n}_k)_i$$

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

- Green formula and its analogue

$$\int p \nabla \cdot \vec{v} dV + \int \vec{v} \cdot \nabla p dV = 0$$

$$\sum_{l=1}^{N_l} \nabla_{\times} \cdot \vec{v}_l p_l W_l = - \sum_{k=1}^{K_j} \vec{v}_k \nabla_{\triangle} p_k V_k$$

W – median-dual cell volume
V – cell volume

- DIV operators (from cells to nodes):

$$(\nabla_{\times} \cdot \vec{v})_j = -\frac{1}{3W_j} \sum_{k=1}^{K_j} \tilde{\vec{v}}_k \cdot (\vec{n}_1 S_1 + \vec{n}_2 S_2 + \vec{n}_3 S_3)_k$$

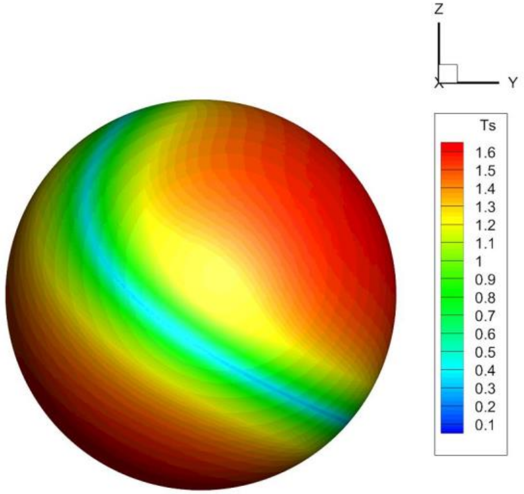
2. Example of cell-nodal operators application in 3D

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

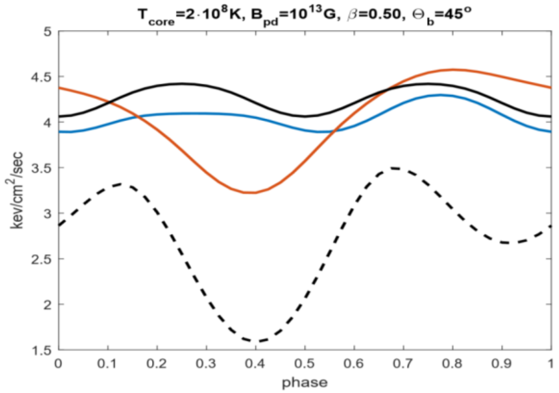
$$(I-\delta_1)\nabla^0_\times \cdot \kappa \cdot \nabla_\triangle (I-\delta_1)T + (I-\delta_1)\nabla_\times \cdot \kappa \cdot \nabla_\triangle T_{core} - \delta_2 \Phi \cdot \vec{n} \sigma T_s^4 = 0$$

$$\nabla \cdot \kappa(\mathrm{B}, \rho, T) \cdot \nabla T = 0$$

$$T|_{in} = T_{core}, \quad \kappa(\mathrm{B}, \rho, T)\nabla_r T + F_s|_{out} = 0$$



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



Kondratyev et al., 2020, Mon. Not. R. Astron. Soc, 497, 2883

3. Gas dynamics with self-gravity

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0 \ ,$$

$$\frac{\partial}{\partial t}(\rho \boldsymbol{v}) + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v}) = -\nabla P - \rho \nabla \phi \ ,$$

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

$$\nabla^2 \phi = 4\pi G \rho \ .$$

- $E = e + \frac{v^2}{2}$ – 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 built 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 $\boldsymbol{M} \to \mathbf{0}$ 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

$$\frac{\rho^{n+1}-\rho^n}{\tau}+\widetilde{\nabla}_\times\cdot(\rho^n\mathbf{v}^n)=0$$

$$\frac{\rho^{n+1}\mathbf{v}^{n+1}-\rho^n\mathbf{v}^n}{\tau}+\widetilde{\nabla}_\times\cdot(\rho^n\mathbf{v}^n\otimes\mathbf{v}^n)+\nabla_\times P^{n+1}=0$$

$$\frac{\rho^{n+1}(e+\frac{\mathbf{v}^2}{2})^{n+1}-\rho^n E^n}{\tau}+\widetilde{\nabla}_\times\cdot\left(\rho^n\mathbf{v}^n\frac{(\mathbf{v}^2)^n}{2}\right)+\nabla_\times\cdot\left((e^{n+1}+\frac{P^{n+1}}{\rho^{n+1}})\rho^{n+1}\mathbf{v}^{n+1}\right)=0$$

- 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

$$\widetilde{\nabla}_\times \cdot \mathbf{F} = \nabla_\times \cdot \mathbf{F} - \frac{1}{12W_j} \sum_{i \in G_j} \left(\left| \frac{\partial \mathbf{F}}{\partial u} \right| (u_i - u_j) |\mathbf{n}_{ij} S_{ij}| \right)$$

$$u = (\rho, \rho \mathbf{v}, \rho E)$$
$$\mathbf{F} = (\rho \mathbf{v}, \rho \mathbf{v} \otimes \mathbf{v}, \rho \mathbf{v} E)$$

- 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 $(\rho\mathbf{v})^{n+1}$ 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))

$$\rho^{n+1}e^{n+1,r+1} - \tau^2\nabla_\times \cdot \left(h^{n+1,r}\nabla_\times P^{n+1,r+1}\right) =$$

$$= \rho^n E^n - \tau\widetilde{\nabla}_\times \cdot \left(\rho^n \mathbf{v}^n \frac{(\mathbf{v}^2)^n}{2}\right) - \tau\nabla_\times \cdot \left(h^{n+1,r}(\rho^n\mathbf{v}^n - \tau\widetilde{\nabla}_\times \cdot (\rho^n\mathbf{v}^n \otimes \mathbf{v}^n))\right)$$

Usage of support operator approach allows to construct a matrix with good properties

Stability condition

$$\tau < min\frac{\Delta x}{|\boldsymbol{v}|}$$

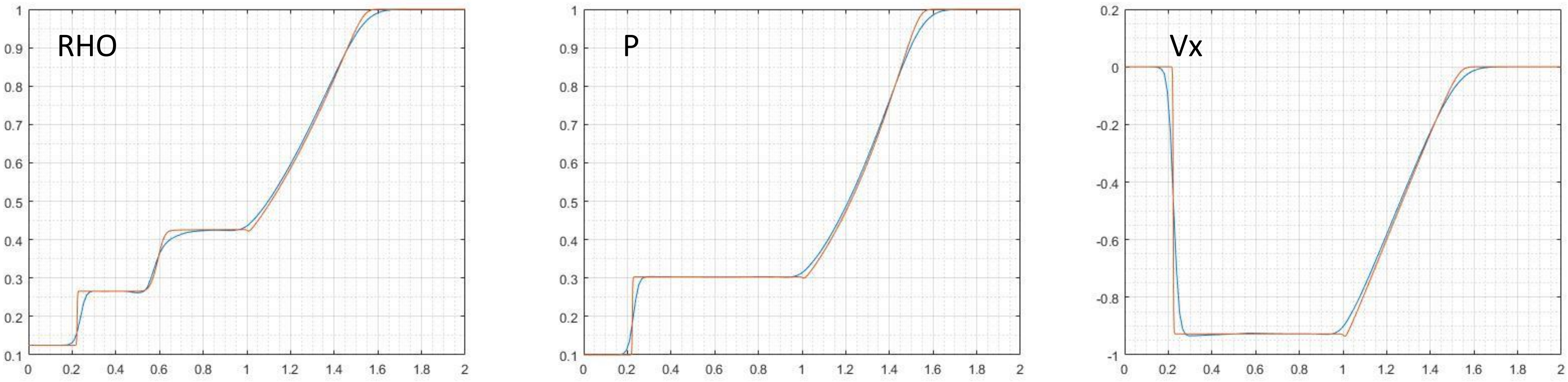
$$h^{n+1,r} = e^{n+1,r} + \frac{P^{n+1,r}}{\rho^{n+1}}$$

$$e^{n+1,r+1} = e(\rho^{n+1}, P^{n+1,r+1})$$

4. Test calculations – Riemann problem

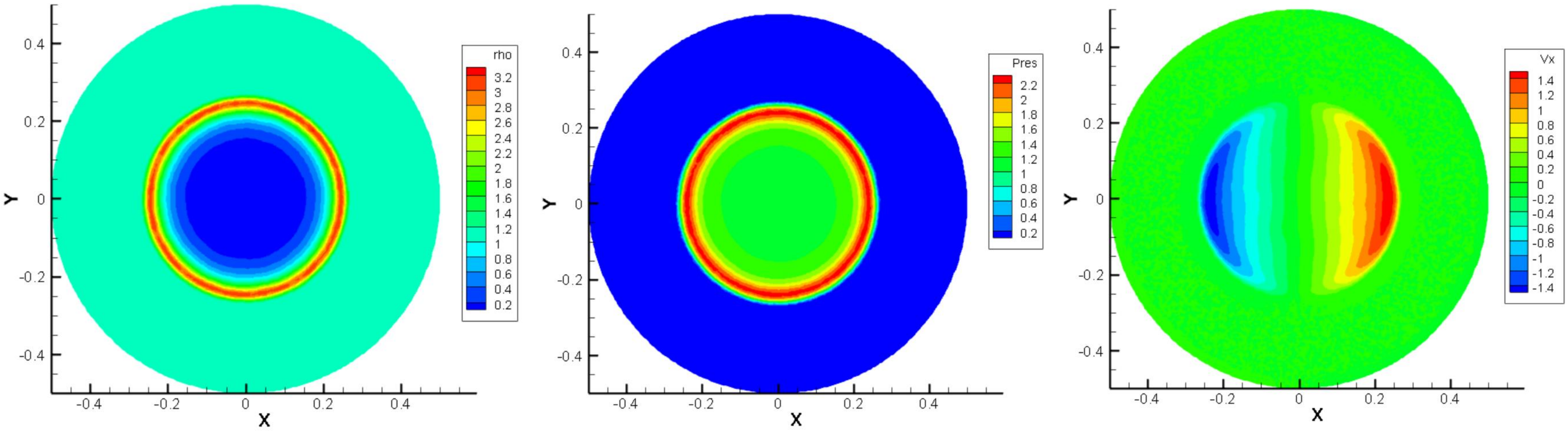
- Sod shock tube (150 nodes, t = 0.44, 0<x<2), comparison to 1D HLL scheme with good resolution

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

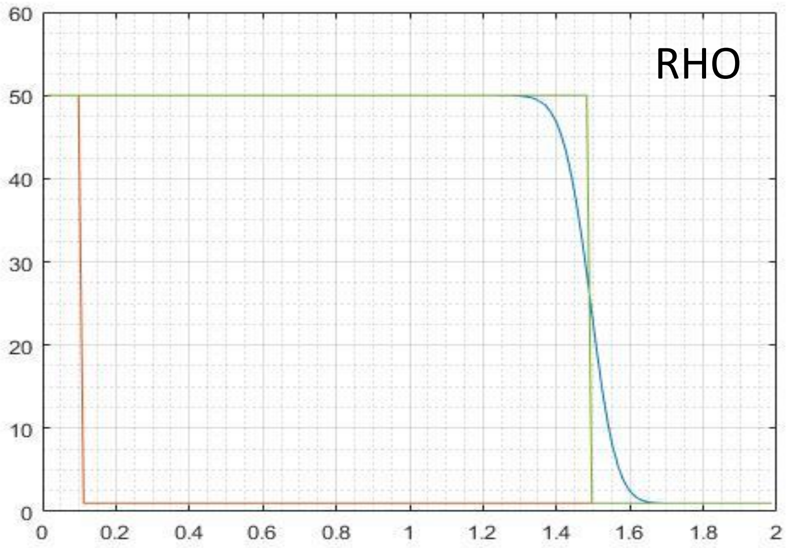


2D: t = 0.067; $\tau = 0.5\tau_{adv} \sim 3 - 4\tau_{cfl}$

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 nodes, t = 139,
Vx = 0.01, x0 = 0.1

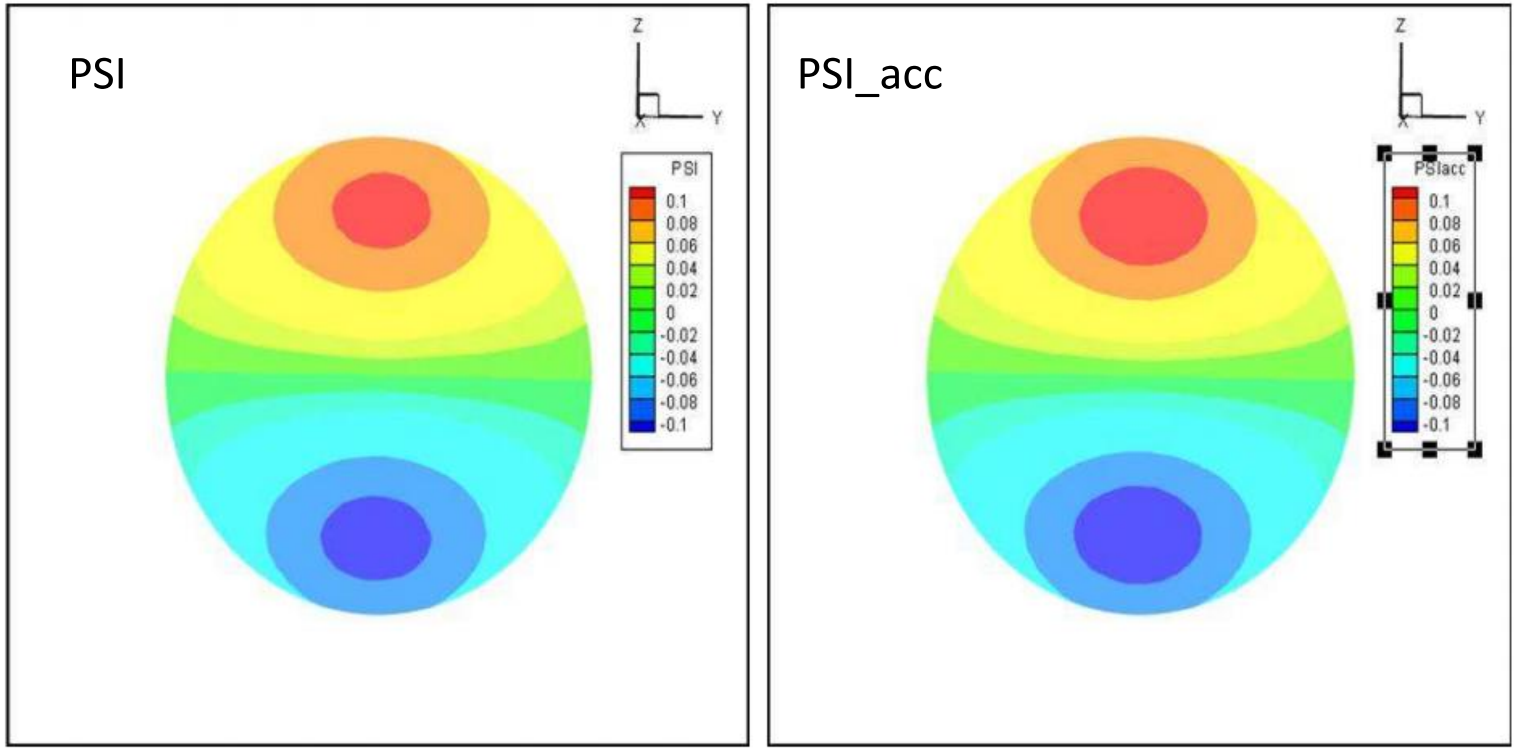
500 time-steps with the semi-implicit scheme
Correspond to 40000 time-steps of an implicit
Godunov-type scheme

Kondratyev I.A., Moiseenko S.G., 2021, in preparation

4. Test problems with self-gravity – Poisson solver

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

- Dirichlet boundary conditions, *G*=1



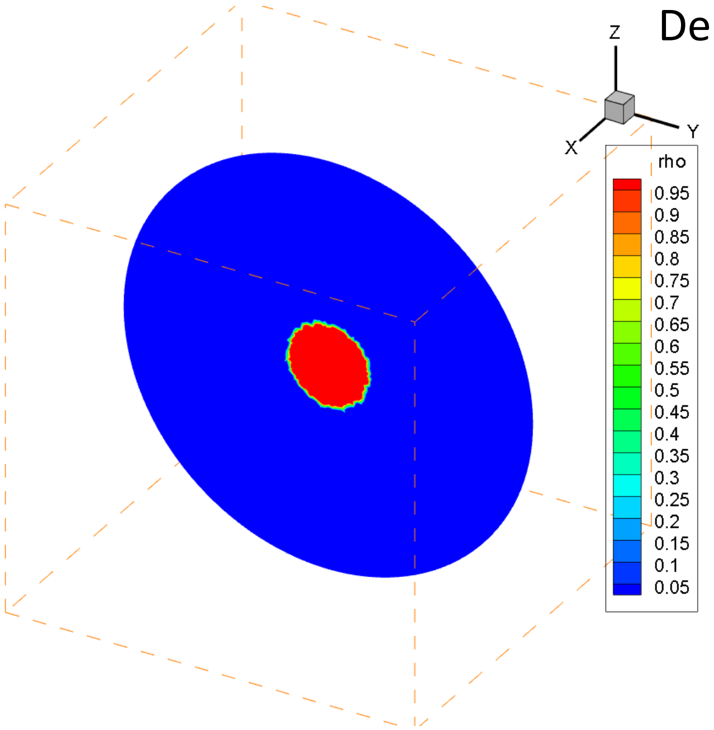
$$(I-\delta)\nabla_\times\cdot\nabla_\times(I-\delta)\psi^n+(I-\delta)\nabla_\times\cdot\nabla_\times\delta\psi_\gamma=4\pi G(I-\delta)\rho^n$$

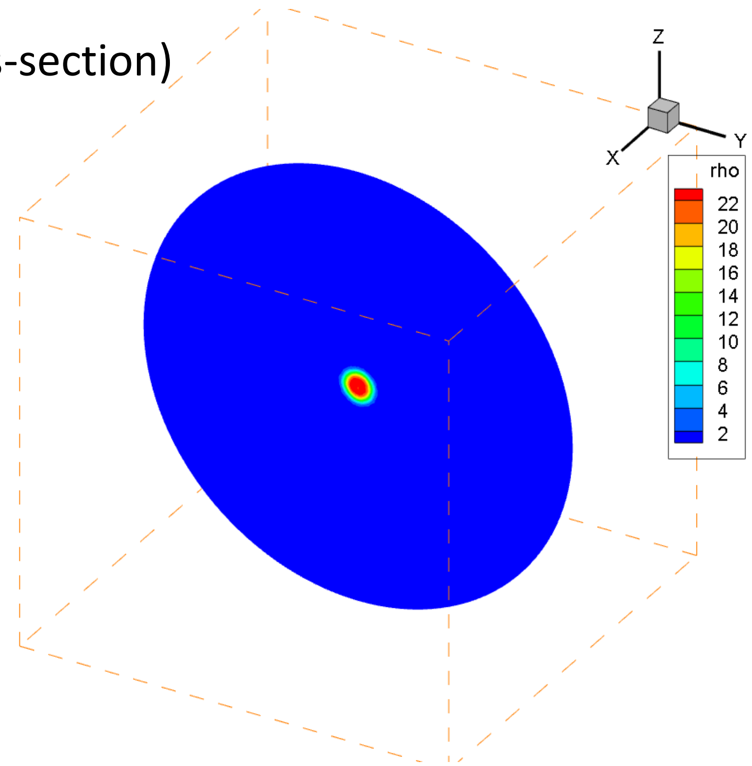
4. Test computations for the dust cloud collapse ($P = 0$)

- At not very large times (r(t)/r0 > 10) a solution on a low-resolution mesh fits well with analytics (Colgate S.A., White R.H., Astrophys J, 143, 626 (1966))

Density (cross-section)

t = 0





t = 1.85

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!