Discrete conservation, entropy functions and induced means

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Summary

- Structure Preserving discretization: motivations and a brief history
- Basic principles and discrete induced equations
- Compressible flows: KEP, EC and PEP formulations
- Extensions and current work
- Future topics

SP discretization: a brief history

The early era: the meteorological community

- Recognization of the nonlinear instability due to the accumulation of aliasing errors (Phillips, 1959)

- Design of *skew-symmetric* splitting to vorticity eq. to control the instability (Arakawa, 1966)

- Application to primitive variable formulations and theoretical analysis (Lilly, 1964, 1965)

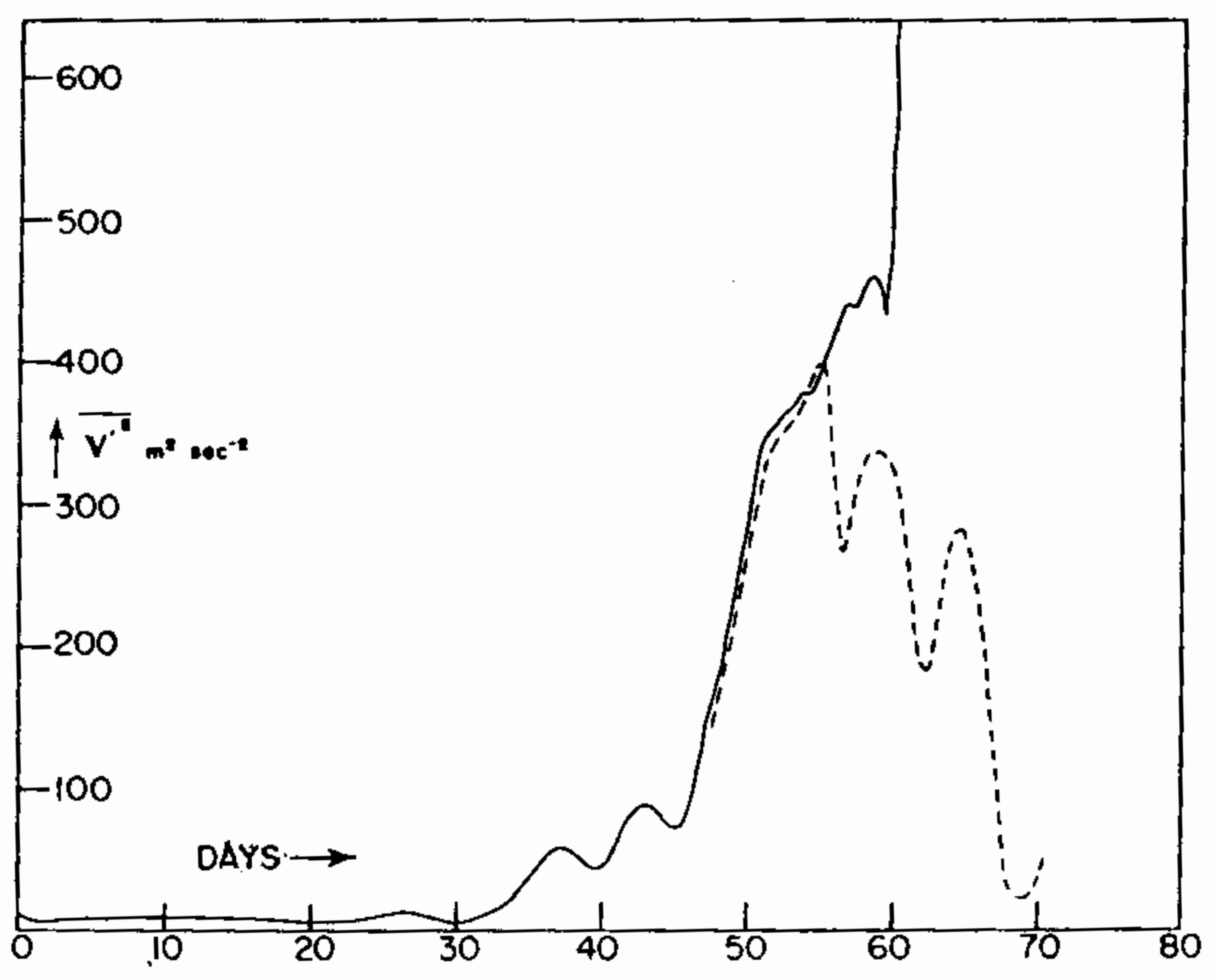

Fig. 1. Disturbance kinetic energy as a function of time. The solid curve was obtained without smoothing, the computations breaking down at about 56 days. The dashed curve was obtained by periodically introducing a filtering procedure.

SP discretization: a brief history

The *skew-symmetric* splitting and the product rule

- Arakawa used splitting techniques and staggered variables to obtain *enstrophy-preserving* (i.e. quadratic-invariants preserving) discretizations

- In modern terms, he devised *skew-symmetric* discretizations, guaranteeing (global) conservation of quadratic invariants

Divergence	$\dfrac{\delta ab}{\delta x}$
Advective	$a\dfrac{\delta b}{\delta x} + b\dfrac{\delta a}{\delta x}$
Skew-symmetric	$\dfrac{1}{2}\left(\dfrac{\delta ab}{\delta x}\right) + \dfrac{1}{2}\left(a\dfrac{\delta b}{\delta x} + b\dfrac{\delta a}{\delta x}\right)$

- Harlow and Welch (1965) used staggered variables to obtain second-order, kinetic-energy preserving (i.e. quadratic-invariants preserving) discretizations using the divergence form

Compressible flows: problem setup

Compressible Euler equations:

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\nabla \cdot \rho \mathbf{u} \\
\frac{\partial \rho \mathbf{u}}{\partial t} &= -\nabla \cdot \rho \mathbf{u}\mathbf{u} - \nabla p \\
\frac{\partial \rho E}{\partial t} &= -\nabla \cdot \rho \mathbf{u} E - \nabla \cdot p \mathbf{u}
\end{aligned}
$$

$$
\begin{aligned}
E &= e + \mathbf{u} \cdot \mathbf{u}/2 \\
p &= p(\rho, T) \\
e &= e(\rho, T)
\end{aligned}
$$

Differences, analogies…

- Kinetic energy is not an invariant, nor a norm of the solution 😐
- Triple products, more *advective* forms 🙂
- No need for staggering (no pressure-decoupling problem) 😐
- More thermodynamic invariants (entropy) and induced properties 🤔

Compressible flows: problem setup

Compressible Euler equations:

General framework:

- Semi-discretized approach: *we focus on spatial discretization*
- FD central (spatial) schemes (uniform Cartesian mesh, periodic BCs): *non dissipative, SBP*

$$\int u \frac{\partial v}{\partial x} \mathrm{d}x = -\int v \frac{\partial u}{\partial x} \mathrm{d}x \longrightarrow \boxed{\sum u_i \delta v_i = -\sum v_i \, \delta u_i}$$

with $\delta u = u_{i+1} - u_{i-1}$ *central difference*

- Negligible temporal errors: *time derivatives can be manipulated at the continuous level*
- Theory will be illustrated for the *1D system* and with *2nd order fluxes* (without loss of generality)

Compressible flows: problem setup

- Under these hypotheses the semi-discrete system of (1D) Euler equations is

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\mathcal{C}_\rho$$
$$\frac{\mathrm{d}\rho u}{\mathrm{d}t} = -\mathcal{C}_{\rho u} - \mathcal{P}_{\rho u}$$
$$\frac{\mathrm{d}\rho E}{\mathrm{d}t} = -\mathcal{C}_{\rho E} - \mathcal{P}_{\rho E}$$

- Locally-conservative discretization: *discrete convective terms admit a 'difference of fluxes' form*

$$\mathcal{C}_{\rho\phi} = \frac{1}{h}\delta^- \mathcal{F}_{\rho\phi}$$

with $\delta^- \mathcal{F}_{i+\frac{1}{2}} = \mathcal{F}_{i+\frac{1}{2}} - \mathcal{F}_{i-\frac{1}{2}}$ *backward difference*

Compressible flows: problem setup

$$\frac{\partial \mathbf{w}}{\partial t} + \frac{\partial \mathbf{f}^j(\mathbf{w})}{\partial x_j} = 0$$

- Compressible Euler equations are a *hyperbolic system of conservation laws*

- Symmetrizable systems of conservation laws admit a *convex entropy function* $U(\mathbf{w})$ and fluxes $F^j(\mathbf{w})$ satisfying

$$\frac{\partial U}{\partial t} + \frac{\partial F^j}{\partial x_j} = 0$$

- *Entropy variables* $\mathbf{v}(\mathbf{w}) = U_{\mathbf{w}}$ are a one-to-one mapping symmetrizing the system

- Expressed in entropy variables, the entropy flux $F(\mathbf{w}(\mathbf{v}))$ has a symmetric Jacobian and admits a potential function such that $\psi_{\mathbf{v}} = F(\mathbf{w}(\mathbf{v}))$

Structure-preserving discretization

Required properties

- KEP: discretized convective terms in mass and momentum equations induce a conservative structure of the convective term in the KE balance

$$\frac{\partial \rho\kappa}{\partial t} = -\frac{\partial \rho u\kappa}{\partial x} - u\frac{\partial p}{\partial x} \qquad \kappa = u^2/2$$

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KEP $\qquad \mathcal{F}_\rho,\, \mathcal{F}_{\rho u} \longrightarrow \sum_i \mathcal{C}_{\rho\kappa}\big|_i = 0$

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- EC: discretized convective terms in mass and energy equations induce a conservative structure of the convective term in the *entropy* balance

$$\frac{\partial \rho s}{\partial t} = -\frac{\partial \rho u s}{\partial x} \qquad s = s(\rho, e)$$

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- PEP: an initial condition with constant distribution of pressure and velocity induce zero pressure and velocity time derivative

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$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} - \frac{1}{\rho}\frac{\partial p}{\partial x}$$

$$\frac{\partial p}{\partial t} = -\frac{\partial pu}{\partial x} - \left(\rho c^2 - p\right)\frac{\partial u}{\partial x}$$

$$p = p(\rho, T)$$

$$c = c(\rho, T)$$

Structure-preserving discretization

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KEP

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KEP schemes - I

'Difference of fluxes' approach (Jameson 2008)

$$\frac{\partial \rho \kappa}{\partial t} = u \frac{\partial \rho u}{\partial t} - \frac{u^2}{2} \frac{\partial \rho}{\partial t}$$

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Enforcing $\sum_i h\mathcal{C}_{\rho\kappa}\big|_i = 0$ gives $\sum_i \left(u\,\delta^-\mathcal{F}_{\rho u} - \frac{u^2}{2}\delta^-\mathcal{F}_{\rho} \right) = 0$

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Using the SBP rule $\sum_i b_i\delta^- a_i = -\sum_i a_i\delta^+ b_i \quad \longrightarrow \quad \sum_i \left(\mathcal{F}_{\rho u}\,\delta^+ u - \mathcal{F}_{\rho}\delta^+ u^2/2\right) = 0$

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Using the SBP rule $\sum_i b_i\delta^- a_i = -\sum_i a_i\delta^+ b_i$ $\longrightarrow$ $\sum_i \left(\mathcal{F}_{\rho u}\,\delta^+ u - \mathcal{F}_{\rho}\delta^+ u^2/2\right) = 0$

For which a sufficient condition is $\mathcal{F}_{\rho u} = \mathcal{F}_{\rho}\frac{1}{2}\frac{\delta^+ u^2}{\delta^+ u} = \mathcal{F}_{\rho}\left(\frac{u_i + u_{i+1}}{2}\right)$

KEP schemes: selected results

- KEP convective fluxes (2nd-order) must satisfy $$\mathcal{F}_{\rho u} = \mathcal{F}_{\rho}\,\overline{u}$$ where $$\overline{u} = \frac{u_i + u_{i+1}}{2}$$

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- In the class of bilinear fluxes $$\mathcal{F}_{\rho} = \xi\,\overline{\rho u} + (1-\xi)\overline{\overline{\rho u}}$$ where $$\overline{\overline{\rho u}} = \frac{\rho_i u_{i+1} + \rho_{i+1} u_i}{2}$$

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- KEP fluxes are designed to induce *global* preservation of kinetic energy, but they are also *locally* conservative! (A kinetic-energy flux always exists!) $$\boxed{\mathcal{F}_{\rho u^2/2} = \mathcal{F}_{\rho}\, \frac{u_i u_{i+1}}{2}}$$

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- Total-energy flux can be built as the sum of internal and kinetic energy fluxes $$\mathcal{F}_{\rho E} = \mathcal{F}_{\rho e} + \mathcal{F}_{\rho}\frac{u_i u_{i+1}}{2}$$

KEP schemes: selected results

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- The general form of the set (KEP) of fluxes is

$$\mathcal{F}_\rho = \mathcal{F}_\rho, \qquad \mathcal{F}^*_{\rho u} = \mathcal{F}_\rho \overline{u} + \overline{p}\,, \qquad \mathcal{F}^*_{\rho E} = \mathcal{F}_{\rho e} + \mathcal{F}_\rho \frac{u_i u_{i+1}}{2} + \overline{\overline{(p,u)}}$$

KEP schemes - II

'*Finite Difference*' approach (Kennedy-Gruber 2008, Pirozzoli 2010, Coppola 2019)

$$\frac{\partial \rho\kappa}{\partial t} = u\frac{\partial \rho u}{\partial t} - \frac{u^2}{2}\frac{\partial \rho}{\partial t} \qquad \longrightarrow \qquad \mathcal{C}_{\rho\kappa} = u\mathcal{C}_{\rho u} - \frac{u^2}{2}\mathcal{C}_{\rho}$$

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$$\mathcal{C}_\rho^D = \frac{\delta \rho u}{\delta x}$$

$$\mathcal{C}_\rho^A = u\frac{\delta \rho}{\delta x} + \rho\frac{\delta u}{\delta x}$$

$$\mathcal{C}_{\rho\phi}^D = \frac{\delta \rho u \phi}{\delta x}$$

$$\mathcal{C}_{\rho\phi}^\phi = \phi\frac{\delta \rho u}{\delta x} + \rho u\frac{\delta \phi}{\delta x}$$

$$\mathcal{C}_{\rho\phi}^u = u\frac{\delta \rho\phi}{\delta x} + \rho\phi\frac{\delta u}{\delta x}$$

$$\mathcal{C}_{\rho\phi}^\rho = \rho\frac{\delta u\phi}{\delta x} + u\phi\frac{\delta \rho}{\delta x}$$

Express the convective terms in mass and momentum eqs. as a linear combination of the various forms

$$\mathcal{C}_\rho = \xi\mathcal{C}_\rho^D + (1-\xi)\mathcal{C}_\rho^A$$

$$\mathcal{C}_{\rho\phi} = \alpha\mathcal{C}^D + \beta\mathcal{C}^\phi + \gamma\mathcal{C}^u + \delta\mathcal{C}^\rho$$

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Enforcing $\sum \mathcal{C}_{\rho\kappa}|_i = 0$

and using $\sum u_i\delta v_i = -\sum v_i\,\delta u_i$ $\longrightarrow$

$$\begin{aligned} \alpha &= \beta = \xi/2 \\ \gamma &= \delta = (1-\xi)/2 \end{aligned}$$

Compressible flows: KEP schemes

FD vs DoF formulations

- For *central* schemes, divergence, advective and 'split' forms are locally conservative (Ducros, 2000, Pirozzoli 2010)
- A correspondence between FD and FV formulations can established. For algebraic (bilinear or trilinear) symmetric interpolations they are <u>equivalent</u>

$$
\begin{aligned}
\xi = 1 \quad &\longrightarrow \quad \mathcal{C}_\rho = \mathcal{C}_\rho^D & \mathcal{F}_\rho &= \overline{\rho u}\,; & \mathcal{F}_{\rho\phi} &= \overline{\phi}\,\overline{\rho u},\\
\xi = 0 \quad &\longrightarrow \quad \mathcal{C}_\rho = \mathcal{C}_\rho^A & \mathcal{F}_\rho &= \overline{\overline{\rho u}}; & \mathcal{F}_{\rho\phi} &= \overline{\phi}\,\overline{\overline{\rho u}},\\
\xi = 1/2 \quad &\longrightarrow \quad \mathcal{C}_\rho = \tfrac{1}{2}\left(\mathcal{C}_\rho^D + \mathcal{C}_\rho^A\right) & \mathcal{F}_\rho &= \overline{\rho}\;\overline{u}\,; & \mathcal{F}_{\rho\phi} &= \overline{\phi}\;\overline{\rho}\;\overline{u}
\end{aligned}
$$

- Jameson (2008) and Kennedy and Gruber (2008) independently formulated an equivalent scheme the same year!

KEP schemes - III

'Entropy variables' approach (Subbareddy and Candler 2009)

Kinetic energy is *not* an entropy function (for compressible flows…). However, analogues of entropy variables can be defined with respect to mass and momentum equations, neglecting pressure

$$U = \rho\kappa \qquad \mathbf{w}^T = (\rho, \rho u) \quad \longrightarrow \quad \mathbf{v}^T = \left(\frac{\partial U}{\partial \mathbf{w}}\right)^T = (-\kappa, u)$$

KEP schemes - III

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The scalar product with the system of equations (neglecting pressure) gives

$$\frac{D\rho\kappa}{Dt} = u\frac{D\rho u}{Dt} - \kappa\frac{D\rho}{Dt}$$

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Semidiscretization gives again

$$\mathcal{F}_{\rho u} = \mathcal{F}_\rho \, \overline{u}$$

and

$$\mathcal{F}_{\rho u^2/2} = \mathcal{F}_\rho \, \frac{u_i u_{i+1}}{2}$$

A selection of KEP schemes

Feiereisen *et al.* 1981	$\mathcal{F}_\rho = \overline{\rho u}, \qquad \mathcal{F}_{\rho u} = \mathcal{F}\rho\,\overline{u}, \qquad \mathcal{F}_p = \overline{\overline{(p, u)}}$	(KEP, PEP)
Kok 2009	$\mathcal{F}_\rho = \overline{\rho}\,\overline{u}, \qquad \mathcal{F}_{\rho u} = \mathcal{F}_\rho\,\overline{u}, \qquad \mathcal{F}_{\rho e} = \mathcal{F}_\rho \overline{e}^G$	(KEP)
Pirozzoli 2010	$\mathcal{F}_\rho = \overline{\rho}\,\overline{u}, \qquad \mathcal{F}_{\rho u} = \mathcal{F}_\rho\,\overline{u}, \qquad \mathcal{F}_{\rho H} = \mathcal{F}_\rho \overline{H}$	(KEP)
KEEP by Kuya *et al.* 2018 (consistent with Coppola *et al.* 2019)	$\mathcal{F}_\rho = \overline{\rho}\,\overline{u}, \qquad \mathcal{F}_{\rho u} = \mathcal{F}_\rho\,\overline{u}, \qquad \mathcal{F}_{\rho e} = \mathcal{F}_\rho \overline{e}$	(KEP)
De Michele and Coppola 2023 (inspired by Kok 2009, consistent with Rozema *et al.* 2014 and 2018)	$\mathcal{F}_\rho = \overline{\rho}^G\,\overline{u}, \qquad \mathcal{F}_{\rho u} = \mathcal{F}_\rho\,\overline{u}, \qquad \mathcal{F}_{\rho e} = \mathcal{F}_\rho \overline{e}^G$	(KEP, PEP)

EC schemes: Tadmor theory

Entropy Conservative fluxes

- *Entropy Conservative* numerical fluxes $\mathcal{F}_{i+\frac{1}{2}}$ satisfy (Tadmor 1987)

$$(\mathbf{v}_{i+1} - \mathbf{v}_i)^T \cdot \mathcal{F}_{i+\frac{1}{2}} = \psi(\mathbf{v}_{i+1}) - \psi(\mathbf{v}_i)$$

Assuming $U = -\dfrac{\rho s}{\gamma - 1}$ for ideal gases the entropy variables are

$$\mathbf{v}^T = \left(\frac{\gamma}{\gamma - 1} - \frac{\log p/\rho^\gamma}{\gamma - 1} - \frac{\rho u^2}{2p}, \frac{\rho u}{p}, -\frac{\rho}{p} \right)$$

and the flux potential is $\psi = \rho u$.

EC schemes

Entropy Conservative fluxes

- Tadmor 1987: EC flux defined as an integral in entropy variables space
- Ismail and Roe 2009: 'affordable' EC fluxes based on the logarithmic mean

$$\overline{\phi}^{\log} = \frac{\phi_{i+1} - \phi_i}{\log \phi_{i+1} - \log \phi_i}$$

- Chandrashekar 2013: KEP and EC fluxes based on the logarithmic mean
- Ranocha and Gassner 2022: KEP, EC and PEP fluxes for ideal gases

$$\mathcal{F}^\rho = \overline{\rho}^{\log}\, \overline{u}, \qquad \mathcal{F}^*_{\rho u} = \mathcal{F}^\rho\, \overline{u} + \overline{p}\,, \qquad \mathcal{F}^*_{\rho E} = \mathcal{F}_\rho \left[\overline{(1/e)}^{\log}\right]^{-1} + \mathcal{F}_\rho \frac{u_i u_{i+1}}{2} + \overline{\overline{(p, u)}}$$

Compressible flows: Real gases

- In the real gases cases the linear link between pressure and internal energy is lost.
- Entropy is an arbitrary function of pressure and density. New averages need to be defined!
- PEP methods are highly challenging (only approximate treatments seem possible)
- EC methods can be obtained with a general approach with potential broad applicability

EC schemes: Real gases

- Starting point: Gibbs relations for temporal derivatives for an arbitrary EOS $e = e(s, v)$

$$\frac{\partial e}{\partial t} = T\frac{\partial s}{\partial t} - p\frac{\partial v}{\partial t} \qquad \longrightarrow \qquad \frac{\partial \rho e}{\partial t} = T\frac{\partial \rho s}{\partial t} + g\frac{\partial \rho}{\partial t}$$

where $T = (\partial e/\partial s)_v$ is the temperature and $g = e - Ts + p/\rho$ is the Gibbs free energy

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where $T = (\partial e/\partial s)_v$ is the temperature and $g = e - Ts + p/\rho$ is the Gibbs free energy

- Substituting spatially discretized terms:

$$\boxed{\mathcal{C}_{\rho e} + \mathcal{P}_{\rho e} = T\mathcal{C}_{\rho s} + g\mathcal{C}_{\rho}}$$

EC schemes: Real gases

- Starting point: Gibbs relations for temporal derivatives for an arbitrary EOS $e = e(s, v)$

$$\frac{\partial e}{\partial t} = T\frac{\partial s}{\partial t} - p\frac{\partial v}{\partial t} \longrightarrow \boxed{\frac{\partial \rho e}{\partial t} = T\frac{\partial \rho s}{\partial t} + g\frac{\partial \rho}{\partial t}}$$

where $T = (\partial e/\partial s)_v$ is the temperature and $g = e - Ts + p/\rho$ is the Gibbs free energy

- Substituting spatially discretized terms:

$$\boxed{\mathcal{C}_{\rho e} + \mathcal{P}_{\rho e} = T\mathcal{C}_{\rho s} + g\mathcal{C}_{\rho}} \longrightarrow$$

- Assuming local conservation for ρ and ρe

$$\frac{1}{h}\delta^- \mathcal{F}_{\rho e} + \frac{1}{h}p\delta^- \overline{u} = T\mathcal{C}_{\rho s} + g\frac{1}{h}\delta^- \mathcal{F}_{\rho}$$

$$\left(p\frac{\partial u}{\partial x} \simeq p\frac{\delta^0 u}{2h} = p\frac{\delta^- \overline{u}}{h}\right)$$

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Compressible flows: Real gases

- Enforcing global conservation of entropy

$$\sum_i \mathcal{C}_{\rho s}\big|_i \, h = \sum_i \left(\frac{1}{T}\,\delta^- \mathcal{F}_{\rho e} - \frac{g}{T}\,\delta^- \mathcal{F}_{\rho} + \frac{p}{T}\,\delta^- \overline{u} \right) = 0$$

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from which

$$\mathcal{F}_{\rho e} = \mathcal{F}_\rho \frac{\delta^+ g/T}{\delta^+ 1/T} - \overline{u}\,\frac{\delta^+ p/T}{\delta^+ 1/T}$$

Internal-energy flux assuring *global conservation* of entropy

Compressible flows: Real gases

- KEP and EC formulations are possible for arbitrary EOS by suitably specifying the internal-energy flux 🙂
- The mass flux is still free (additional properties can be enforced) 🙂
- High-order extension is straightforward 🙂
- The formulation admits an entropy flux (it is also *locally conservative!*) 🙂
- The formulation is potentially singular (local fixes are available, as in the case of perfect gases) 🤔

Thermally-Perfect (TP) gases

- TP gases still use the perfect-gas EoS: $p = \rho R T$ with internal energy and entropy given by

$$e = \int_{T_{\rm ref}}^{T} c_v(T')\,\mathrm{d}T' + e_{\rm ref}, \qquad s = \int_{T_{\rm ref}}^{T} \frac{c_v(T')}{T'}\,\mathrm{d}T' - R\log\left(\rho/\rho_{\rm ref}\right) + s_{\rm ref}$$

for which

$$g = \omega(T) + RT\log\rho; \qquad \omega(T) = \int_{T_{\rm ref}}^{T} c_v(T')\,\mathrm{d}T' - T\int_{T_{\rm ref}}^{T} \frac{c_v(T')}{T'}\,\mathrm{d}T' + T(R - R\log\rho_{\rm ref} - s_{\rm ref}) + e_{\rm ref}$$

- Fixing the mass flux as $\mathcal{F}_\rho = \overline{\rho}^{\log}\overline{u}$ gives the simplified EC flux

$$\mathcal{F}_{\rho e} = \mathcal{F}_\rho \frac{\delta^+\omega(T)/T}{\delta^+ 1/T}$$

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It reduces to the Ranocha's flux for ideal gases

$$\mathcal{F}_{\rho e} = \mathcal{F}_\rho \frac{\delta^{+}\log(1/e)}{\delta^{+}1/e}$$

Numerical results I: real gases

Transcritical double shear layer

- The initial conditions for the transcritical double shear layer test are

$$\begin{cases} u(x,y^{\pm},0) &= u_0\left[1 \mp A\tanh\left(\dfrac{y}{\delta}\right)\right] \\ v(x,y,0) &= \epsilon \sin\left(\dfrac{k\pi}{L_x}x\right)e^{-4y^2/\delta} \\ T(x,y^{\pm},0) &= T_0\left[1 \pm B\tanh\left(\dfrac{y}{\delta}\right)\right] \end{cases}$$

$$\begin{aligned} &A = B = 3/8 \\ &\epsilon = 0.1 \\ &\delta = 1/15 \\ &k = 3 \\ &u_0 = 20\,\mathrm{m/s} \\ &T_0 = 110\,\mathrm{K} \end{aligned}$$

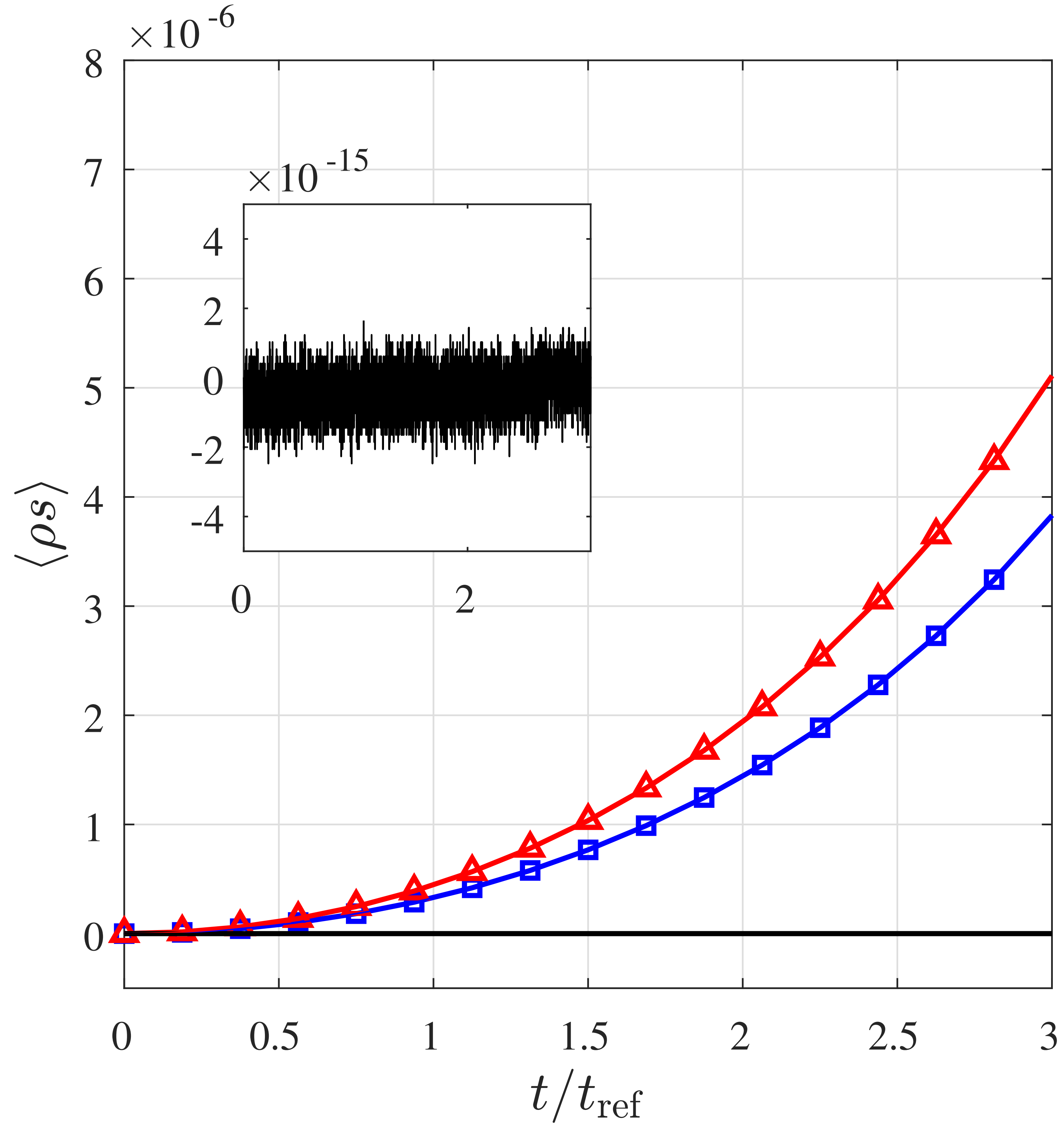
- Spatial domain $L_x = 0.5\,\mathrm{m},\ L_y = 0.25\,\mathrm{m},\ N_x \times N_y = 32 \times 16$
- Periodic boundary conditions are used
- Time integration: RK4 with CFL = 0.005

Numerical results I: real gases

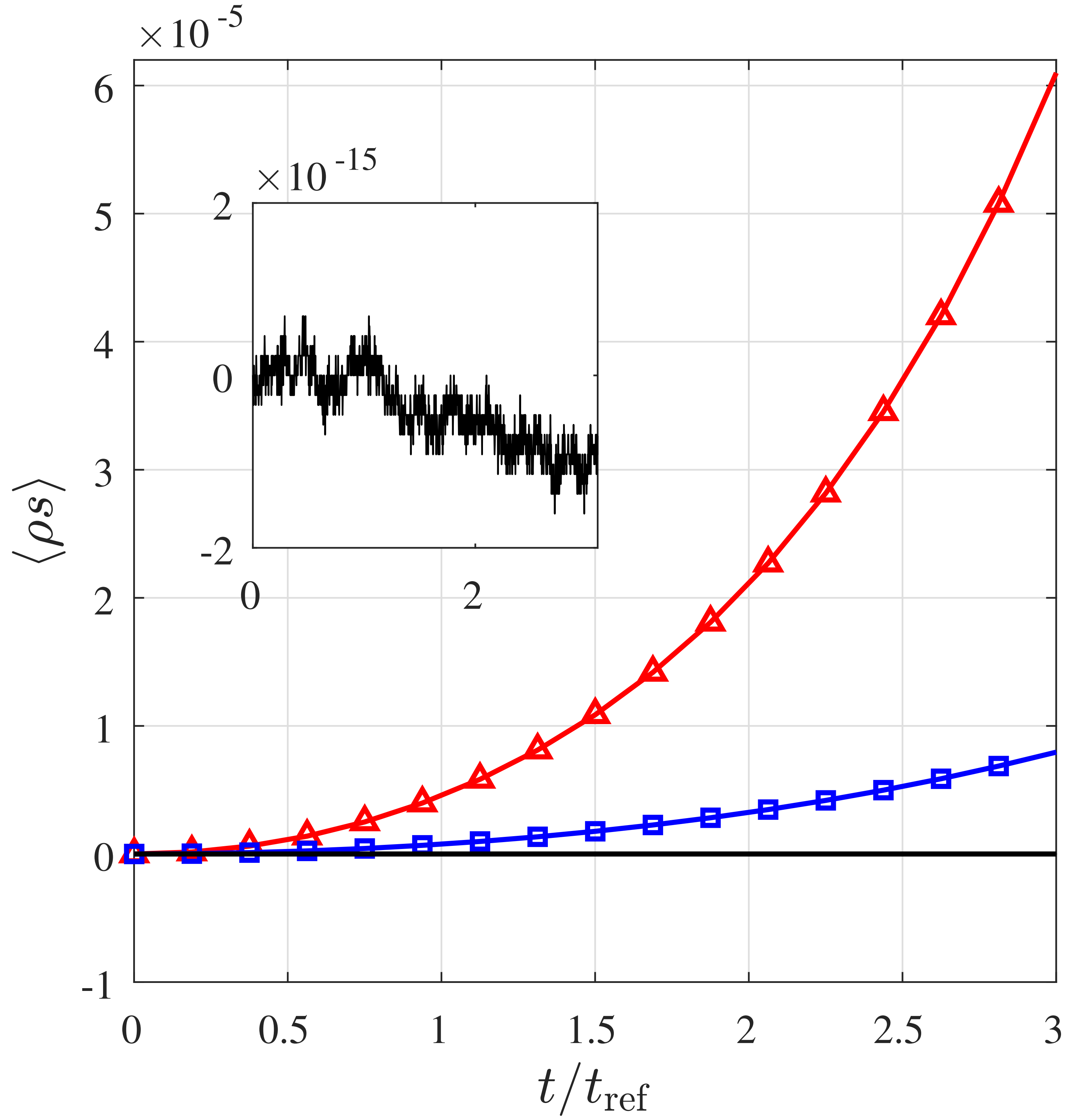
$$\mathcal{F}_{\rho e} = -\frac{\delta^+(g/T)}{\delta^+(1/T)}\mathcal{F}_\rho - \frac{\delta^+(p/T)}{\delta^+(1/T)}\overline{u}$$

$$\mathcal{F}_{\rho e} = \mathcal{F}_\rho \overline{e}^H$$

$$\mathcal{F}_{\rho e} = \mathcal{F}_\rho \left[\overline{\left(\frac{1}{e}\right)}^{log}\right]^{-1}$$



(a) Van der Waals (4th order)



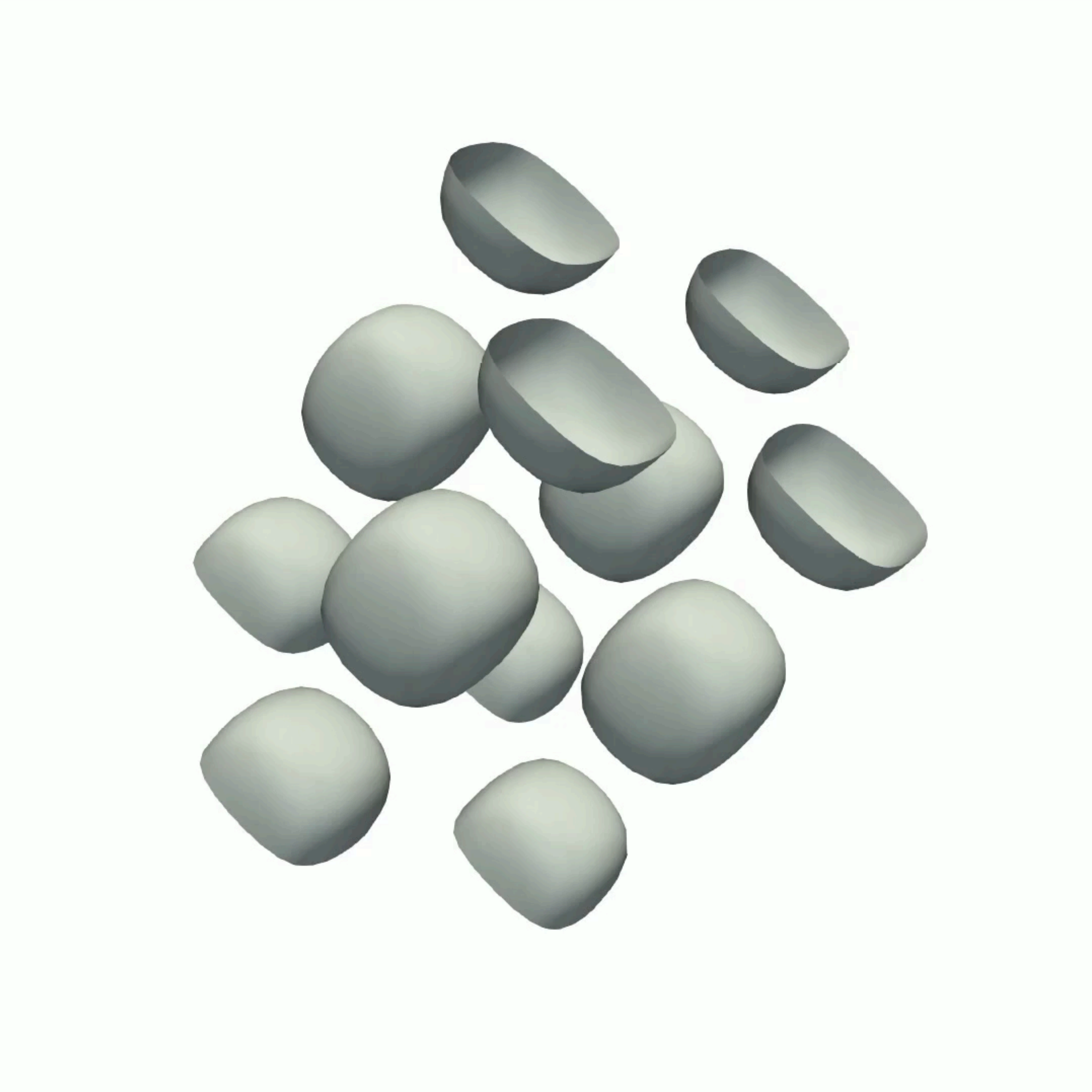
(b) Peng-Robinson (2nd order)

Numerical results - II: TP gases

Compressible (inviscid) TGV

- The initial conditions for the TGV test are

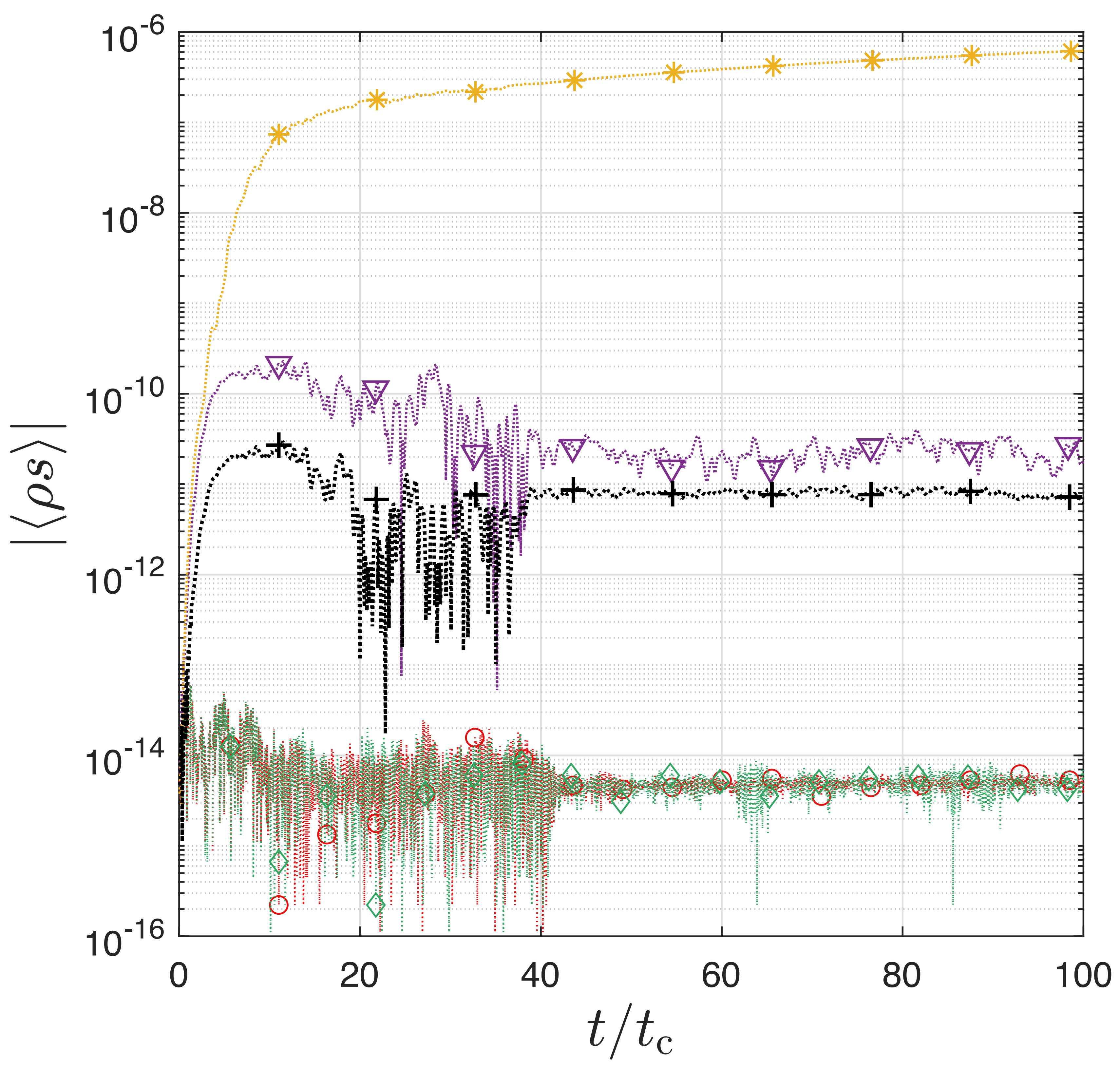
$$\rho(x,y,z,0) = \rho_0$$
$$u(x,y,z,0) = u_0 \sin x \cos y \cos z$$
$$v(x,y,z,0) = -u_0 \cos x \sin y \cos z$$
$$w(x,y,z,0) = 0$$
$$p(x,y,z,0) = p_0 + \frac{\rho_0 u_0^2}{16} (\cos 2x + \cos 2y)(\cos 2z + 2)$$



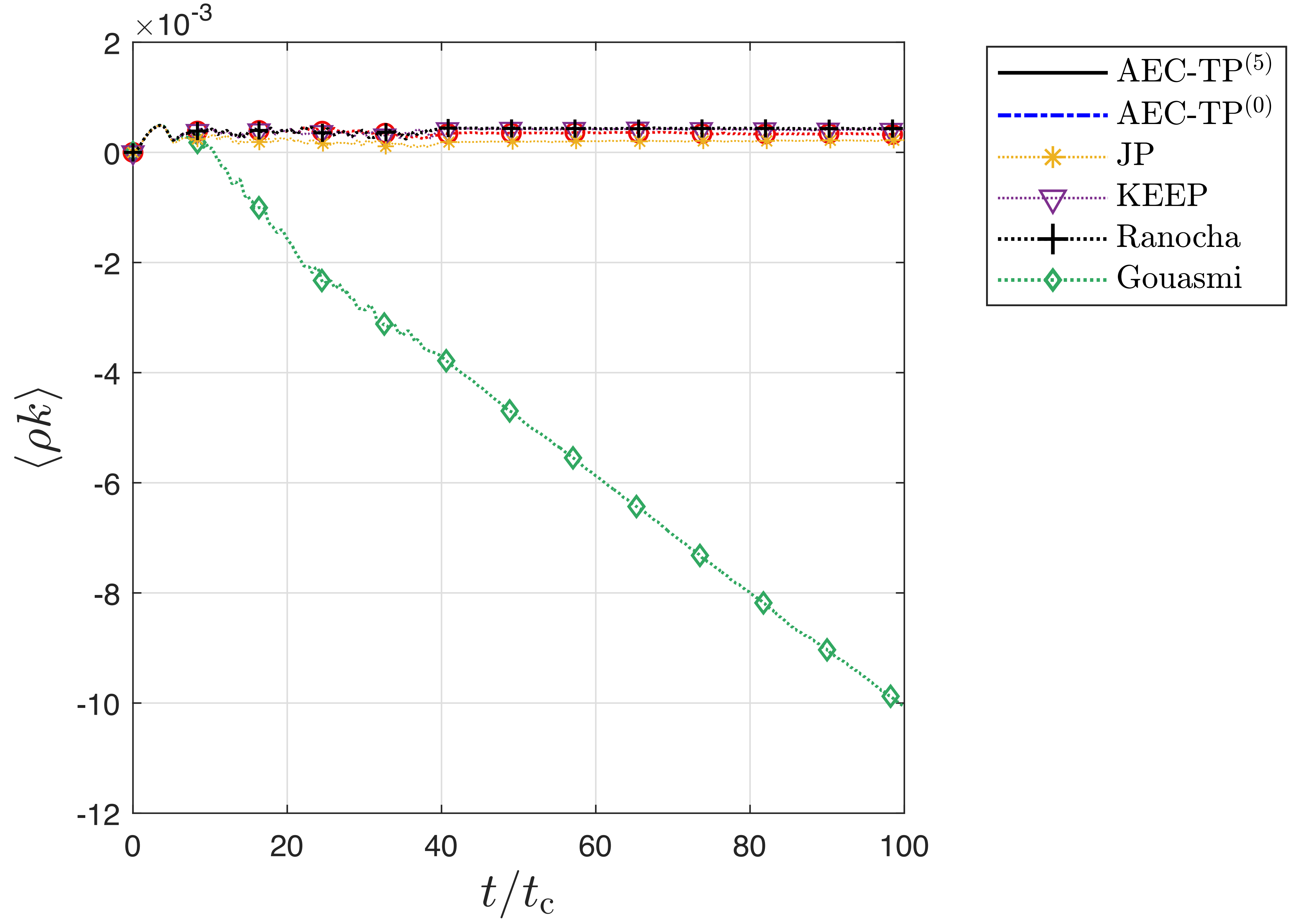
- Spatial domain has size $L = 2\pi$ and is discretized with 32x32x32 points
- 6th order explicit schemes are used (STREAmS-2.0), with periodic BCs
- Time integration: RK4 with CFL = 0.1

Numerical results - II: TP gases

Compressible (inviscid) TGV



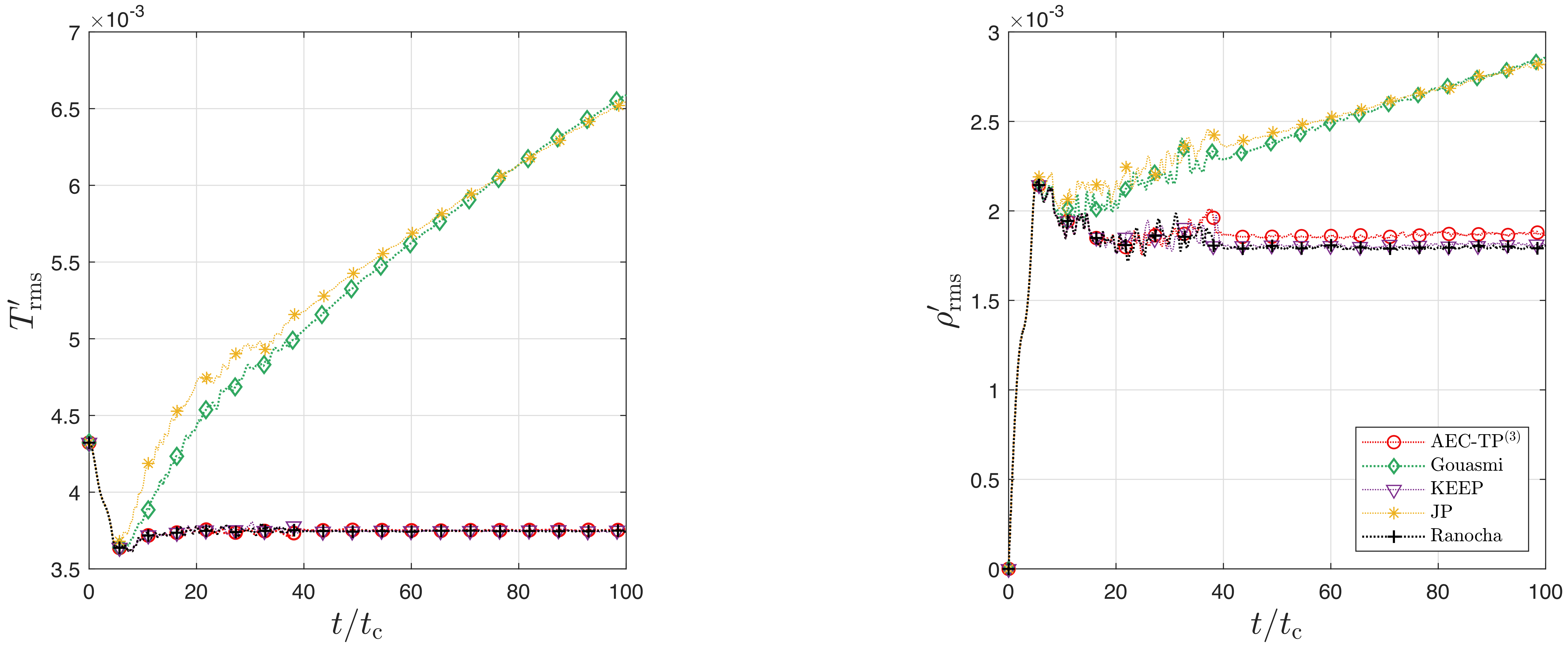
Entropy conservation



KE evolution

Numerical results - II:TP gases

Compressible (inviscid) TGV



Temperature fluctuations

Density fluctuations

Generalized FD formulations

What about Finite Differences?

- The introduction of more general averages in the definition of EC numerical fluxes naturally leads to the question of FD compatible formulations

- Classical FD formulations can be associated only with algebraic (bilinear or trilinear) interpolations. Differences are due to the failure of the *product rule*

- For arbitrary nonlinear flux functions, classical FD formulations need to include suitable *nonlinear* transformations, for which the *chain rule* plays a role

Generalized FD formulations

- An example of a nonlinear transformation involving the chain rule is

$$\rho = \left(\frac{1}{\rho}\right)^{-1} = \left(\frac{\mathrm{d}\log\rho}{\mathrm{d}\rho}\right)^{-1} = \frac{\mathrm{d}\rho}{\mathrm{d}\log\rho}$$

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- Using it in the evaluation of the mass flux and applying classical FD:

$$\frac{\partial \rho u}{\partial x} = \frac{\partial}{\partial x}\left(\frac{\mathrm{d}\rho}{\mathrm{d}\log\rho}u\right) \rightarrow \frac{\delta}{\delta x}\left(\frac{\delta\rho}{\delta\log\rho}u\right) \rightarrow \frac{\delta\left(\overline{\rho}^{\log}u\right)}{\delta x}$$

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- Employing split forms and various difference operators leads to the classical EC schemes based on the logarithmic mean, and generate new ones!

Generalized FD formulations

- A sufficiently general set of nonlinear transformations is given by

$$\phi = \frac{\beta}{\beta+1}\frac{\mathrm{d}\phi^{\beta+1}}{\mathrm{d}\phi^{\beta}}$$

- Many nonlinear averages can be generated

  - This approach can be used to obtain more EC, KEP and PEP methods within a FD approach, even based on biased (non central) operators

- $\beta = 1 \quad \rightarrow \quad$ Arithmetic mean:

$$\frac{1}{2}\frac{\mathrm{d}\phi^2}{\mathrm{d}\phi} \approx \frac{1}{2}\frac{\delta\phi^2}{\delta\phi} \quad \rightarrow \quad \frac{1}{2}\frac{\delta_{2\mathrm{pt}}\phi^2}{\delta_{2\mathrm{pt}}\phi} = \frac{1}{2}\frac{\phi_a^2-\phi_b^2}{\phi_a-\phi_b} = \frac{\phi_a+\phi_b}{2} = \overline{\phi}$$

- $\beta = 0 \quad \rightarrow \quad$ Logarithmic mean:

$$\frac{\mathrm{d}\phi}{\mathrm{d}\log\phi} \approx \frac{\delta\phi}{\delta\log\phi} \quad \rightarrow \quad \frac{\delta_{2\mathrm{pt}}\phi}{\delta_{2\mathrm{pt}}\log\phi} = \frac{\phi_a-\phi_b}{\log\phi_a-\log\phi_b} = \overline{\phi}^{(\log)}$$

- $\beta = -\frac{1}{2} \quad \rightarrow \quad$ Geometric mean:

$$-\frac{\mathrm{d}\sqrt{\phi}}{\mathrm{d}(1/\sqrt{\phi})} \approx -\frac{\delta\sqrt{\phi}}{\delta(1/\sqrt{\phi})} \quad \rightarrow \quad \frac{\delta_{2\mathrm{pt}}\sqrt{\phi}}{\delta_{2\mathrm{pt}}(1/\sqrt{\phi})} = \frac{\sqrt{\phi_a}-\sqrt{\phi_b}}{\frac{1}{\sqrt{\phi_a}}-\frac{1}{\sqrt{\phi_b}}} = \sqrt{\phi_a\phi_b} = \overline{\phi}^G$$

- $\beta = -2 \quad \rightarrow \quad$ Harmonic mean:

$$2\frac{\mathrm{d}\phi^{-1}}{\mathrm{d}\phi^{-2}} \approx \frac{\delta\phi^{-1}}{\delta\phi^{-2}} \quad \rightarrow \quad \frac{\delta_{2\mathrm{pt}}\phi^{-1}}{\delta_{2\mathrm{pt}}\phi^{-2}} = \frac{\frac{1}{\phi_a}-\frac{1}{\phi_b}}{\frac{1}{\phi_a^2}-\frac{1}{\phi_b^2}} = 2\frac{\phi_b\phi_a}{\phi_b+\phi_a} = \overline{\phi}^H$$

Future work

Topics for the future

- SP methods is an active and important field, with exciting challenges and expanding applications
- Possible future topics include
  - Refinement of existing theories: singularity of the fluxes, efficient implementation…
  - Explore new structural properties e.g. positivity preserving, multicomponent flows…
  - Temporal integration
  - Unstructured meshes
  - …