A fully-discrete kinetic energy preserving and entropy conservative scheme for compressible flows

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Conservation laws

Consider the system

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{f}(\mathbf{U}) = 0, \qquad \mathbf{f} = (\mathbf{f}_1, \mathbf{f}_2, ..., \mathbf{f}_n)$$
$$\mathbf{U}(\mathbf{x}, 0) = \mathbf{U}_0$$

Entropy framework: Assume there exists $(\eta(\mathbf{U}), \mathbf{q}(\mathbf{U}))$ with entropy variables $\mathbf{V} = \eta'$ satisfying $(q_k')^\top = \mathbf{V}^\top \mathbf{f}_k'$, then

$$\begin{aligned} \frac{\partial \eta}{\partial t} + \nabla \cdot \mathbf{q} &= 0 \qquad \text{(for smooth solutions)} \\ \frac{\partial \eta}{\partial t} + \nabla \cdot \mathbf{q} &\leq 0 \qquad \text{(for discontinous solutions)} \end{aligned}$$

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$$\frac{\partial \eta}{\partial t} + \nabla \cdot \mathbf{q} \;\leq\; 0 \qquad \text{(for discontinous solutions)}$$

Compressible Euler equations

In 1D we have

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{U})}{\partial x} = 0$$

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}, \quad \mathbf{f}(\mathbf{U}) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (E+p)u \end{pmatrix}$$

ρ : density

u : velocity

p : pressure

E : total energy

e : internal energy

$$E = \frac{1}{2}\rho u^2 + \rho e, \qquad e = \frac{p}{\rho(\gamma - 1)}$$

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$$E = \frac{1}{2}\rho u^2 + \rho e, \qquad e = \frac{p}{\rho(\gamma - 1)}$$

Choose the entropy pair

$$\eta = -\frac{\rho s}{\gamma - 1}, \quad q = \eta u, \quad s = \log\left(\frac{p}{\rho^\gamma}\right), \qquad \mathbf{V} = \begin{pmatrix} \frac{\gamma - s}{\gamma - 1} - \beta u^2 \\ 2\beta u \\ -2\beta \end{pmatrix}, \quad \beta = \frac{\rho}{2p}$$

(Harten '83, Hughes '86)

Compressible Euler equations

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AIM 1:
Construct a **fully-discrete entropy conservative scheme** for the Euler equations.

Evolution of total kinetic energy

$$\mathcal{K} = \frac{1}{2}\rho u^2 \quad \implies \quad \frac{\partial \mathcal{K}}{\partial t} = -\frac{1}{2}u^2\frac{\partial \rho}{\partial t} + u\frac{\partial \rho u}{\partial t}$$

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Integrating and ignoring BC terms

$$\frac{\mathsf{d}}{\mathsf{d}t}\int \mathcal{K}\mathsf{d}x = \int p\frac{\partial u}{\partial x}\mathsf{d}x$$

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AIM 2:
Construct a **fully-discrete kinetic energy preserving scheme** for the Euler equations, which evolves $\mathcal{K}$ in a consistent manner.

Existing arsenal of methods

- Entropy conservative/stable flux construction (Tadmor)
- High-order entropy conservative fluxes (LeFloch et al.)
- High-order entropy stable fluxes (Fjordholm et al.)
- Entropy conservative flux for Euler (Roe et al.)
- Kinetic energy preserving flux (Jameson)
- Kinetic energy preserving and entropy conservative flux (Chandrashekar)

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- Kinetic energy preservation with split forms (Feiereisen, Kennedy et al., Pirozzoli)
- Kinetic energy preserving DG schemes (Gassner et al.)
- Kinetic energy and entropy preserving scheme in split form (Kuya et al.)
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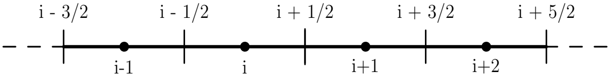
Fully-discrete scheme



$$I_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}], \qquad x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}} \equiv \Delta x$$

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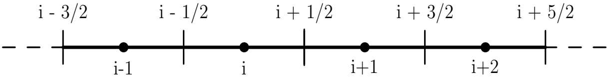

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Define the vector of averaged entropy variables

$$\widetilde{\mathbf{V}}(\mathbf{U}^*, \mathbf{U}^{**}), \qquad \mathbf{V}_i^{n+\frac{1}{2}} = \widetilde{\mathbf{V}}(\mathbf{U}_i^n, \mathbf{U}_i^{n+1}), \qquad \mathbf{U}_i^n \approx \mathbf{U}(x_i, t^n)$$

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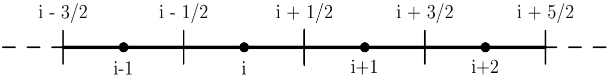

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Consider the semi-implicit scheme

$$\frac{\mathbf{U}_i^{n+1} - \mathbf{U}_i^n}{\Delta t} + \frac{\mathbf{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}} - \mathbf{F}_{i-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta x} = 0$$

where

$$\mathbf{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \mathbf{F}(\mathbf{V}_i^{n+\frac{1}{2}}, \mathbf{V}_{i+1}^{n+\frac{1}{2}}) \qquad \longrightarrow \text{written in terms of } \widetilde{\mathbf{V}}$$

Entropy conservation

We have the entropy relation

$$\frac{\partial \eta(\mathbf{U})}{\partial t} = \left\langle \mathbf{V}, \frac{\partial \mathbf{U}}{\partial t} \right\rangle = -\left\langle \mathbf{V}, \frac{\partial \mathbf{f}}{\partial x} \right\rangle = -\frac{\partial q}{\partial x}$$

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Need to satisfy two consistency conditions at the discrete level

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Need to satisfy two consistency conditions at the discrete level

- Temporal

Entropy conservation

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Need to satisfy two consistency conditions at the discrete level

- Temporal
- Spatial

Entropy conservation

We have the entropy relation

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Temporal (LeFloch et al. 2000): Find $\widetilde{\mathbf{V}}(\mathbf{U}^*, \mathbf{U}^{**})$ satisfying

$$\left\langle \widetilde{\mathbf{V}}(\mathbf{U}^*, \mathbf{U}^{**}), (\mathbf{U}^{**} - \mathbf{U}^*) \right\rangle = \eta(\mathbf{U}^{**}) - \eta(\mathbf{U}^*)$$

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Spatial (Tadmor '84): Find a numerical flux $\mathbf{F}$ satisfying

$$\left\langle \Delta \mathbf{V}_{i+\frac{1}{2}}, \mathbf{F}_{i+\frac{1}{2}} \right\rangle = \Delta \Psi_{i+\frac{1}{2}}, \quad \Psi = \left\langle \mathbf{V}, \mathbf{f} \right\rangle - q$$

where $\Delta(.)_{i+\frac{1}{2}} = (.)_{i+1} - (.)_i$.

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where $\Delta(.)_{i+\frac{1}{2}} = (.)_{i+1} - (.)_i$.

Need to construct $\widetilde{\mathbf{V}}$ and $\mathbf{F}$ for Euler equations.

Kinetic energy preservation

Recall the evolution equation

$$\frac{\mathsf{d}}{\mathsf{d}t}\int \mathcal{K}\mathsf{d}x = -\int \frac{1}{2}u^2\frac{\partial \rho}{\partial t}\mathsf{d}x + \int u\frac{\partial \rho u}{\partial t}\mathsf{d}x = \int p\frac{\partial u}{\partial x}\mathsf{d}x$$

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Temporal (Subbareddy et al. 2009): If the time-averaged velocity is chosen as

$$u^{n+\frac{1}{2}} = u(\mathbf{V}^{n+\frac{1}{2}}) = \frac{\sqrt{\rho^n}u^n + \sqrt{\rho^{n+1}}u^{n+1}}{\sqrt{\rho^n} + \sqrt{\rho^{n+1}}}$$

then the following holds

$$\frac{\mathcal{K}_i^{n+1} - \mathcal{K}_i^n}{\Delta t} = -\frac{1}{2}(u_i^{n+\frac{1}{2}})^2\frac{\rho_i^{n+1} - \rho_i^n}{\Delta t} + -\frac{1}{2}u_i^{n+\frac{1}{2}}\frac{(\rho u)_i^{n+1} - (\rho u)_i^n}{\Delta t}$$

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Spatial (Jameson 2008): If the inviscid flux $\mathbf{F}_{i+\frac{1}{2}} = \begin{pmatrix} F^\rho, & F^m, & F^e \end{pmatrix}^\top_{i+\frac{1}{2}}$ is chosen as

$$F^m_{i+\frac{1}{2}} = p_{i+\frac{1}{2}} + \overline{u}_{i+\frac{1}{2}} F^\rho_{i+\frac{1}{2}}$$

for any consistent approximation $p_{i+\frac{1}{2}}$, $F^\rho_{i+\frac{1}{2}}$, $F^e_{i+\frac{1}{2}}$, then

$$\sum_i \left[\frac{1}{2}(u_i)^2 \frac{F^\rho_{i+\frac{1}{2}} - F^\rho_{i-\frac{1}{2}}}{\Delta x}\right] - \sum_i \left[(u_i)\frac{F^m_{i+\frac{1}{2}} - F^m_{i-\frac{1}{2}}}{\Delta x}\right] = \sum_i p_{i+\frac{1}{2}} \frac{\Delta u_{i+\frac{1}{2}}}{\Delta x}$$

Constructing $\widetilde{\mathbf{V}}$

Define the time averaging and difference operators

$$\{\{(.)\}\}^{n+\frac{1}{2}} = \frac{(.)^{n+1} + (.)^{n}}{2}, \quad [\![(.)]\!]^{n+\frac{1}{2}} = (.)^{n+1} - (.)^{n}, \quad \ddot{(.)}^{n+\frac{1}{2}} = \frac{(.)^{n+1} - (.)^{n}}{\log(.)^{n+1} - \log(.)^{n}}$$

Need to satisfy two conditions

- For entropy conservation

$$\left\langle \mathbf{V}^{n+\frac{1}{2}}, [\![\mathbf{U}]\!]^{n+\frac{1}{2}} \right\rangle = [\![\eta]\!]^{n+\frac{1}{2}}$$

- For kinetic energy preservation

$$u^{n+\frac{1}{2}} = u(\mathbf{V}^{n+\frac{1}{2}}) = \frac{\sqrt{\rho^{n}}u^{n} + \sqrt{\rho^{n+1}}u^{n+1}}{\sqrt{\rho^{n}} + \sqrt{\rho^{n+1}}}$$

Constructing $\widetilde{\mathbf{V}}$

Step 1: Introduce the parameter vector

$$\mathbf{Z} = \begin{pmatrix} Z_1, & Z_2, & Z_3 \end{pmatrix}^\top = \begin{pmatrix} \sqrt{\rho}, & \sqrt{\rho}u, & p \end{pmatrix}^\top$$

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Step 2: Re-write the relation $\left\langle \mathbf{V}^{n+\frac{1}{2}}, [\![\mathbf{U}]\!]^{n+\frac{1}{2}} \right\rangle = [\![\eta]\!]^{n+\frac{1}{2}}$ in terms of $\mathbf{Z}$.

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Step 3: Compare coefficients of jumps $[\![Z_1]\!]^{n+\frac{1}{2}}$, $[\![Z_2]\!]^{n+\frac{1}{2}}$, $[\![Z_3]\!]^{n+\frac{1}{2}}$ to get

$$\beta^{n+\frac{1}{2}} = \frac{\{\{\rho\}\}^{n+\frac{1}{2}}}{2(\ddot{p})^{n+\frac{1}{2}}}, \qquad s^{n+\frac{1}{2}} = \{\{s\}\}^{n+\frac{1}{2}} + \gamma\left(1 - \frac{\{\{\rho\}\}^{n+\frac{1}{2}}}{(\ddot{\rho})^{n+\frac{1}{2}}}\right)$$

$$\boxed{u^{n+\frac{1}{2}} = \frac{\{\{Z_2\}\}^{n+\frac{1}{2}}}{\{\{Z_1\}\}^{n+\frac{1}{2}}} = \frac{\sqrt{\rho^n}u^n + \sqrt{\rho^{n+1}}u^{n+1}}{\sqrt{\rho^n} + \sqrt{\rho^{n+1}}}}$$

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Step 4: Evaluate $\mathbf{V}^{n+\frac{1}{2}} = \widetilde{\mathbf{V}}(\beta^{n+\frac{1}{2}},\ s^{n+\frac{1}{2}},\ u^{n+\frac{1}{2}})$.

Constructing $\widetilde{\mathbf{V}}$

Such constructions need not unique and depends on

- Choice of algebraic relation
- Choice of parameter vector $\mathbf{Z}$
- Choice of variables whose jump coefficients are compared

Subbareddy et al. used KE relation, $\mathbf{Z} = \left(\sqrt{\rho}, \quad \sqrt{\rho}u\right)^\top$ and $[\![\mathbf{Z}]\!]$
$\longrightarrow$ full-discrete kinetic energy preserving scheme

Gouasmi et al. used EC relation, $\mathbf{Z} = \mathbf{V}$ and $[\![\rho]\!]$, $[\![u]\!]$, $[\![p]\!]$
$\longrightarrow$ full-discrete entropy conservative scheme

Other options out there in the wild?

Euler fluxes

Euler fluxes

Entropy conservative flux (Roe et al.):

$$\mathbf{Z} = \begin{pmatrix} Z_1 & Z_2 & Z_3 \end{pmatrix}^\top = \sqrt{\frac{\rho}{p}} \begin{pmatrix} 1 & u & p \end{pmatrix}^\top$$

$$\mathbf{F} = \begin{pmatrix} F^\rho \\ F^m \\ F^e \end{pmatrix} = \begin{pmatrix} \overline{Z_2}\widehat{Z_3} \\ \dfrac{\overline{Z_3}}{\overline{Z_1}} + \dfrac{\overline{Z_2}}{\overline{Z_1}} F^\rho \\ F^e \end{pmatrix}, \; F^e = \frac{1}{2\overline{Z_1}} \left[\frac{(\gamma+1)}{(\gamma-1)} \frac{F^\rho}{\widehat{Z_1}} + \overline{Z_2} F^m \right]$$

where for $\phi > 0$

$$\overline{\phi} = \frac{\phi_{i+1} + \phi_i}{2}, \qquad \widehat{\phi} = \frac{\phi_{i+1} - \phi_i}{\ln(\phi_{i+1}) - \ln(\phi_i)}$$

ROE-EC flux

Kinetic energy preserving and entropy conservative flux (Chandrashekar):

$$\mathbf{F} = \begin{pmatrix} F^\rho \\ F^m \\ F^e \end{pmatrix} = \begin{pmatrix} \widehat{\rho}\overline{u} \\ \tilde{p} + \overline{u}F^\rho \\ F^e \end{pmatrix}, \; F^e = \left[\frac{1}{2(\gamma-1)\widehat{\beta}} - \frac{1}{2}\overline{|u|^2} \right] F^\rho + \overline{u}F^m$$

where

$$\tilde{p} = \frac{\overline{\rho}}{2\overline{\beta}}$$

KEPEC flux

Euler fluxes

Kinetic energy preserving and entropy conservative flux (Chandrashekar):

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where

$$\tilde{p} = \frac{\overline{\rho}}{2\overline{\beta}}$$

KEPEC flux

Kinetic energy preserving flux (Gassner et al.):
KEPEC flux with $\tilde{p} = \overline{p}$

KEP flux

Density wave: test for accuracy

$\rho = 2 + \sin(4\pi x), \quad u = 1, \quad p = 1$
KEPEC flux, Newton-GMRES solver, CFL $= 1.5$, $T_f = 10$

N	L^1		L^2		L^∞	
	error	rate	error	rate	error	rate
40	1.23e-0	-	1.36e-0	-	1.92e-0	-
80	4.12e-1	1.58	4.59e-1	1.57	6.96e-1	1.47
160	1.01e-1	2.02	1.17e-1	1.98	2.01e-1	1.79
320	2.60e-2	1.96	2.91e-2	2.00	4.67e-2	2.10
640	6.55e-3	2.00	7.28e-3	2.00	1.07e-2	2.13

Isentropic vortex

$$\rho = \left[1 - \frac{\beta^2(\gamma-1)}{8\gamma\pi^2}\exp\left(1-r^2\right)\right]^{\frac{1}{(\gamma-1)}}$$

$$u = M\cos(\alpha) - \frac{\beta(y-y_c)}{2\pi}\exp\left(\frac{1-r^2}{2}\right)$$

$$v = M\sin(\alpha) + \frac{\beta(x-x_c)}{2\pi}\exp\left(\frac{1-r^2}{2}\right)$$

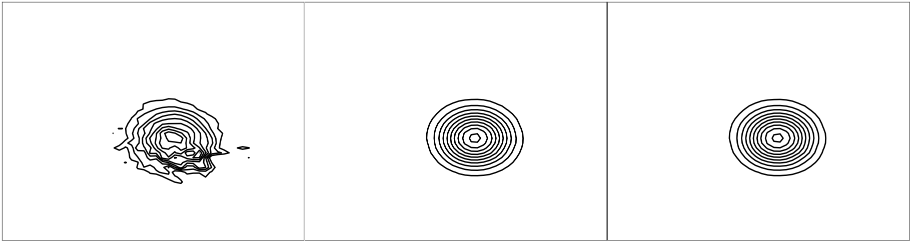
$$r = \sqrt{(x-x_c)^2+(y-y_c)^2}$$

Ω: $[-5,5]\times[-5,5]$ with final time t=100.

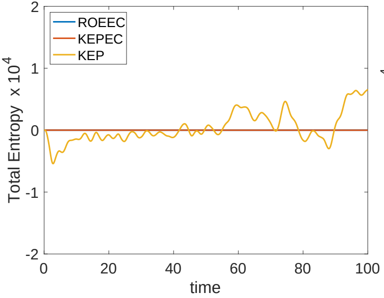
- Total kinetic energy is preserved
- Total entropy is preserved (identically zero)

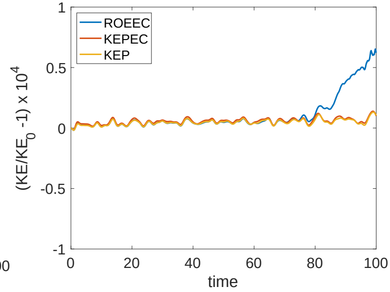
$$p = \rho^\gamma \quad (x_c, y_c) = (0,0) \quad \beta = 5 \quad \alpha = 0^\circ$$

Isentropic vortex: M=0.5, (50 x 50)

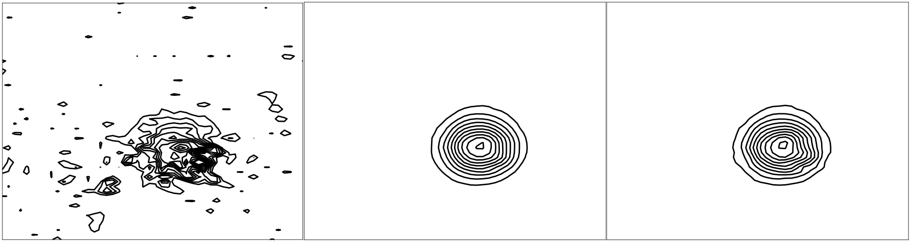


ROE-EC **KEPEC** **KEP**

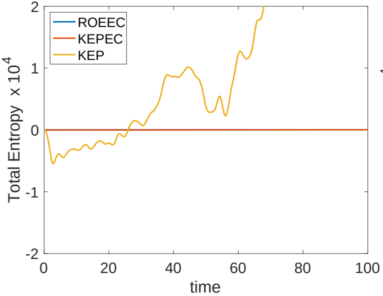


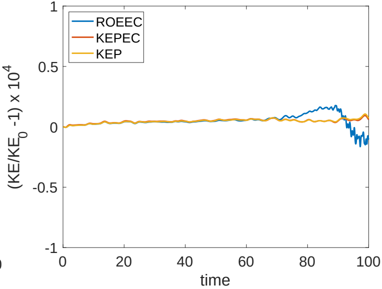


Isentropic vortex: M=1, (50 x 50)

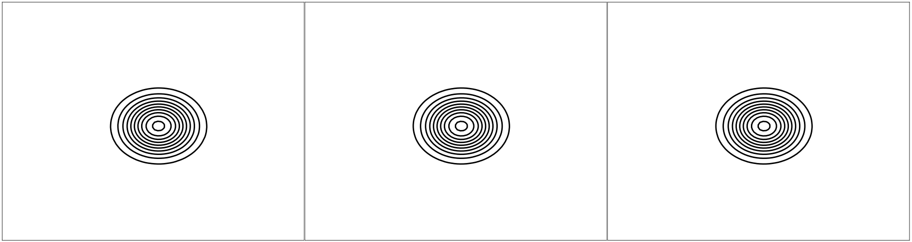


ROE-EC **KEPEC** **KEP**

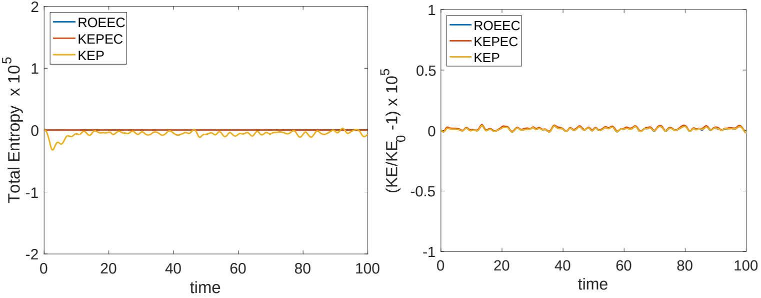




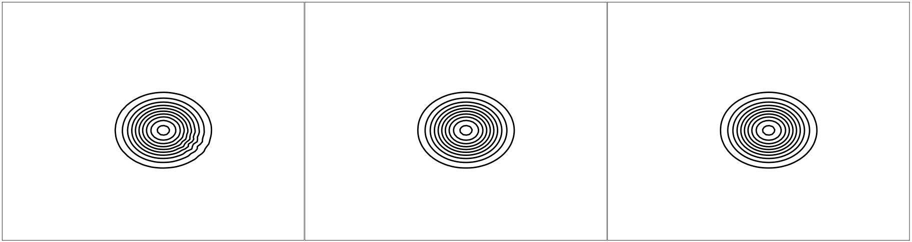
Isentropic vortex: M=0.5, (100 x 100)



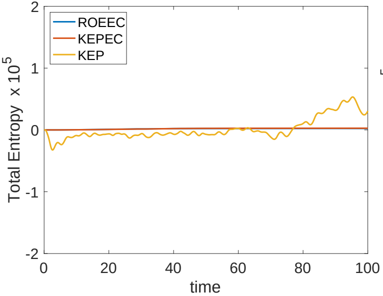
ROE-EC KEPEC KEP

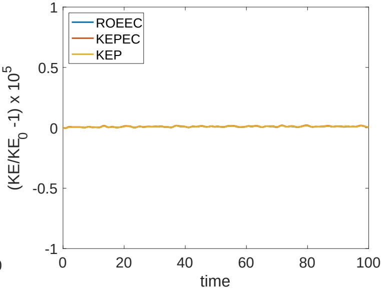


Isentropic vortex: M=1, (100 x 100)



ROE-EC KEPEC KEP





Conclusions

- Proposed a fully-discrete KEPEC scheme
- Can be used on unstructured grids
- Useful for DNS of turbulent flows
  - Viscous discretization available in 1D for KEP and ES
  - KEP or ES discretization (but not both) in higher-dimensions?

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Questions?

Viscous relations

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} = \frac{\partial \mathbf{g}}{\partial x}$$

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (E+p)u \end{pmatrix}, \quad \mathbf{g} = \begin{pmatrix} 0 \\ \tau \\ u\tau + \kappa \frac{\partial \theta}{\partial x} \end{pmatrix}, \quad \tau = \frac{4}{3}\mu \frac{\partial u}{\partial x}$$

Entropy relation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int \eta \mathrm{d}x = -\int \left[\frac{8\mu}{3}\beta \left(\frac{\partial u}{\partial x}\right)^2 + \frac{\kappa}{R\theta^2}\left(\frac{\partial \theta}{\partial x}\right)^2\right] \mathrm{d}x \leq 0$$

Kinetic energy evolution:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int \mathcal{K} \mathrm{d}x = \underbrace{\int p \frac{\partial u}{\partial x} \mathrm{d}x}_{\text{work by pressure forces}} - \underbrace{\int \frac{4}{3}\mu \left(\frac{\partial u}{\partial x}\right)^2 \mathrm{d}x}_{\text{dissipation by viscous forces}}$$