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

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SIAM CSE
Spokane, 27 February 2019
Conservation laws

Consider the system
\[
\frac{\partial U}{\partial t} + \nabla \cdot f(U) = 0, \quad f = (f_1, f_2, \ldots, f_n)
\]
\[U(x, 0) = U_0\]

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

\[
\frac{\partial \eta}{\partial t} + \nabla \cdot q = 0 \quad \text{(for smooth solutions)}
\]
\[
\frac{\partial \eta}{\partial t} + \nabla \cdot q \leq 0 \quad \text{(for discontinuous solutions)}
\]
Conservation laws

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

\[
\begin{align*}
\frac{\partial \eta}{\partial t} + \nabla \cdot q & = 0 \quad \text{(for smooth solutions)} \\
\frac{\partial \eta}{\partial t} + \nabla \cdot q & \leq 0 \quad \text{(for discontinuous solutions)}
\end{align*}
\]
In 1D we have

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

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

\[
E = \frac{1}{2} \rho u^2 + \rho e, \quad e = \frac{p}{\rho(\gamma - 1)}
\]

\( \rho \): density  
\( u \): velocity  
\( p \): pressure  
\( E \): total energy  
\( e \): internal energy
Compressible Euler equations

In 1D we have

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

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

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

Choose the entropy pair

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

(Harten '83, Hughes '86)
Compressible Euler equations

In 1D we have

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

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

$\rho$: density
$u$: velocity
$p$: pressure
$E$: total energy
$e$: internal energy
$s$: specific entropy

AIM 1:
Construct a fully-discrete entropy conservative scheme for the Euler equations.
Evolution of total kinetic energy

\[ K = \frac{1}{2} \rho u^2 \quad \implies \quad \frac{\partial K}{\partial t} = -\frac{1}{2} u^2 \frac{\partial \rho}{\partial t} + u \frac{\partial \rho u}{\partial t} \]
Evolution of total kinetic energy

\[ K = \frac{1}{2} \rho u^2 \quad \Rightarrow \quad \frac{\partial K}{\partial t} = -\frac{1}{2} u^2 \frac{\partial \rho}{\partial t} + u \frac{\partial \rho u}{\partial t} \]

Integrating and ignoring BC terms

\[ \frac{d}{dt} \int K \, dx = \int p \frac{\partial u}{\partial x} \, dx \]
Evolution of total kinetic energy

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Integrating and ignoring BC terms

\[ \frac{d}{dt} \int K \, dx = \int p \frac{\partial u}{\partial x} \, dx \]

**AIM 2:**
Construct a **fully-discrete kinetic energy preserving scheme** for the Euler equations, which evolves \( K \) 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.)*
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FDKEPEC
Fully-discrete scheme

\[ I_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}], \quad x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}} \equiv \Delta x \]
Fully-discrete scheme

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

Define the vector of averaged entropy variables

\[ \tilde{V}(\text{U}^*, \text{U}**) \]

\[ \tilde{V}_i^{n+\frac{1}{2}} = \tilde{V}(\text{U}_i^n, \text{U}_i^{n+1}) \]

\[ \text{U}_i^n \approx \text{U}(x_i, t^n) \]
Fully-discrete scheme

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Define the vector of averaged entropy variables

\[ \tilde{V}(U^*, U^{**}), \quad V_i^{n+\frac{1}{2}} = \tilde{V}(U_i^n, U_i^{n+1}), \quad U_i^n \approx U(x_i, t^n) \]

Consider the semi-implicit scheme

\[
\frac{U_i^{n+1} - U_i^n}{\Delta t} + \frac{F_i^{n+\frac{1}{2}} - F_i^{-\frac{1}{2}}}{\Delta x} = 0
\]

where

\[ F_i^{n+\frac{1}{2}} = F(V_i^{n+\frac{1}{2}}, V_i^{n+\frac{1}{2}}) \]

\[ \rightarrow \text{written in terms of } \tilde{V} \]
Entropy conservation

We have the entropy relation

\[
\frac{\partial \eta(U)}{\partial t} = \langle V, \frac{\partial U}{\partial t} \rangle = -\langle V, \frac{\partial f}{\partial x} \rangle = - \frac{\partial q}{\partial x}
\]
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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

\[ \frac{\partial \eta(U)}{\partial t} = \langle V, \frac{\partial U}{\partial t} \rangle = -\langle V, \frac{\partial f}{\partial x} \rangle = - \frac{\partial q}{\partial x} \]

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

\[ \langle \tilde{V}(U^*, U^{**}), (U^{**} - U^*) \rangle = \eta(U^{**}) - \eta(U^*) \]

\( \eta \) is the entropy function.
Entropy conservation

We have the entropy relation

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\frac{\partial \eta(U)}{\partial t} = \left\langle V, \frac{\partial U}{\partial t} \right\rangle = -\left\langle V, \frac{\partial f}{\partial x} \right\rangle = -\frac{\partial q}{\partial x}
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Spatial (Tadmor ’84): Find a numerical flux \( F \) satisfying

\[
\left\langle \Delta V_{i+\frac{1}{2}}, F_{i+\frac{1}{2}} \right\rangle = \Delta \Psi_{i+\frac{1}{2}}, \quad \Psi = \left\langle V, f \right\rangle - q
\]

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

We have the entropy relation

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\frac{\partial \eta(U)}{\partial t} = \left\langle V, \frac{\partial U}{\partial t} \right\rangle = -\left\langle V, \frac{\partial f}{\partial x} \right\rangle = -\frac{\partial q}{\partial x}
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where \( \Delta(\cdot)_{i+\frac{1}{2}} = (\cdot)_i + 1 - (\cdot)_i \).

Need to construct \( \tilde{V} \) and \( F \) for Euler equations.
Kinetic energy preservation

Recall the evolution equation

$$\frac{d}{dt} \int \mathcal{K} \, dx = - \int \frac{1}{2} u^2 \frac{\partial \rho}{\partial t} \, dx + \int u \frac{\partial \rho u}{\partial t} \, dx = \int p \frac{\partial u}{\partial x} \, dx$$
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Temporal (Subbareddy et al. 2009): If the time-averaged velocity is chosen as

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

then the following holds

\[ \frac{K_{i}^{n+1} - K_{i}^{n}}{\Delta t} = -\frac{1}{2} \left( u_i^{n+\frac{1}{2}} \right)^2 \frac{\rho_{i}^{n+1} - \rho_{i}^{n}}{\Delta t} + \frac{1}{2} u_i^{n+\frac{1}{2}} \frac{(\rho u)_i^{n+1} - (\rho u)_i^{n}}{\Delta t} \]
Kinetic energy preservation

Recall the evolution equation

\[ \frac{d}{dt} \int \mathcal{K} \, dx = - \int \frac{1}{2} u^2 \frac{\partial \rho}{\partial t} \, dx + \int u \frac{\partial \rho u}{\partial t} \, dx = \int \rho \frac{\partial u}{\partial x} \, dx \]

Spatial (Jameson 2008): If the inviscid flux \( F_{i+\frac{1}{2}} = (F^\rho, \quad F^m, \quad F^e)_{i+\frac{1}{2}} \) is chosen as

\[ F^m_{i+\frac{1}{2}} = p_{i+\frac{1}{2}} + \bar{u}_{i+\frac{1}{2}} F^\rho_{i+\frac{1}{2}} \]

for any consistent approximation \( p_{i+\frac{1}{2}}, \quad F^\rho_{i+\frac{1}{2}}, \quad F^e_{i+\frac{1}{2}} \), 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 $\tilde{V}$

Define the time averaging and difference operators

$$\langle \{(.\} \rangle n+\frac{1}{2} = \frac{(.)^{n+1} + (.)^{n}}{2}, \quad \llbracket (. \rrbracket)^{n+\frac{1}{2}} = (.)^{n+1} - (.)^{n}, \quad (\cdot)^{n+\frac{1}{2}} = \frac{(.)^{n+1} - (.)^{n}}{\log(.)^{n+1} - \log(.)^{n}}$$

Need to satisfy two conditions

- For entropy conservation

$$\langle \mathbf{V}^{n+\frac{1}{2}}, \llbracket \mathbf{U} \rrbracket^{n+\frac{1}{2}} \rangle = \llbracket \eta \rrbracket^{n+\frac{1}{2}}$$

- 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 $\tilde{V}$

**Step 1:** Introduce the parameter vector

$$Z = (Z_1, Z_2, Z_3)^\top = (\sqrt{\rho}, \sqrt{\rho u}, p)^\top$$
Constructing $\tilde{V}$

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$$Z = (Z_1, Z_2, Z_3)^\top = (\sqrt{\rho}, \sqrt{\rho u}, p)^\top$$

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

**Step 1:** Introduce the parameter vector

$$Z = (Z_1, Z_2, Z_3)\top = (\sqrt{\rho}, \sqrt{\rho}u, p)\top$$

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

**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

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

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

**Step 1:** Introduce the parameter vector

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

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

Such constructions need not unique and depends on

- Choice of algebraic relation
- Choice of parameter vector $Z$
- Choice of variables whose jump coefficients are compared

Subbareddy et al. used KE relation, $Z = \begin{pmatrix} \sqrt{\rho} \\ \sqrt{\rho}u \end{pmatrix}^\top$ and $[Z]$

$\longrightarrow$ full-discrete kinetic energy preserving scheme

Gouasmi et al. used EC relation, $Z = V$ and $[\rho], [u], [p]$

$\longrightarrow$ full-discrete entropy conservative scheme

Other options out there in the wild?
Euler fluxes

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

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FDKEPEC
Euler fluxes

Entropy conservative flux (Roe et al.):

\[ Z = (Z_1, Z_2, Z_3)^\top = \sqrt{\frac{\rho}{p}} (1, u, p)^\top \]

\[ F = \begin{pmatrix} F^\rho \\ F^m \\ F^e \end{pmatrix} = \begin{pmatrix} Z_2 \hat{Z}_3 \\ \frac{Z_3}{Z_1} + \frac{Z_2}{Z_1} F^\rho \\ \frac{Z_3}{Z_1} \end{pmatrix}, \quad F^e = \frac{1}{2Z_1} \left[ \frac{(\gamma + 1)}{(\gamma - 1)} \hat{Z}_1 + \hat{Z}_2 F^m \right] \]

where for \( \phi > 0 \)

\[ \overline{\phi} = \frac{\phi_{i+1} + \phi_i}{2}, \quad \hat{\phi} = \frac{\phi_{i+1} - \phi_i}{\ln(\phi_{i+1}) - \ln(\phi_i)} \]

ROE-EC flux
Euler fluxes

Kinetic energy preserving and entropy conservative flux (Chandrashekar):

\[
F = \begin{pmatrix} F^\rho \\ F^m \\ F^e \end{pmatrix} = \begin{pmatrix} \tilde{\rho} u + \bar{u} F^\rho \\ \tilde{\beta} - \frac{1}{2} |u|^2 \end{pmatrix}, \quad F^e = \frac{1}{2(\gamma - 1)} \tilde{\beta} - \frac{1}{2} |u|^2 
\]

where

\[
\tilde{\rho} = \frac{\bar{\rho}}{2\beta}
\]

KEPEC flux
Euler fluxes

Kinetic energy preserving and entropy conservative flux (Chandrashekar):

\[
F = \begin{pmatrix}
F^\rho \\
F^m \\
F^e
\end{pmatrix} = \begin{pmatrix}
\tilde{\rho}u \\
\tilde{\rho}uF^\rho \\
\frac{1}{2(\gamma - 1)}\tilde{\beta} - \frac{1}{2}|u|^2
\end{pmatrix} F^\rho + \bar{u}F^m,
\]

where

\[
\tilde{\rho} = \frac{\bar{\rho}}{2\bar{\beta}}.
\]

KEPEC flux

Kinetic energy preserving flux (Gassner et al.):

KEPEC flux with \(\tilde{\rho} = \bar{\rho}\)

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, \( T_f = 10 \)

<table>
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<th>( L^1 ) error</th>
<th>( L^1 ) rate</th>
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Isentropic vortex

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

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

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

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

\[ \Omega: [-5, 5] \times [-5, 5] \text{ with final time } t=100. \]

- 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: $M = 0.5$, $(50 \times 50)$
Isentropic vortex: $M=1$, $(50 \times 50)$
Isentropic vortex: $M=0.5$, $(100 \times 100)$
Isentropic vortex: $M=1$, $(100 \times 100)$
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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  - Can be done in the DG setup (Andrew’s talk)
- Can we preserve other analytical relations (as done by Kuya et al.)?
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Questions?
Viscous relations

\[ \frac{\partial U}{\partial t} + \frac{\partial f}{\partial x} = \frac{\partial g}{\partial x} \]

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

Entropy relation:

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

Kinetic energy evolution:

\[ \frac{d}{dt} \int \kappa \, dx = \int p \frac{\partial u}{\partial x} \, dx - \int \frac{4}{3} \mu \left( \frac{\partial u}{\partial x} \right)^2 \, dx \]

- work by pressure forces
- dissipation by viscous forces