Uniformly high-order bound-preserving OEDG schemes for two-phase flows

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The model: Kapila model

Model

- 2 phases, equation of state $p_i = p_i(\rho_i, e_i)$
- volume fractions $\alpha_1 \in [0,1]$, $\alpha_2 \in [0,1]$, $\alpha_1 + \alpha_2 = 1$
- Density $\rho = \alpha_1 \rho_1 + \alpha_2 \rho_2$
- Velocity equilibrium: one velocity u
- Energy: $E = e + \frac{1}{2}\rho u^2$, $e = \alpha_1 e_1 + \alpha_2 e_2$
- Pressure equilibrium: $p = p_1(\rho_1, e_1) = p_2(\rho_2, e_2)$

$$\begin{split} \frac{\partial \alpha_1}{\partial t} + u \frac{\partial \alpha_1}{\partial x} &= K \frac{\partial u}{\partial x} \\ \frac{\partial \alpha_1 \rho_1}{\partial t} + \frac{\partial (\alpha_1 \rho_1 u)}{\partial x} &= 0 \\ \frac{\partial \alpha_2 \rho_2}{\partial t} + \frac{\partial (\alpha_2 \rho_2 u)}{\partial x} &= 0 \\ \frac{\partial E}{\partial t} + \frac{\partial}{\partial x} \left[u(E+p) \right] &= 0 \end{split}$$

Strictly hyperbolic, $\lambda = u, u, u \pm a$,

$$\frac{1}{\rho a^2} = \frac{\alpha_1}{\rho_1 a_1^2} + \frac{\alpha_2}{\rho_2 a_2^2}.$$

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Justification

Starting from Baer and Nunziato model i = 1, 2

$$\begin{split} \frac{\partial \alpha_i}{\partial t} &+ u_l \frac{\partial \alpha_1}{\partial x} = \lambda \left(p_i - p_{\overline{i}} \right) \\ \frac{\partial \alpha_i \rho_i}{\partial t} &+ \frac{\partial (\alpha_i \rho_i u^i)}{\partial x} = \\ \frac{\partial \alpha_i \rho_i u_i}{\partial t} &+ \frac{\partial (\alpha_i \rho_i u_i^2 + \alpha_i p_i)}{\partial x} = u_l \frac{\partial \alpha_i}{\partial x} + \mu \left(u_i - u_{\overline{i}} \right) \\ \frac{\partial E_i}{\partial t} &+ \frac{\partial}{\partial x} \left[u_l (E_i + p_i) \right] = p_l u_l \frac{\partial \alpha_i}{\partial x} + \mu p_i \left(p_i - p_{\overline{i}} \right) + \mu u_i \left(u_i - u_{\overline{i}} \right) \\ p_l &= \sum_i \alpha_i p_i, u_l = \sum_i \alpha_i u_i / \rho. \end{split}$$

If λ/μ bounded and $\lambda\to+\infty$ then 1 the BN model "converges" towards Kapila's model.

¹Angelo Murrone and Hervé Guillard. "A five equation reduced model for compressible two-phase flow problems". In: J. Comput. Phys. 202.2 (2005), pp. 664–698.

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$$\begin{aligned} \frac{\partial \alpha_i}{\partial t} + u_l \frac{\partial \alpha_1}{\partial x} &= \lambda (p_i - p_{\bar{i}}) \\ \frac{\partial \alpha_i \rho_i}{\partial t} + \frac{\partial (\alpha_i \rho_i u^i)}{\partial x} &= \\ \frac{\partial \alpha_i \rho_i u_i}{\partial t} + \frac{\partial (\alpha_i \rho_i u_i^2 + \alpha_i p_i)}{\partial x} &= u_l \frac{\partial \alpha_i}{\partial x} + \mu (u_i - u_{\bar{i}}) \\ \frac{\partial E_i}{\partial t} + \frac{\partial}{\partial x} [u_l (E_i + p_i)] &= p_l u_l \frac{\partial \alpha_i}{\partial x} + \mu p_i (p_i - p_{\bar{i}}) + \mu u_i (u_i - u_{\bar{i}}) \\ p_l &= \sum_i \alpha_i p_i, u_l = \sum_i \alpha_i u_i / \rho. \end{aligned}$$

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Interpretation

The interpretation of the α equation and the term $K = \alpha_1 \alpha_2 \times \ldots$: Take the Lagrangian derivative of

$$p_1(\rho_1, s_1) - p_2(\rho_2, s_2) = 0$$

along isentropes $s_i = cte$.

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Questions

- How to define shocks? In², some arguments are given to define shock relations: Hugoniot curve for each phase, and pressure equilibrium.
- Invariant domain:

 $\mathcal{D} = \{\alpha_i \rho_i \geq 0, \alpha_i \in [0, 1], e \geq 0\}$

How to design numerical scheme that respect that

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dG framework

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Numerical scheme

Rewrite Kapila's model as:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = \chi \mathbf{z}_1 \frac{\partial u}{\partial x}$$

with

$$U = \begin{pmatrix} \alpha_1 \\ \alpha_1 \rho_1 \\ \alpha_2 \rho_2 \\ \rho u \\ E \end{pmatrix}, \ F = \begin{pmatrix} \alpha_1 u \\ \alpha_1 \rho_1 u \\ \alpha_2 \rho_2 u \\ \rho u^2 + p \\ u(E + p) \end{pmatrix} \text{ and } \mathbf{z}_1 = \chi \alpha_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$
$$\chi = \frac{K}{\alpha_1} + 1 = \frac{\frac{1}{Z_1}}{\frac{\alpha_1}{Z_1} + \frac{\alpha_2}{Z_2}}.$$

Numerical scheme: do dG

•
$$\Omega = \bigcup I_j, I_j = [x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}], j = 1, \dots, N_x.$$

• $\mathbb{V}_h^K := \left\{ \mathbf{v} \in L^2(\Omega) : \mathbf{v}|_{I_j} \in \mathbb{P}^K(I_j) \quad \forall I_j \in \Omega \right\},$
• $\mathbf{U}_h(x, t) = \sum_{k=0}^K \mathbf{U}_j^{(k)}(t)\phi_j^{(k)}(x) \quad \forall x \in I_j, \text{ where } \left\{\phi_j^{(k)}(x)\right\}_{k=0}^K \text{ is a basis of } \mathbb{P}^K(I_j), \text{ and } \mathbf{U}_j^{(k)}(t) \text{ is the corresponding } k \text{th degree of freedom.}$
Formally:

$$\int_{l_j} \frac{\partial \mathbf{U}_h}{\partial t} \phi_j^{(k)}(\mathbf{x}) d\mathbf{x} + \widehat{\mathbf{F}}(\mathbf{U}_{j+\frac{1}{2}}^-, \mathbf{U}_{j+\frac{1}{2}}^+) \phi_j^{(k)}(\mathbf{x}_{j+\frac{1}{2}}) - \widehat{\mathbf{F}}(\mathbf{U}_{j-\frac{1}{2}}^-, \mathbf{U}_{j-\frac{1}{2}}^+) \phi_j^{(k)}(\mathbf{x}_{j-\frac{1}{2}}) - \int_{l_j} \mathbf{F}(\mathbf{U}_h) \frac{\partial \phi_j^{(k)}(\mathbf{x})}{\partial \mathbf{x}} d\mathbf{x} = \int_{l_j} \left(\chi \right)_h (\mathbf{z}_1)_h \frac{\partial u_h}{\partial \mathbf{x}} \phi_j^{(k)}(\mathbf{x}) d\mathbf{x},$$
(1)

where the superscripts "–" and "+" represent the left- and right-hand side limits at a cell interface, respectively, and $\widehat{F}(U^-, U^+)$ is the numerical flux.

In this work, we use the HLL flux

Meaning of the non conservative integral

$$\int_{l_j} (\chi)_h(\alpha_1)_h \frac{\partial u_h}{\partial x} \phi_j^{(k)}(x) dx = \lim_{\varepsilon \to 0^+} \int_{x_j - \frac{1}{2} + \varepsilon}^{x_j + \frac{1}{2} - \varepsilon} (\chi)_h(\alpha_1)_h \frac{\partial u_h}{\partial x} \phi_j^{(k)}(x) dx + \lim_{\varepsilon \to 0^+} \int_{x_j - \frac{1}{2} + \varepsilon}^{x_j - \frac{1}{2} + \varepsilon} (\chi)_h(\alpha_1)_h \frac{\partial u_h}{\partial x} \phi_j^{(k)}(x) dx + \lim_{\varepsilon \to 0^+} \int_{x_j + \frac{1}{2} - \varepsilon}^{x_j + \frac{1}{2} - \varepsilon} (\chi)_h(\alpha_1)_h \frac{\partial u_h}{\partial x} \phi_j^{(k)}(x) dx.$$
(2)

so

$$\lim_{\varepsilon \to 0^+} \int_{x_{j-\frac{1}{2}}^{+\varepsilon}}^{x_{j+\frac{1}{2}}^{-\varepsilon}} (\chi)_h(\alpha_1)_h \frac{\partial u_h}{\partial x} \phi_j^{(k)}(x) \mathrm{d}x \approx \Delta x \sum_{\nu=1}^Q \omega_\nu(\chi \alpha_1)_j^{[\nu]} \left(\frac{\partial u}{\partial x}\right)_j^{[\nu]} \phi_j^{(k)}(x_j^{[\nu]}).$$
(3)

and:

$$\lim_{\varepsilon \to 0^+} \int_{x_{j+\frac{1}{2}} - \varepsilon}^{x_{j+\frac{1}{2}} + \varepsilon} (\chi)_h(\alpha_1)_h \frac{\partial u_h}{\partial x} \phi_j^{(k)}(x) \mathrm{d}x \approx \omega_{j+\frac{1}{2}}^- (\chi \alpha_1)_{j+\frac{1}{2}}^- \llbracket u \rrbracket_{j+\frac{1}{2}} \phi_j^{(k)}(x_{j+\frac{1}{2}}) + \omega_{j+\frac{1}{2}}^+ (\chi \alpha_1)_{j+\frac{1}{2}}^+ \llbracket u \rrbracket_{j+\frac{1}{2}} \phi_{j+1}^{(k)}(x_{j+\frac{1}{2}}),$$
(4)

with:

$$\omega_{j+\frac{1}{2}}^{-} = \frac{-a_{j+\frac{1}{2}}^{-}}{a_{j+\frac{1}{2}}^{+} - a_{j+\frac{1}{2}}^{-}}, \quad \omega_{j+\frac{1}{2}}^{+} = \frac{a_{j+\frac{1}{2}}^{+}}{a_{j+\frac{1}{2}}^{+} - a_{j+\frac{1}{2}}^{-}}$$

Here, $a_{j+\frac{1}{2}}^-$ and $a_{j+\frac{1}{2}}^+$ respectively denote the wave speeds estimated in the HLL flux at the interface $x = x_{j+\frac{1}{2}}$.

so . . .

$$\int_{I_{j}} \phi_{j}^{(k)}(\mathbf{x}) d\mathbf{x} \frac{\partial \mathbf{U}_{j}^{(k)}}{\partial t} = \Delta \mathbf{x} \sum_{\nu=1}^{Q} \omega_{\nu} \mathbf{F}(\mathbf{U}_{j}^{[\nu]}) \frac{\partial \phi_{j}^{(k)}(\mathbf{x}_{j}^{[\nu]})}{\partial \mathbf{x}} + \Delta \mathbf{x} \sum_{\nu=1}^{Q} \omega_{\nu} (\chi \alpha_{1})_{j}^{[\nu]} \left(\frac{\partial u}{\partial \mathbf{x}} \right)_{j}^{[\nu]} \phi_{j}^{(k)}(\mathbf{x}_{j}^{[\nu]}) \\
- \frac{a_{j+\frac{1}{2}}^{+} \mathbf{F}(\mathbf{U}_{j+\frac{1}{2}}^{-}) - a_{j+\frac{1}{2}}^{-} \mathbf{F}(\mathbf{U}_{j+\frac{1}{2}}^{+}) + a_{j+\frac{1}{2}}^{+} a_{j+\frac{1}{2}}^{-} (\mathbf{U}_{j+\frac{1}{2}}^{+} - \mathbf{U}_{j+\frac{1}{2}}^{-})}{a_{j+\frac{1}{2}}^{+} - a_{j+\frac{1}{2}}^{-}} \phi_{j}^{(k)}(\mathbf{x}_{j+\frac{1}{2}}) \\
+ \frac{a_{j-\frac{1}{2}}^{+} \mathbf{F}(\mathbf{U}_{j-\frac{1}{2}}^{-}) - a_{j-\frac{1}{2}}^{-} \mathbf{F}(\mathbf{U}_{j-\frac{1}{2}}^{+}) + a_{j+\frac{1}{2}}^{+} a_{j-\frac{1}{2}}^{-} (\mathbf{U}_{j-\frac{1}{2}}^{+} - \mathbf{U}_{j-\frac{1}{2}}^{-})}{a_{j-\frac{1}{2}}^{+} - a_{j-\frac{1}{2}}^{-}} \\
+ (\chi \alpha_{1})_{j+\frac{1}{2}}^{-} \frac{a_{j+\frac{1}{2}}^{-} [\mathbf{U}]_{j+\frac{1}{2}}^{+}}{a_{j+\frac{1}{2}}^{+} - a_{j+\frac{1}{2}}^{-}} \phi_{j}^{(k)}(\mathbf{x}_{j+\frac{1}{2}}) + (\chi \alpha_{1})_{j-\frac{1}{2}}^{+} \frac{a_{j-\frac{1}{2}}^{+} [\mathbf{U}]_{j-\frac{1}{2}}^{-}}{a_{j-\frac{1}{2}}^{+}} \phi_{j}^{(k)}(\mathbf{x}_{j-\frac{1}{2}}). \quad (5)$$

Time discretisation: OEDG

• Runge Kutta, for example SSP RK

• To stabilize discontinuities: post processing technique³

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}\hat{t}} \int_{I_j} \mathbf{U}_\sigma \phi_j^{(k)}(x) \mathrm{d}x + \sum_{m=0}^K \beta_j \frac{\sigma_j^m (\mathbf{U}_h^{n,\ell+1})}{\Delta x} \int_{I_j} (\mathbf{U}_\sigma - P^{m-1} \mathbf{U}_\sigma) \phi_j^{(k)}(x) \mathrm{d}x = 0, \\ \mathbf{U}_\sigma(x,0) = \mathbf{U}_h^{n,\ell+1}(x), \end{cases}$$
(6)

The damping coefficient $\sigma_i^m(\mathbf{U}_h)$ is defined as

$$\sigma_j^m(\mathbf{U}_h) := \max_{1 \le q \le 5} \sigma_j^m(\mathbf{U}_h^{(q)})$$

with

$$\sigma_{j}^{m}(\mathbf{U}_{h}^{(q)}) = \begin{cases} 0, & \text{if } \mathbf{U}_{h}^{(q)} \equiv \overline{\mathbf{U}}_{\Omega}^{(q)}, \\ \frac{(2m+1)\Delta \mathbf{x}^{m}}{(2K-1)m!} \frac{\left\| \left[\partial_{\mathbf{x}}^{m}\mathbf{U}_{h}^{(q)} \right] \right]_{j-\frac{1}{2}} + \left\| \left[\partial_{\mathbf{x}}^{m}\mathbf{U}_{h}^{(q)} \right] \right]_{j+\frac{1}{2}} \right|}{2 \left\| \mathbf{U}_{h}^{(q)} - \overline{\mathbf{U}}_{\Omega}^{(q)} \right\|_{L^{\infty}(\Omega)}}, & \text{otherwise}, \end{cases}$$

where $U_h^{(q)}$ is the *q*th component of \mathbf{U}_h , and $\overline{U}_{\Omega}^{(q)} = \frac{1}{|\Omega|} \int_{\Omega} U_h^{(q)}(x) dx$ represents the global average of $U_h^{(q)}$ over the entire computational domain Ω .

³M. Peng, Z. Sun, and K. Wu. "OEDG: Oscillation-eliminating discontinuous Galerkin method for hyperbolic conservation laws". In: Mathematics of Computation (Published electronicaly July 30, 2024). in press.

Some properties

Equilibrium condition:

if
$$u^{n}(x) \equiv u_{0}, \quad p^{n}(x) \equiv p_{0},$$
 then $u^{n+1}(x) \equiv u_{0}, \quad p^{n+1}(x) \equiv p_{0}.$ (7)

Result

The fully-discrete OEDG scheme with an SSP RK method maintains the condition (7) condition around an isolated material interface:

$$\text{if} \quad u_{\sigma}^n(x)\equiv u_0, \quad p_{\sigma}^n(x)\equiv p_0, \quad \text{then} \quad u_{\sigma}^{n+1}(x)\equiv u_0, \quad p_{\sigma}^{n+1}(x)\equiv p_0.$$

Preserving the invariance domain

We use Zhang and Shu's technique⁴:

- Show that the average values stay in the invariant domain if they are at the previous time step
- Onstruct a bound preserving polynomial approximation
- all this under a CFL like condition

⁴Xiangxiong Zhang and Chi-Wang Shu. "On positivity-preserving high order discontinuous Galerkin schemes for compressible Euler equations on rectangular meshes". In: <u>Journal of Computational Physics</u> 229.23 (2010), pp. 8918–8934.

Preserving the invariance domain

Case of the volume fraction

$$\begin{aligned} (\overline{\alpha}_{1})_{j}^{n+1} = (\overline{\alpha}_{1})_{j}^{n} + \frac{\tau}{\Delta x} \left(\Delta x \sum_{\nu=1}^{Q} \omega_{\nu} (\chi \alpha_{1})_{j}^{[\nu]} \left(\frac{\partial u}{\partial x} \right)_{j}^{[\nu]} \right. \\ & - \frac{a_{j+\frac{1}{2}}^{+} (\alpha_{1}u)_{j+\frac{1}{2}}^{-} - a_{j+\frac{1}{2}}^{-} (\alpha_{1}u)_{j+\frac{1}{2}}^{+} + a_{j+\frac{1}{2}}^{+} a_{j+\frac{1}{2}}^{-} (\alpha_{1})_{j+\frac{1}{2}}^{+} - (\alpha_{1})_{j+\frac{1}{2}}^{-})}{a_{j+\frac{1}{2}}^{+} - a_{j+\frac{1}{2}}^{-}} \\ & + \frac{a_{j-\frac{1}{2}}^{+} (\alpha_{1}u)_{j-\frac{1}{2}}^{-} - a_{j-\frac{1}{2}}^{-} (\alpha_{1}u)_{j+\frac{1}{2}}^{+} + a_{j+\frac{1}{2}}^{+} a_{j-\frac{1}{2}}^{-} ((\alpha_{1})_{j+\frac{1}{2}}^{+} - (\alpha_{1})_{j-\frac{1}{2}}^{-})}{a_{j-\frac{1}{2}}^{+} - a_{j-\frac{1}{2}}^{-}} \\ & + (\chi \alpha_{1})_{j+\frac{1}{2}}^{-} \frac{a_{j+\frac{1}{2}}^{-} [u]_{j+\frac{1}{2}}^{-} + (\chi \alpha_{1})_{j-\frac{1}{2}}^{+} \frac{a_{j+\frac{1}{2}}^{+} [u]_{j-\frac{1}{2}}^{-}}{a_{j+\frac{1}{2}}^{+} - a_{j-\frac{1}{2}}^{-}} \right), \end{aligned}$$

where $(\overline{\alpha}_1)_j^n := \frac{1}{\Delta x} \int_{I_j} (\alpha_1)_{\sigma}^n(x) dx$

We have:

Result

Consider the $\mathbb{P}^{\mathcal{K}}\text{-}\mathsf{based}$ OEDG method for the 1D Kapila five-equation model. If

$$(\widehat{lpha}_1)_j^{[lpha]} := (lpha_1)_{\sigma}^n (\widehat{x}_j^{[lpha]}) \in [0,1], \quad (lpha_1)_j^{[
u]} := (lpha_1)_{\sigma}^n (x_j^{[
u]}) \in [0,1] \quad orall j, lpha,
u_j$$

then the scheme (8) preserves $(\overline{lpha}_1)_j^{n+1} \in [0,1]$ under the CFL condition

$$\frac{\tau}{\Delta x} \le \frac{1}{\mathcal{A}_1 + \mathcal{A}_2},\tag{9}$$

where

$$\mathcal{A}_{1} = \Delta x \max\left\{ \left\| \chi \frac{\partial u}{\partial x} \right\|_{\infty}, \ \left\| \chi_{2} \frac{\partial u}{\partial x} \right\|_{\infty} \right\},$$

$$\mathcal{A}_{2} = \frac{1}{\widehat{\omega}_{1}} \max_{j} \left\{ \left| \mathbf{a}_{j+\frac{1}{2}}^{\pm} \right| + \max\left\{ (\chi)_{j+\frac{1}{2}}^{\mp}, \ (\chi_{2})_{j+\frac{1}{2}}^{\mp} \right\} \left| \llbracket u \rrbracket_{j+\frac{1}{2}} \right| \right\}.$$
 (10)

About the CFL condition

Utilizing the inverse inequalities for polynomials of degree K, we have:

$$\begin{split} \left\| \chi_{\ell} \frac{\partial u_{h}}{\partial x} \right\|_{L^{\infty}(I_{j})} &\leq \| \chi_{\ell} \|_{\infty} \left\| \frac{\partial u_{h}}{\partial x} \right\|_{L^{\infty}(I_{j})} \\ &\leq C_{1}(\Delta x)^{-\frac{1}{2}} \| \chi_{\ell} \|_{\infty} \left\| \frac{\partial u_{h}}{\partial x} \right\|_{L^{2}(I_{j})} \\ &\leq C_{2}(\Delta x)^{-\frac{3}{2}} \| \chi_{\ell} \|_{\infty} \| u_{h} \|_{L^{2}(I_{j})} \\ &\leq C_{2}(\Delta x)^{-1} \| \chi_{\ell} \|_{\infty} \| u_{h} \|_{L^{\infty}(I_{j})}, \quad \ell \in \{1, 2\}, \end{split}$$

where C_1 and C_2 are positive constants depending solely on the polynomial degree K. It follows that

$$\mathcal{A}_1 \le C_2 \|u_h\|_{\infty} \max\{\|\chi\|_{\infty}, \|\chi_2\|_{\infty}\},\$$

which implies the time step constraint (9) is indeed a reasonable CFL-type condition.

Bound preserving

Shu-Wu's technique⁵

$$\mathcal{D} = \underbrace{\{\alpha_1 \in [0,1]\}}_{\mathcal{D}_1} \cap \underbrace{\{\alpha_1 \rho_1 \ge 0, u \in \mathbb{R}, \alpha_2 \rho_2 \ge o, e \ge 0\}}_{\mathcal{D}_2}$$
$$(\alpha_1 \rho_1, \alpha_2 \rho_2, u, E) \in \mathcal{D}_1 \iff \forall u_\star, \begin{pmatrix} \alpha_1 \rho_1 \\ \alpha_2 \rho_2 \\ u, \\ E \end{pmatrix}^T \underbrace{\begin{pmatrix} u_\star^2/2 \\ u_\star^2/2 \\ -u_\star \\ 1 \end{pmatrix}}_{\mathbf{n}_\star} \ge 0$$

HLL flux satisfies

Result

For any $\mathbf{U} \in \mathcal{G}_*$ and $q \in \{1,2\}$, the following inequalities hold:

$$\begin{split} &\mathsf{F}_q(\mathsf{U}) \cdot \mathsf{n}_\ell > \sigma_q^-\mathsf{U} \cdot \mathsf{n}_\ell, \quad -\mathsf{F}_q(\mathsf{U}) \cdot \mathsf{n}_\ell > -\sigma_q^+\mathsf{U} \cdot \mathsf{n}_\ell, \qquad \ell = 1, 2, \\ &\mathsf{F}_q(\mathsf{U}) \cdot \mathsf{n}_* > \sigma_a^-\mathsf{U} \cdot \mathsf{n}_*, \quad -\mathsf{F}_q(\mathsf{U}) \cdot \mathsf{n}_* > -\sigma_a^+\mathsf{U} \cdot \mathsf{n}_* \qquad \forall \mathsf{u}_* \in \mathbb{R}^2, \end{split}$$

and

$$\begin{split} \sigma_1^- &= \min\{u-c, \ 0\}, \qquad \sigma_1^+ &= \max\{u+c, \ 0\}, \\ \sigma_2^- &= \min\{v-c, \ 0\}, \qquad \sigma_2^+ &= \max\{v+c, \ 0\}. \end{split}$$

⁵Kailiang Wu and Chi-Wang Shu. "Geometric quasilinearization framework for analysis and design of bound-preserving schemes". In: SIAM Rev. 65.4 (2023), pp. 1031–1073.

Result

Consider the $\mathbb{P}^{{\sf K}}\text{-}{\sf based}$ OEDG method for the 1D Kapila five-equation model. If

$$\widehat{\mathbf{U}}_{j}^{[\alpha]} := \mathbf{U}_{\sigma}^{n}(\widehat{\mathbf{x}}_{j}^{[\alpha]}) \in \mathcal{D}, \quad \mathbf{U}_{j}^{[\nu]} := \mathbf{U}_{\sigma}^{n}(\mathbf{x}_{j}^{[\nu]}) \in \mathcal{D} \quad \forall j, \alpha, \nu,$$

then the scheme (8) preserves $\overline{\mathbf{U}}_{j}^{n+1}\in\mathcal{D}$ under the CFL condition

$$\frac{\Delta t}{\Delta x} \le \min\left\{\frac{\widehat{\omega}_1}{\max_j \left\{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-\right\}}, \frac{1}{\mathcal{A}_1 + \mathcal{A}_2}\right\},\tag{11}$$

where \mathcal{A}_1 and \mathcal{A}_2 are given in (10).

Final step: get $\widehat{\mathbf{U}}_{j}^{[\alpha]} := \mathbf{U}_{\sigma}^{n}(\widehat{x}_{j}^{[\alpha]}) \in \mathscr{D}$

Shu and Zhang⁶ **Step 1.** First, enforce the volume fraction $0 \le \alpha_1 \le 1$ and partial density $z_\ell \rho_\ell \ge \epsilon_\ell$ with $\epsilon_\ell = \min \{ (\overline{\alpha_\ell \rho_\ell})_j^n, 10^{-13} \}$. Modify the OEDG solution $(\mathbf{U}_{\sigma}^n)_j(x)$ as

$$\widetilde{\mathbf{U}}_{j}(x) = \overline{\mathbf{U}}_{j}^{n} + \theta_{\min}\left((\mathbf{U}_{\sigma}^{n})_{j}(x) - \overline{\mathbf{U}}_{j}^{n}\right) \quad \text{with} \quad \theta_{\min} = \min\left\{\theta_{\alpha_{1}}, \theta_{\alpha_{1}\rho_{1}}, \theta_{z_{2}\rho_{2}}\right\},$$
(12)

where

$$\theta_{z} = \min\left\{\frac{1 - (\overline{\alpha}_{1})_{j}^{n}}{\max_{x \in \mathbb{S}_{j}}\left((\alpha_{1})_{\sigma}^{n}\right)_{j}(x) - (\overline{\alpha}_{1})_{j}^{n}}, \ \frac{(\overline{\alpha}_{1})_{j}^{n}}{(\overline{\alpha}_{1})_{j}^{n} - \min_{x \in \mathbb{S}_{j}}\left((\alpha_{1})_{\sigma}^{n}\right)_{j}(x)}, \ 1\right\},$$

$$\theta_{\alpha_{\ell}\rho_{\ell}} = \min\left\{\frac{(\overline{\alpha_{\ell}\rho_{\ell}})_{j}^{n} - \epsilon_{\ell}}{(\overline{\alpha_{\ell}\rho_{\ell}})_{j}^{n} - \min_{\mathsf{x}\in\mathbb{S}_{j}}\left((\alpha_{\ell}\rho_{\ell})_{\sigma}^{n}\right)_{j}(\mathsf{x})}, \ 1\right\}, \quad \ell \in \{1,2\}.$$

Step 2. Next, enforce the internal energy $\mathcal{E} \geq \epsilon_3$ with $\epsilon_3 = \min \{\mathcal{E}(\overline{\mathbf{U}}_j^n), 10^{-13}\}$. Modify $\widetilde{\mathbf{U}}_j(x)$ as

$$\mathbf{U}_{j}(x) = \overline{\mathbf{U}}_{j}^{n} + \theta_{\rho e} \left(\widetilde{\mathbf{U}}_{j}(x) - \overline{\mathbf{U}}_{j}^{n} \right) \quad \text{with} \quad \theta_{\rho e} = \min \left\{ \frac{\mathscr{E}(\overline{\mathbf{U}}_{j}^{n}) - \epsilon_{3}}{\mathscr{E}(\overline{\mathbf{U}}_{j}^{n}) - \min_{x \in \mathbb{S}_{j}} \mathscr{E}(\widetilde{\mathbf{U}}_{j}(x))}, 1 \right\}.$$
(13)

⁶Xiangxiong Zhang and Chi-Wang Shu. "On positivity-preserving high order discontinuous Galerkin schemes for compressible Euler equations on rectangular meshes". In: <u>Journal of Computational Physics</u> 229.23 (2010), pp. 8918–8934.

Overview

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Equation of state

Each fluid follow a gamma model

Accuracy test

$$(\rho_1, \rho_2, u, p, \alpha_1) = (1, 1.5 + 0.4\cos(\pi x), 1 + 0.4\cos(\pi x), 1, 0.5 + 0.4\sin(\pi x)).$$

The specific heat ratios $\gamma_1 = 1.4$ and $\gamma_2 = 1.6$. The problem is simulated until t = 0.05 in computational domain is [0, 2] with periodic boundary conditions.

N _x	l ¹ error	order	<i>I</i> ² error	order	I^∞ error	order
P ² -BP-OEDG-AVE						
40	2.64E-04	-	4.84E-04	-	3.59E-03	-
80	8.56E-06	4.95	1.42E-05	5.09	8.71E-05	5.36
160	9.87E-07	3.12	1.45E-06	3.30	8.32E-06	3.39
320	2.93E-07	1.75	4.04E-07	1.84	2.06E-06	2.01
640	9.07E-08	1.69	1.21E-07	1.73	4.89E-07	2.07
1280	2.53E-08	1.84	3.44E-08	1.82	1.08E-07	2.18
P ² -BP-OEDG						
40	4.54E-04	-	7.60E-04	-	5.16E-03	-
80	1.10E-05	5.37	2.08E-05	5.19	1.65E-04	4.97
160	4.66E-07	4.56	9.52E-07	4.45	7.90E-06	4.38
320	3.42E-08	3.77	8.61E-08	3.47	1.21E-06	2.71
640	3.26E-09	3.39	9.59E-09	3.17	1.83E-07	2.72
1280	3.43E-10	3.25	9.00E-10	3.41	1.58E-08	3.53

Table: Numerical errors in the mixture density ρ at t = 0.05 and the corresponding convergence orders for the \mathbb{P}^2 -BP-OEDG-AVE schemeand our \mathbb{P}^2 -BP-OEDG scheme.

BP-OEDG-AVE scheme⁷

⁷Fan Zhang and Jian Cheng. "Analysis on physical-constraint-preserving high-order discontinuous Galerkin method for solving Kapila's five-equation model". In: J. Comput. Phys. 492 (2023), p. 112417.

N _x	l^1 error	order	I^2 error	order	I^∞ error	order
₽ ³ -BP-OEDG-AVE						
40	1.99E-04	-	2.81E-04	-	1.34E-03	-
80	2.62E-05	2.93	3.76E-05	2.90	1.49E-04	3.17
160	6.12E-06	2.10	1.06E-05	1.83	5.67E-05	1.39
320	1.60E-06	1.94	3.63E-06	1.55	2.96E-05	0.94
640	4.11E-07	1.96	1.23E-06	1.56	1.33E-05	1.15
1280	1.07E-07	1.95	3.94E-07	1.64	5.36E-06	1.31
₽ ³ -BP-OEDG						
40	2.34E-06	—	3.17E-06	-	1.01E-05	-
80	5.15E-08	5.51	8.18E-08	5.28	3.72E-07	4.76
160	2.20E-09	4.55	4.23E-09	4.27	2.58E-08	3.85
320	9.71E-11	4.50	2.25E-10	4.23	2.14E-09	3.59
640	4.26E-12	4.51	1.10E-11	4.36	1.45E-10	3.88
1280	2.02E-13	4.40	4.80E-13	4.51	5.75E-12	4.66

Table: Numerical errors in the mixture density ρ at t = 0.05 and the corresponding convergence orders for the \mathbb{P}^3 -BP-OEDG-AVE scheme and our \mathbb{P}^3 -BP-OEDG scheme.

Strong interface interaction problem

$$(\rho_1, \rho_2, u, p, \alpha_1) = \begin{cases} \left(0.3884, 1, 27.1123\sqrt{10^5}, 10^7, 10^{-10}\right), & x < 0.2, \\ \left(0.1, 1, 0, 10^5, 10^{-10}\right), & 0.2 < x < 0.3, \\ \left(0.1, 1, 0, 10^5, 1 - 10^{-10}\right), & x > 0.3. \end{cases}$$

The specific heat ratios $\gamma_1 = \frac{5}{3}$ and $\gamma_2 = 1.4$. The computational domain [0, 1] is divided into 200 uniform cells with outflow boundary conditions.



Figure: Numerical results obtained by \mathbb{P}^2 -BP-OEDG and \mathbb{P}^3 -BP-OEDG with 200 uniform cells. Left: mixture density ρ ; right: volume fraction α_1 .

$$(\rho_1, \rho_2, u, e, \alpha) = \begin{cases} (1, \ 0.001, \ 0, \ 10^{-1}, \ 1 - 10^{-10}), & x < 3, \\ (1, \ 0.001, \ 0, \ 10^{-7}, \ 10^{-10}), & \text{otherwise.} \end{cases}$$

The specific heat ratios $\gamma_1 = \gamma_2 = \frac{5}{3}$. The computational domain [0, 9] is divided into 400 uniform cells with the outflow boundary conditions. Final time t = 6. The reference solution is computed by \mathbb{P}^2 -BP-OEDG with 10,000 uniform cells.



Figure: Numerical results obtained by the BP-OEDG-AVE scheme and our BP-OEDG scheme with 400 uniform cells. Left: \mathbb{P}^2 ; right: \mathbb{P}^3 .

Lax like problem

$$(\rho_1, \rho_2, u, p, \alpha_1) = \begin{cases} (0.445, 0.5, 0.698, 3.528, x + 0.5), & x < 0, \\ (0.445, 0.5, 0, 0.571, x + 0.5), & x > 0. \end{cases}$$

The specific heat ratios $\gamma_1 = 1.4$ and $\gamma_2 = 1.6$. The computational domain is [-0.5, 0.5] with outflow boundary conditions. Final time: t = 0.17.



Figure: Numerical results obtained by \mathbb{P}^2 -BP-OEDG-AVE scheme and our \mathbb{P}^2 -BP-OEDG scheme with 1000 uniform cells. The reference solution is computed by the VFRoe-ncv scheme⁹ with 100,000 uniform cells. Left: mixture density ρ ; right: volume fraction α_1 .

⁸Angelo Murrone and Hervé Guillard. "A five equation reduced model for compressible two-phase flow problems". In: J. Comput. Phys. 202.2 (2005), pp. 664–698.

⁹Angelo Murrone and Hervé Guillard. "A five equation reduced model for compressible two-phase flow problems". In: J. Comput. Phys. 202.2 (2005), pp. 664–698.

About the CFL condition



(bottom). From left to right: Moving interface, Shock interface, and LeBlanc.

Richtmyer-Meshkov Instability

Initial position of the gas-gas interface: $x = 2.9 - 0.1 \sin (2\pi (y + 0.25)), y \in [0, 1]$.



Figure: A schematic of the computational domain for Richtmyer-Meshkov instability problem.

Richtmyer-Meshkov Instability

The initial conditions are

$$(\rho_1, \rho_2, u, v, \rho, \alpha_1) = \begin{cases} \left(1, 5.04, 0, 0, 1, 10^{-6}\right), & \mathsf{SF}_6, \gamma = 1.093\\ \left(1, 5.04, 0, 0, 1, 1 - 10^{-6}\right), & \mathsf{pre-shock air}, \gamma = 1.4\\ \left(1.411, 5.04, -0.39, 0, 1.628, 1 - 10^{-6}\right), & \mathsf{post-shock air}, \gamma = 1.4 \end{cases}$$

- Initially, a planar shock wave with a Mach number of 1.24 is positioned at x = 3.2 in air
- moving from right to left
- Domain: $[0, 4] \times [0, 1]$, mesh 1000×250 .
- Boundary conditions:
 - periodic on upper/bottom edges
 - Left is outflow, right: set to post-flow conditions.



Figure: The mixture density ρ obtained by $\mathbb{P}^3\text{-}\mathsf{BP}\text{-}\mathsf{OEDG}$ with 1000 \times 250 uniform cells at different time instances.

shock-helium bubble interaction

 $d_1 = 50$ mm, $d_2 = 25$ mm, $d_3 = 100$ mm, $d_4 = 300$ mm, and $d_5 = 89$ mm.



Initial conditions:

- · The bubble is in thermodynamical equilibrium with surounding air
- A shock wave with a Mach number of 1.22 propagates to the left and hits a helium bubble
- bubble: contaminated with 28% of air.
- Initial conditions are:
 - Helium bubbleρ₁ = 1.4, ρ₂ = 0.25463, u = 0, v = 0, p = 10⁵, α₁ = 10⁻⁶,
 Air: pre-shock ρ₁ = 1.4, ρ₂ = 0.25463, u = 0, v = 0, p = 10⁵, α₁ = 1 10⁻⁶,
 - Air: pre-shock $\rho_1 = 1.4$, $\rho_2 = 0.25463$, u = 0, v = 0, $p = 10^5$, $\alpha_1 = 1 10^{-6}$, post-shock: $\rho_1 = 1.92691$, $\rho_2 = 0.25463$, u = -113.5, v = 0, $p = 1.5698 \times 10^5$, $\alpha_1 = 1 - 10^{-6}$, for post-shock air.

•
$$\gamma_{\it air} = 1.4, \ \gamma_{\it HE} = 1.648$$

solid wall on top/bottom, left is outflow, right is set to post-shock



Figure: 900 \times 267 uniform cells.



Figure: 900 \times 267 uniform cells.



Triple point: 2D Riemann problem

In $[0,7] \times [0,3]$ with 840 \times 360 uniform cells:

$$(\rho_1, \rho_2, u, v, p, \alpha_1) = \begin{cases} \left(1, 1, 0, 0, 1, 1 - 10^{-6}\right), & x \leq 1, \\ \left(1, 1, 0, 0, 0.1, 10^{-6}\right), & x > 1 \text{ and } y < 1.5, \\ \left(0.125, 1, 0, 0, 0.1, 1 - 10^{-6}\right), & \text{otherwise.} \end{cases}$$

- $\gamma_1 = 1.5$ and $\gamma_2 = 1.4$
- Solid wall on top/bottom
- Ouflow on right and left
- Times: *t* = 2.4 and *t* = 5





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- A novel high-order bound-preserving oscillation-eliminating discontinuous Galerkin (BP-OEDG) method with the Harten-Lax-van Leer (HLL) flux for the Kapila five-equation model.
- Preserves isolated contact
- Provably: $\alpha \in [0,1]$, time/space discrete. Carefull discretisation of the α equation
- Bound preserving on $\alpha_i \rho_i$ and internal energy
- Under an almost classical CFL condition.
- Robust

¹⁰Ruifang Yan, Rémi Abgrall, and Kailiang Wu. "Uniformly high-order bound-preserving OEDG schemes for two-phase flows". In: Mathematical Models & Methods in Applied Sciences 34.13 (2024), pp. 2537–2610.



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What has not been done: respect the Saurel-Gavryliuk shock relations.

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