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A high-order matrix-free finite element method for hyperbolic problems

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Outline

1. Mass-matrix-free FEM
   - FEM-type Residual Distribution (RD) in space
   - Deferred-correction (DeC) type time-stepping
2. Applications to Lagrangian hydrodynamics
3. Structure preserving RD scheme (IDP-RD)
4. Advection-diffusion problems
   - DeC + Multirate time integration

Part I: Matrix-free FEM

Finite element approximation

Consider a hyperbolic PDE: $\frac{\partial U}{\partial t} + \nabla_x \cdot \mathbf{f}(U) = 0$

Polynomial interpolation in space: $U \approx U_h = \sum_{i=1}^{N} U_i(t)\varphi_i(x)$

FEM method requires a linear solver with a global sparse mass matrix:

$$\mathbf{M}\frac{d\mathbf{U}}{dt} + \mathbf{F} = \mathbf{0}$$

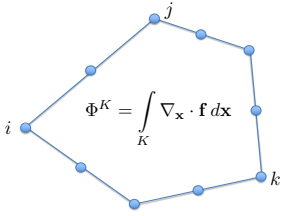
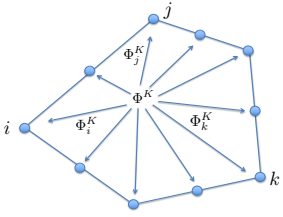
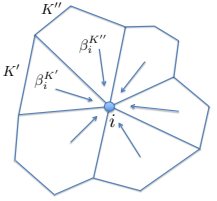
Matrix-free FEM framework

- *Diagonal mass matrix* and high-order:

$$\mathbf{D}\frac{d\mathbf{U}}{dt} + \mathbf{R} = \mathbf{0}$$

- No mass matrix $\Rightarrow$ No linear solver!
- Our ”matrix-free” idea is different from e.g. ”partial assembly” (avoids storing the matrix)

RD for steady problem $\nabla_x \cdot \mathbf{f}(U) = 0$

Step 1: Define the total residual on element K	Step 2: Compute the distribution coefficients β_i^K	Step 3: Gather the residuals at every DOF
		
$\Phi_i^{K,\alpha} = \int_K \nabla \cdot f(U_h)\varphi_i \, d\mathbf{x} + V_i^K$ $\sum_{i \in K} V_i^K = 0$ (1st order art. viscosity) $\Phi^K = \sum_{i \in K} \Phi_i^{K,\alpha} \equiv \int_K \nabla \cdot f(U_h)\, d\mathbf{x}$	$\Phi_i^K = \beta_i^K \Phi^K$ $\sum_{i \in K} \beta_i^K = 1$ Distribution coeff. β_i^K ensure upwinding, conservation and stabilization.	$\sum_{K \ni i} \Phi_i^K(U_h) = 0$ High-order scheme in space because Φ^K is high-order!

Computation of residuals

- Monotonicity-preserving residual (first order):

$$\Phi_i^{K,\alpha}(U_h) = -\int_K \nabla_x \varphi_i \cdot \mathbf{f}^h \, d\mathbf{x} + \int_{\partial K} \mathbf{f}^h \cdot \mathbf{n} \, \varphi_i \, d\gamma + \alpha_K (U_i - \bar{U}_K),$$

  where $\bar{U}_K = \frac{1}{N_K} \sum_{j \in K} U_j$, N_K is the number of DOFs in K, and

$$\alpha_K = \max_{i \in K} \rho\big(\nabla_{\mathbf{U}} \mathbf{f}(U)\big) \|\mathbf{n}_i\|, \quad \mathbf{n}_i = \int_K \nabla \varphi_i \, d\mathbf{x}.$$

  Here, $\rho(A)$ is the spectral radius of the matrix A.

- Higher order of accuracy + monotonicity is achieved e.g. by setting

$$\beta_i^K(U_h) = \frac{\max\left(\frac{\Phi_i^{K,\alpha}}{\Phi^K}, 0\right)}{\sum_{j \in K} \max\left(\frac{\Phi_j^{K,\alpha}}{\Phi^K}, 0\right)}.$$

- Later in this talk: alternative definition of β_i^K via invariant domain preservation

Matrix-free FEM for time-dependent problems

- Define a functional $\mathcal{L}$ to be

$$\mathcal{L}_i(U) = \left(\frac{\partial U}{\partial t} + \nabla_x \cdot \mathbf{f}(U), \varphi_i\right)_{L^2([t^n, t^{n+1}]\times\Omega)}. \tag{1}$$

- A high-order approximation of $\mathcal{L}$ is given by

$$\mathcal{L}_i^H(U) = \sum_j \mathbf{M}_{ij}\left(U_j(t^{n+1}) - U_j(t^n)\right) + \int_{t^n}^{t^{n+1}} \mathcal{I}_H\left(\int_\Omega \nabla_x \cdot \mathbf{f}(U_h)\,\varphi_i\,dx\right) dt. \tag{2}$$

- A low-order approximation of $\mathcal{L}$ is given by

$$\mathcal{L}_i^L(U) = \underbrace{\mathbf{D}_i\left(U_i(t^{n+1}) - U_i(t^n)\right)}_{\text{lumped mass matrix}} + \int_{t^n}^{t^{n+1}} \mathcal{I}_L\left(\int_\Omega \nabla_x \cdot \mathbf{f}(U_h)\,\varphi_i\,dx\right) dt. \tag{3}$$

A Useful Lemma[1]

Lemma

Let $\mathcal{L}^L, \mathcal{L}^H : \mathbb{R}^N \to \mathbb{R}^N$ be a pair of operators which satisfy the following conditions for any norm, $\|\cdot\|$, on $\mathbb{R}^N$.

1. *There exist at least one nontrivial element of $Ker(\mathcal{L}^H)$.*
2. *The operator $\mathcal{L}^L$ is invertible and coercive in the sense that there exist some $C_1 > 0$ such that for any $v, \bar{v} \in \mathbb{R}^N$ $C_1\|v - \bar{v}\| \leq \|\mathcal{L}^L v - \mathcal{L}^L \bar{v}\|$.*
3. *The operator $\mathcal{L}^L - \mathcal{L}^H$ has Lipschitz constant $C_2 \in (0, C_1)$.*

Then, the operator $\mathcal{L}^H$ is invertible and the unique element $y^* \in Ker(\mathcal{L}^H)$ can be obtained, for any initial guess with $m \in \mathbb{N}_0$, via the iteration $\mathcal{L}^L y^{(m+1)} = \mathcal{L}^L y^{(m)} - \mathcal{L}^H y^{(m)}$. The error of the iterative procedure is given by $\|y^{m+1} - y^*\| \leq \left(\frac{C_2}{C_1}\right)^{m+1} \|y^0 - y^*\|$.

[1] Abgrall 2017; Lohmann 2019; Kuzmin and Hajduk 2023.

High order in time + RD

- High order in time:
  - Define sub-steps on $[t_n, t_{n+1}]$: $t_n = t_{n,0} < t_{n,1} < t_{n,M} = t_{n+1}$.
  - Define $(U_{n,0}, \ldots, U_{n,M})$.

Iterative timestepping method (deferred-correction type)

$$\mathcal{L}^L(U_{n,m}^{(r+1)}) = \mathcal{L}^L(U_{n,m}^{(r)}) - \mathcal{L}^H(U_{n,m}^{(r)}), \quad m = 1, \ldots, M$$

- $\mathcal{L}^L$ – low order operator (explicit)
- $\mathcal{L}^H$ – high order operator (implicit)
- resulting timestepping method is **explicit and high order**

Definition of the low-order operator $\mathcal{L}^L$

For any $\sigma \in K$, define $\mathcal{L}^1_\sigma$ as:

$$\mathcal{L}^L_\sigma(U^{(r)}) = \mathcal{L}^L_\sigma(U^{n,1,r}, \dots, U^{n,M,r})$$
$$= \begin{pmatrix} |C_\sigma|\big(U^{n,M,r}_\sigma - U^{n,0}_\sigma\big) + \sum_{K|\sigma\in K} \int_{t_{n,0}}^{t_{n,M}} \mathcal{I}_L\big(\Phi^{K,\alpha}_\sigma(U^{(r)}), s\big)\, ds \\ \vdots \\ |C_\sigma|\big(U^{n,1,r}_\sigma - U^{n,0}_\sigma\big) + \sum_{K|\sigma\in K} \int_{t_{n,0}}^{t_{n,1}} \mathcal{I}_L\big(\Phi^{K,\alpha}_\sigma(U^{(r)}), s\big)\, ds \end{pmatrix},$$

In order to make the operator $\mathcal{L}^L_\sigma$ explicit in time, we set

$$\mathcal{I}_L\big(\Phi^{K,\alpha}_\sigma(U^{(r)}), s\big) = \Phi^{K,\alpha}_\sigma(U^{n,0}).$$

Definition of the high-order operator $\mathcal{L}^H$

The operator $\mathcal{L}^2_\sigma$ is defined as[2]

$$\mathcal{L}^H_\sigma(U^{(r)}) = \mathcal{L}^H_\sigma(U^{n,1,r}, \dots, U^{n,M,r})$$
$$= \begin{pmatrix} \sum_{K|\sigma\in K} \Big(\int_K \varphi_\sigma \big(U^{n,M,r}_\sigma - U^{n,0}_\sigma\big)\, d\mathbf{x} + \int_{t_{n,0}}^{t_{n,M}} \mathcal{I}_H\big(\Phi^{K,\alpha}_\sigma(U^{(r)}), s\big)\, ds \Big) \\ \vdots \\ \sum_{K|\sigma\in K} \Big(\int_K \varphi_\sigma \big(U^{n,1,r}_\sigma - U^{n,0}_\sigma\big)\, d\mathbf{x} + \int_{t_{n,0}}^{t_{n,1}} \mathcal{I}_H\big(\Phi^{K,\alpha}_\sigma(U^{(r)}), s\big)\, ds \Big) \end{pmatrix},$$

where $\mathcal{I}_H$ is the interpolating polynomial of degree M.

[2] R. Abgrall, P. Bacigaluppi, ST. High-order residual distribution scheme for the time-dependent Euler equations of fluid dynamics. *CAMWA, 2018*

Resulting high-order RD scheme

For $m = 1, \dots, M$:

$$|C_\sigma|\big(U_\sigma^{n,m,r+1} - U_\sigma^{n,m,r}\big) = -\sum_{K \ni \sigma} \beta_\sigma^K \sum_{\sigma' \in K} \Big(\int_K \varphi_{\sigma'}\big(U^{n,m,r} - U^{n,0}\big)\, d\mathbf{x} + \int_{t_{n,0}}^{t_{n,m}} \mathcal{I}_H\big(\Phi_{\sigma'}^{K,\alpha}(U^{n,0,r}), \dots, \Phi_{\sigma'}^{K,\alpha}(U^{n,M,r}), s\big)\, ds \Big)$$

$$\Phi_{\sigma'}^K = \text{red}$$

About β_i^K coefficients

- Definition commonly used since Abgrall & Roe 2003:

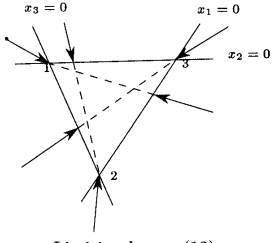
$$\beta_i^K(U_h) = \frac{\max\left(\hat{\beta}_i^K, 0\right)}{\sum_{j\in K} \max\left(\hat{\beta}_j^K, 0\right)}, \qquad \hat{\beta}_i^K = \frac{\Phi_i^{K,\alpha}}{\Phi^K}$$

- It was derived for 2D, $Q1$ triangles, for steady-state problems
- Seems to generalize and works OK in 2D with $Q1/Q2$ quads
- Drawback: accuracy suffers on higher-order elements in time-dependent problems
- In Part III of this talk: rethinking the meaning of β_i^K via convex limiting for arbitrary high order elements

Here, we simply offer two examples for the case $N = 3$, presenting the vectors $\boldsymbol{\beta} = (\beta_1, \beta_2, \beta_3)$ and $\hat{\boldsymbol{\beta}} = (\hat{\beta}_1, \hat{\beta}_2, \hat{\beta}_3)$ as the barycentric coordinates of a point in space with respect to an equilateral triangle. To ensure boundedness, we insist that, for all j, $0 \leqslant \hat{\beta}_j \leqslant 1$, so that the point $\boldsymbol{\beta}$ lies within the triangle, or on its boundary. A weaker condition, constraining the point $\boldsymbol{\beta}$ to a finite neighborhood of the triangle, seems possible but has not yet been explored.

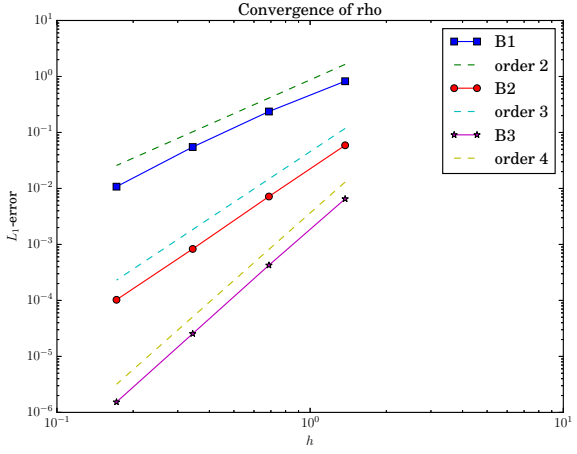
If the monotone weights are all positive, then $\boldsymbol{\beta}$ already lies within the triangle, and it is natural to take simply $\hat{\boldsymbol{\beta}} = \boldsymbol{\beta}$. If $\boldsymbol{\beta}$ lies outside the triangle, one possibility is simply to project $\boldsymbol{\beta}$ onto the boundary of the triangle. For example, we may take

$$\hat{\beta}_j = \frac{\beta_j^+}{\sum_j \beta_j^+} \quad \text{with} \quad x^+ = \max(0, x) \tag{12}$$



Limiting by eqn(12)

Convergence in 2D for Eulerian formulation: isentropic vortex[3]



[3] R. Abgrall, P. Bacigaluppi, ST. High-order residual distribution scheme for the time-dependent Euler equations of fluid dynamics. *CAMWA, 2018*

Part II: Lagrangian hydrodynamics[4]

[4] Credits: Steven Walton, Nathaniel Morgan

Lagrangian hydrodynamics

Consider the compressible Euler equations which, in the Lagrangian reference frame, with $\frac{\mathrm{d}}{\mathrm{d}t} := \partial_t + \boldsymbol{u} \cdot \nabla$ and $(t, \boldsymbol{x}) \in [0, T] \times \Omega_t \subseteq \mathbb{R}^+ \times \mathbb{R}^3$, $T > 0$ are given by the system

$$\begin{aligned} \frac{1}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}t} &= \nabla \cdot \boldsymbol{u} \\ \rho\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} &= \nabla \cdot \boldsymbol{\sigma} \\ \rho\frac{\mathrm{d}e}{\mathrm{d}t} &= \boldsymbol{\sigma} : \nabla \boldsymbol{u}, \end{aligned} \tag{4}$$

and are complemented by an equation of motion

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{u}, \tag{5}$$

where $\boldsymbol{x} = \boldsymbol{x}(t)$, $\boldsymbol{u} = \boldsymbol{u}(t, \boldsymbol{x})$, $e = e(t, \boldsymbol{x})$, $\rho = \rho(t, \boldsymbol{x})$ and $\boldsymbol{\sigma} = \sigma(t, \boldsymbol{x})$ denote the position, velocity, specific internal energy, density and the stress tensor, respectively.

FE discretization[5]

- kinematic space (d-dimensional) $\mathcal{V} \subset [H^1(\Omega_0)]^d$ with basis $\{\varphi_i\}_{i=1}^{N_u}$
- continuous FE for velocity:

$$u_h(\mathbf{X}, t) = \sum_{i=1}^{N_u} u_i(t)\varphi_i(\mathbf{X}),$$

  N_u — number of DOFs in Ω_0.
- thermodynamic space $\mathcal{E} \subset L_2(\Omega_0)$ with basis $\{\psi_j\}_{j=1}^{N_e}$
- piecewise-continuous elements for energy, so that on any mesh element K:

$$e_h^K(\mathbf{X}, t) = \sum_{j=1}^{N_e^K} e_j^K(t)\psi_j(\mathbf{X}),$$

  N_e^K — number of DOFs in K.

[5] V.A. Dobrev, T.V. Kolev, R.N. Rieben. High-order finite element methods for Lagrangian hydrodynamics. SIAM J. Sci. Comput. 34 (2012), 606–641.

Full System Discretization

- We can now write the fully discretized Euler equations.
- For $k = 0, \ldots, K$ and $m = 1, \ldots, M$

$$\begin{aligned} \mathcal{L}_i^L(\boldsymbol{u}_{n,m}^{(k+1)}) &= \mathcal{L}_i^L(\boldsymbol{u}_{n,m}^{(k)}) - \mathcal{L}_i^H(\boldsymbol{u}_{n,m}^{(k)}), \\ \mathcal{L}_i^L(e_{n,m}^{(k+1)}) &= \mathcal{L}_i^L(e_{n,m}^{(k)}) - \mathcal{L}_i^H(e_{n,m}^{(k)}), \\ \mathcal{L}^L(\boldsymbol{x}_{n,m}^{(k+1)}) &= \mathcal{L}^L(\boldsymbol{x}_{n,m}^{(k)}) - \mathcal{L}^H(\boldsymbol{x}_{n,m}^{(k)}), \\ \rho^{(k+1)} &= \rho_0 \frac{|\det \boldsymbol{J}_0|}{|\det \boldsymbol{J}_{n,m}^{(k+1)}|}. \end{aligned} \tag{6}$$

Second order in time

For $k = 0, 1$:

$$|m_i^{\mathcal{V}}|(u_i^{k+1} - u_i^k) + \sum_{K \ni i} \left\{ \mathcal{M}_i^{\mathcal{V}} \cdot (\boldsymbol{u}^k - \boldsymbol{u}^n) + \frac{\Delta t}{2} \left(\int_K \left(\nabla \cdot \boldsymbol{\sigma}^k + \nabla \cdot \boldsymbol{\sigma}^n \right) \varphi_i \, dx \right) \right\} = 0,$$

$$|m_i^{\mathcal{E}}|(e^{k+1} - e^k) + \sum_{K \ni i} \left\{ \mathcal{M}_i^{\mathcal{E}} \cdot (\boldsymbol{e}^k - \boldsymbol{e}^n) + \frac{\Delta t}{2} \left(\int_K \left((\sigma : \nabla \boldsymbol{u})^k + (\sigma : \nabla \boldsymbol{u})^n \right) \psi_i \, dx + \varepsilon_i^k + \varepsilon_i^n \right) \right\} = 0,$$

$$x_i^{k+1} - x_i^n - \Delta t \frac{u_i^k + u_i^n}{2} = 0.$$

Artificial Viscosity

- The stress tensor has the form
$$\sigma = -p\mathbf{I} + \sigma_a$$
- Let $\varepsilon = \frac{1}{2}(\nabla \boldsymbol{u} + \nabla^t \boldsymbol{u})$ denote the symmetric gradient tensor, c_s denotes the sound speed and $\ell = \ell(\boldsymbol{x})$ is a characteristic length. Following[6], we define the artificial viscosity to be
$$\boldsymbol{\sigma}_a = \mu\varepsilon.$$
The coefficient μ is a function defined at the quadrature points which we define to be
$$\mu = \mathcal{S}(a\delta\mathbf{u})\rho\ell\Big(bc_s + \ell|\delta\boldsymbol{u}^*|\Big)$$
where $\delta\boldsymbol{u}^* = \min_{\mathbf{x}} \delta\boldsymbol{u}(\boldsymbol{x})$, $\delta\boldsymbol{u}(\boldsymbol{x}) = \frac{(\boldsymbol{u}-\bar{\boldsymbol{u}})\cdot\varepsilon\cdot(\boldsymbol{u}-\bar{\boldsymbol{u}})}{\|\boldsymbol{u}-\bar{\boldsymbol{u}}\|^2}$ and $\bar{\boldsymbol{u}}$ denoting the velocity average.

[6] VonNeumann and Richtmyer 2004; Campbell and M.J. Shashkov 2001; CARAMANA and Loubère 2006; CARAMANA, Burton, et al. 1998; CARAMANA, M.J. Shashkov, and Whalen 1998; Lipnikov and M. Shashkov 2010.

Artificial Viscosity

- The coefficient function b is a measure of vorticity[7].
- The function

$$\mathcal{S}(a\delta\mathbf{u}) = \Big(1 + \exp(a\delta\mathbf{u})\Big)^{-1}$$

  serves a sigmoidal limiter on the artificial viscosity, with a a tuneable parameter defining the transition width of the activation function which is typically set to one.

- The length scale is is given $\ell(x) = \ell_0 \frac{\|J_0^{-1} J \cdot (\boldsymbol{u} - \bar{\boldsymbol{u}})\|}{\|\boldsymbol{u} - \bar{\boldsymbol{u}}\|}$, with the initial length $\ell_0 = \frac{1}{p}|H|^{1/3}$ the cubed root of the volume of an element $H \in \mathcal{H}$ in the initial configuration scaled by the inverse of the kinematic polynomial order.

[7] Dobrev, Kolev, and Rieben 2012.

Taylor-Green Vortex

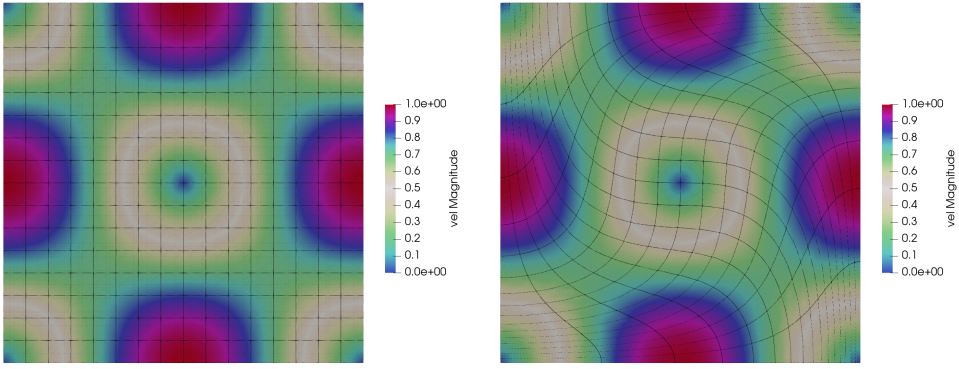


Figure: Q4Q3 simulation of the Taylor-Green Vortex. The mesh is 16x16x1. The velocity field is shown at $t = 0.0$ (left) and $t = 0.5$ (right).

Sedov

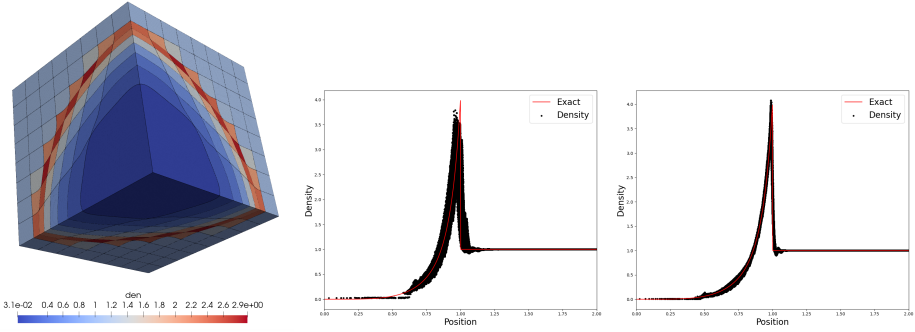


Figure: **Q4Q3** simulation of the Sedov problem. **Left:** Density (cell-averages). **Center:** Scatter plot of density at Gauss quadrature points. On an **8x8x8** mesh, we reach 94.6%of the analytic maximum peak. **Right:** Scatter plot of density at Gauss quadrature points. On a **16x16x16** mesh, we reach 101.5% of the analytic maximum peak.

Triple Point

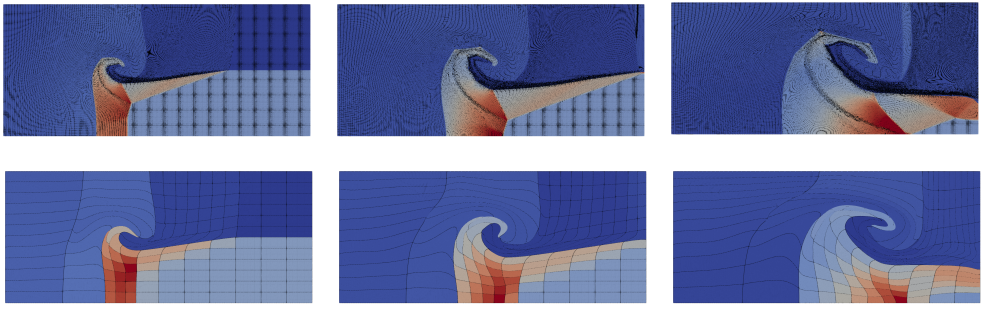


Figure: Density (cell averages) at $t = 2, 3$ and 4.3 for Triple Point problem. **Top:** Q1Q0 solution with $\sim$**173k** nodes. **Bottom:** Q4Q3 solution with $\sim$**12k** nodes.

Triple Point

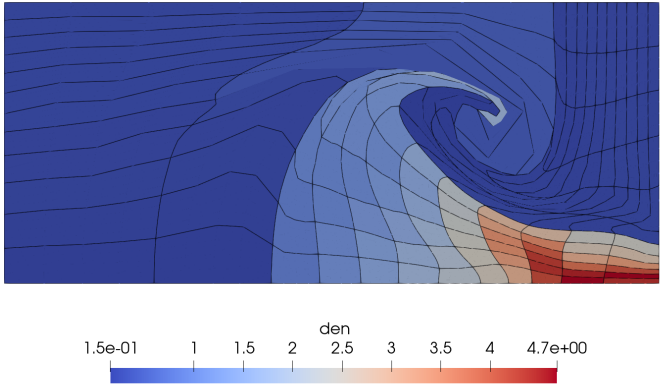


Figure: Q4Q3 simulation of the Triple Point problem. The mesh is 12x12x1. The cell-average density is shown at $t = 5.0$.

Part III: Structure-preserving matrix-free RD scheme[8]

[8] Credits: Jean-Luc Guermond, Eric Tovar, Matthias Maier, Steven Walton

Structure preserving RD scheme[9]

Structure preserving, or Invariant Domain Preserving (IDP) schemes ensure the following important properties at the discrete level:

- conservation
- positivity, bounds
- entropy inequality
- asymptotics, equilibria, etc.

IDP framework:

1. Construct a low-order (LO) RD scheme with provable IDP properties
2. Construct a high-order (HO) scheme possibly violating IDP properties
3. ”Blend” LO and HO schemes via convex limiting
4. Connection with β_i^K coefficients for RD framework

[9] Based on the work by Kuzmin, Guermond, et al.

Low-order scheme

LO IDP scheme based on graph viscosity approach of Guermond et al:

$$m_i \frac{u_i^{L,n+1} - u_i^n}{\tau} = -\sum_{j \in I(S_i)} f(u_j) c_{ij} + \overbrace{\sum_{j \in I(S_i)} d_{ij}^{L,n}(u_j^n - u_i^n)}^{\text{graph artificial viscosity}}, \tag{7}$$

where $m_i = \sum_{K \ni i} m_i^K = \sum_{K \ni i} \int_K \varphi_i \, d\mathbf{x}$, $c_{ij} = \int_D \varphi_i \nabla \varphi_j \, d\mathbf{x}$.
This scheme can be written in terms on residual distribution:

$$m_i \frac{u_i^{L,n+1} - u_i^n}{\tau} + \sum_{K \ni i} \beta_i^{K,L} \Phi^K = 0, \tag{8}$$

where

$$\Phi_i^{K,L} = \sum_{j \in K} \left[f(u_j) c_{ij}^K - d_{ij}^{K,L,n}(u_j^n - u_i^n) \right], \quad \beta_i^{K,L} = \frac{\Phi_i^{K,L}}{\Phi^K}, \quad \Phi^K = \sum_{j \in K} \Phi_j^{K,L} = \int_K \nabla \cdot f(u) \, d\mathbf{x}.$$

High-order scheme

HO scheme written in terms of residual distribution (lumped mass for now, can be modified to account for full mass matrix or DeC time iterations):

$$m_i \frac{u_i^{H,n+1} - u_i^n}{\tau} + \sum_{K \ni i} \beta_i^{K,H} \Phi^K = 0. \tag{9}$$

Here $\beta_i^{K,H}$ are high-order distribution coefficients TBD.

Take the difference between HO and LO schemes:

$$\begin{aligned} u_i^{H,n+1} &= 1 \cdot u_i^{L,n+1} - \frac{\tau}{m_i} \sum_{K \ni i} (\beta_i^{K,H} - \beta_i^{K,L}) \Phi^K \\ &= \sum_{K \ni i} \frac{m_i^K}{m_i} u_i^{L,n+1} + \frac{\tau}{m_i} \sum_{K \ni i} (\beta_i^{K,L} - \beta_i^{K,H}) \Phi^K \\ &= \sum_{K \ni i} \frac{m_i^K}{m_i} \left(u_i^{L,n+1} + \frac{\tau}{m_i^K} (\beta_i^{K,L} - \beta_i^{K,H}) \Phi^K \right) \end{aligned}$$

RD blending and IDP limiter

High-order update:

$$u_i^{H,n+1} = \sum_{K \ni i} \frac{m_i^K}{m_i} \left(u_i^{L,n+1} + \frac{\tau}{m_i^K} (\beta_i^{K,L} - \beta_i^{K,H}) \Phi^K \right) \tag{10}$$

RD schemes often use *blending* of high-order and low-order schemes by means of the distribution coefficients, namely, we can define

$$\beta_i^{K,H} = \theta^K \beta_i^{K,G} + (1 - \theta^K) \beta_i^{K,L}, \tag{11}$$

where

- $\beta_i^{K,G}$ corresponds to a high-order Galerkin scheme
- $\theta^K \in [0, 1]$ is the blending parameter
- $\theta^K = 0$ returns a low order scheme
- $\theta^K = 1$ returns a high-order scheme
- this blending preserves the conservation condition $\sum_{i \in K} \beta_i^{K,H} = 1$.

Substituting this blended coefficient for $\beta_i^{K,H}$ into (10), we get

$$
\begin{aligned}
u_i^{H,n+1} &= \sum_{K\ni i} \frac{m_i^K}{m_i}\Big(u_i^{L,n+1} + \frac{\tau}{m_i^K}(\beta_i^{K,L} - \beta_i^{K,H})\Phi^K\Big) \\
&= \sum_{K\ni i} \frac{m_i^K}{m_i}\Big(u_i^{L,n+1} + \frac{\tau}{m_i^K}(\beta_i^{K,L} - \theta^K\beta_i^{K,G} - (1-\theta^K)\beta_i^{K,L})\Phi^K\Big) \\
&= \sum_{K\ni i} \frac{m_i^K}{m_i}\Big(u_i^{L,n+1} + \frac{\tau}{m_i^K}(\cancel{\beta_i^{K,L}} - \theta^K\beta_i^{K,G} - \cancel{\beta_i^{K,L}} + \theta^K\beta_i^{K,L})\Phi^K\Big) \\
&= \sum_{K\ni i} \frac{m_i^K}{m_i}\underbrace{\Big(u_i^{L,n+1} + \theta^K\frac{\tau}{m_i^K}(\beta_i^{K,L} - \beta_i^{K,G})\Phi^K\Big)}_{\theta^K \text{ is the IDP limiter!}} \qquad (12)
\end{aligned}
$$

Conclusion

The RD blending parameter has the meaning of the IDP limiter, hence we can use standard techniques of Guermond et al to enforce IDP property in RD schemes!

IDP limiting[10]

High-order solution as a convex combination:

$$u_i^{H,n+1} = \sum_{K \ni i} \frac{m_i^K}{m_i} \left(u_i^{L,n+1} + \theta^K \frac{\tau}{m_i^K} (\beta_i^{K,L} - \beta_i^{K,G}) \Phi^K \right) = \sum_{K \ni i} \frac{m_i^K}{m_i} \underbrace{\left(u_i^{L,n+1} + \theta^K P_i^K \right)}_{\text{make IDP}} \tag{13}$$

Lemma (Guermond 2018)

Let $\Psi(u)$ be a quasi-concave function. Assume that the limiting parameters θ_K are such that $\Psi(u_i^{L,n+1} + \theta^K P_i^K) \geq 0$, then $\Psi(u_i^{H,n+1}) \geq 0$.

IDP limiter is defined by

$$\theta^K = \begin{cases} 1, & \text{if } \Psi(u_i^{L,n+1} + P_i^K) \geq 0, \\ \max\{\theta \in [0,1] \text{ s. t. } \Psi(u_i^{L,n+1} + \theta P_i^K) \geq 0\}, & \text{otherwise.} \end{cases}$$

[10] Guermond et al

Local bounds

- Line search is generally required to compute the limiter.
- There are a few exceptions, e.g. enforcing local bounds, leading to algebraic expressions for the limiter.
- Define the IDP functionals $\Psi_+ = u - u_i^{\min} \geq 0$ and $\Psi_- = u_i^{\max} - u \geq 0$.
  The limiter is given by

$$\theta^K = \begin{cases} \min\left(\dfrac{|u_i^{\min} - u_i^{L,n+1}|}{|P_i^K| + \epsilon}, 1\right), & \text{if } u_i^{L,n+1} + P_i^K < u_i^{\min} \\ 1, & \text{if } u_i^{\min} \leq u_i^{L,n+1} + P_i^K \leq u_i^{\max} \\ \min\left(\dfrac{u_i^{\max} - u_i^{L,n+1}}{|P_i^K| + \epsilon}, 1\right), & \text{if } u_i^{\max} < u_i^{L,n+1} + P_i^K \end{cases}$$

Sod problem

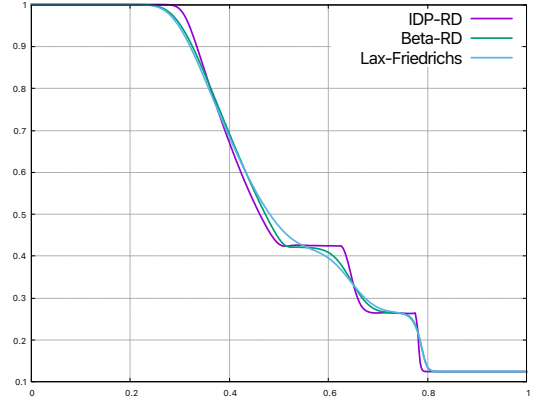


Figure: Sod shock tube test, 200 cells, quadratic Bernstein polynomials

Shu-Osher problem

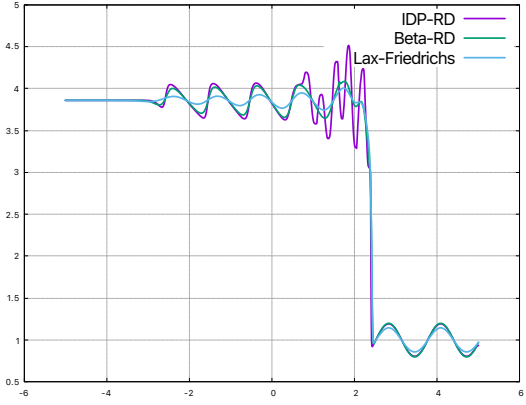


Figure: Shu-Osher test, 800 cells, quadratic Bernstein polynomials

Woodward-Colella problem

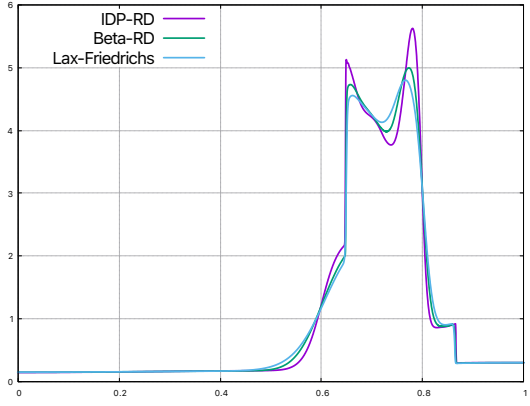


Figure: Woodward-Colella test, 1600 cells, quadratic Bernstein polynomials

Part IV (WIP): Advection-Diffusion Problems, IMEX, MRI...

Advection-Diffusion Problems

- 1D advection-diffusion equation

$$\frac{\partial v}{\partial t} + \frac{\partial f(v)}{\partial x} = \mu \frac{\partial^2 v}{\partial x^2}. \tag{14}$$

- The Galerkin residual is given by

$$\Phi_i^{K,\alpha} = \underbrace{\int_K (v_h^{n,m,k} - v_h^n)\varphi_i \, d\mathbf{x}}_{\text{additional term for time-dependent problems}} + \underbrace{\int_{t^n}^{t^{n,m}} \Big(\int_K \Big(\frac{\partial f(v)}{\partial x} - \mu \frac{\partial^2 v}{\partial x^2} \Big) \varphi_i \, d\mathbf{x} \Big) \, dt}_{\text{space-time integral}}.$$

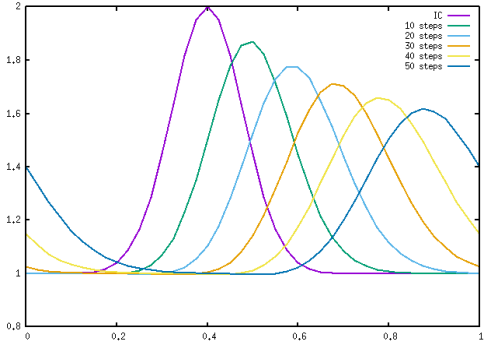
- The space-time RD scheme then results in an *explicit, matrix-free method*:

$$\boldsymbol{v}_i^{n,m,k+1} = \boldsymbol{v}_i^{m,n,k} - \frac{1}{|m_i|} \sum_{K \ni i} \Phi_i^K, \quad \text{where} \quad \Phi_i^K = \beta_i^K \Phi^K, \quad \Phi^K = \sum_{i \in K} \Phi_i^{K,\alpha}. \tag{15}$$

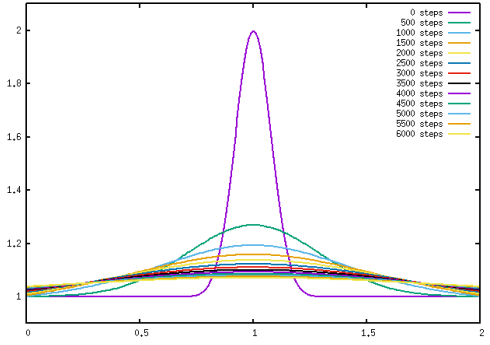
Results

Model advection-diffusion PDE:

$$u_t + au_x = \mu u_{xx} \tag{16}$$



advection-diffusion



pure diffusion

Convergence

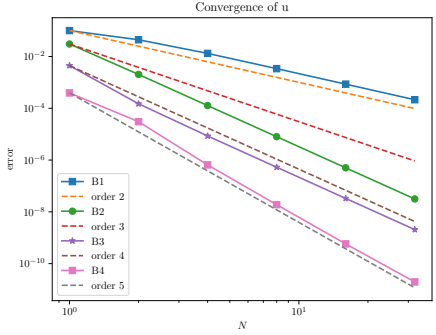


Figure: Convergence analysis for pure diffusion with RD solver.

Multirate time integration

$$y' = \underbrace{f^{\{s\}}(t,y)}_{\text{diffusion (slow) – Implicit}} + \underbrace{f^{\{f\}}(t,y)}_{\text{advection (fast) – DeC+MF-FEM}}$$

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A CLASS OF MULTIRATE INFINITESIMAL GARK METHODS*

ADRIAN SANDU†

Abstract. Differential equations arising in many practical applications are characterized by multiple time scales. Multirate time integration seeks to solve them efficiently by discretizing each scale with a different, appropriate time step, while ensuring the overall accuracy and stability of the numerical solution. In a seminal paper, Knoth and Wolke [*Appl. Numer. Math.*, 28 (1998), pp. 327–341] proposed a hybrid solution approach: discretize the slow component with an explicit Runge–Kutta method, and advance the fast component via a modified fast differential equation. The idea led to the development of multirate infinitesimal step (MIS) methods by Wensch, Knoth, and Galant [*BIT*, 49 (2009), pp. 449–473]. Günther and Sandu [*Numer. Math.*, 133 (2016), pp. 497–524] explained MIS schemes as a particular case of multirate General-structure Additive Runge–Kutta (MR-GARK) methods. The hybrid approach offers extreme flexibility in the choice of the numerical solution process for the fast component. This work constructs a family of multirate infinitesimal GARK schemes (MRI-GARK) that extends the hybrid dynamics approach in multiple ways. Order conditions theory and stability analyses are developed, and practical explicit and implicit methods of up to order four are constructed. Numerical results confirm the theoretical findings. We expect the new MRI-GARK family to be most useful for systems of equations with widely disparate time scales, where the fast process is dispersive, and where the influence of the fast component on the slow dynamics is weak.

$$y' = f(t,y) = f^{\{s\}}(t,y) + f^{\{f\}}(t,y), \qquad y(t_0) = y_0. \tag{1.1}$$

Definition 2.2 (MRI-GARK methods for additively partitioned systems). *A multirate infinitesimal GARK (MRI-GARK) scheme applied to the additively partitioned system* (1.1) *advances the solution from t_n to $t_{n+1} = t_n + H$ as follows:*

$$Y_1^{\{s\}} = y_n, \tag{2.2a}$$

$$\begin{cases} v(0) = Y_i^{\{s\}}, \\ T_i = t_n + c_i^{\{s\}} H, \\ v' = \Delta c_i^{\{s\}} f^{\{f\}}\left(T_i + \Delta c_i^{\{s\}}\theta,\, v\right) + \sum_{j=1}^{i+1} \gamma_{i,j}\left(\frac{\theta}{H}\right) f^{\{s\}}\left(T_j,\, Y_j^{\{s\}}\right) \\ \qquad \text{for } \theta \in [0,H], \\ Y_{i+1}^{\{s\}} = v(H), \qquad i = 1,\ldots,s^{\{s\}}, \end{cases} \tag{2.2b}$$

$$y_{n+1} = Y_{s^{\{s\}}+1}^{\{s\}}. \tag{2.2c}$$

Linear combinations of the slow function values are added as forcing to the modified fast ODE system (2.2b)*; in order to use only already computed slow stages, one needs $\gamma_{i,j}(\tau) = 0$ for $j > i$.*

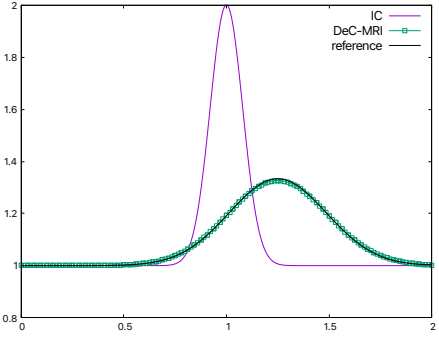
The implicit trapezoidal method is the slow component (2.1a) of the following second order *implicit* MRI-GARK scheme (2.2):

$$\begin{aligned} &v(0) = y_n; \quad v' = f^{\{f\}}(v) + f^{\{s\}}\left(y_n\right), \quad \theta \in [0,H]; \quad Y_2^{\{s\}} = v(H), \\ &y_{n+1} = Y_2^{\{s\}} - \tfrac{1}{2} f^{\{s\}}(y_n) + \tfrac{1}{2} f^{\{s\}}\left(y_{n+1}\right); \\ &\widehat{y}_{n+1} = Y_2^{\{s\}} - f^{\{s\}}(y_n) + f^{\{s\}}\left(y_{n+1}\right). \end{aligned} \tag{2.7}$$

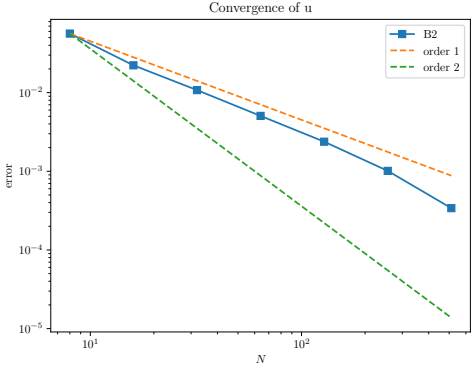
Results

Model advection-diffusion PDE:

$$u_t + a u_x = \mu u_{xx} \tag{17}$$



64 cells



convergence

Conclusions & work in progress...

1. RD is a flexible framework to construct high-order schemes for hyperbolic PDEs
2. Mass-matrix-free FEM
3. Easily extends to higher order in space and time
4. IDP property enforced via distribution coefficients
5. WIP: Consider more IDP functionals (e.g., entropy inequality)
6. WIP: 2D/3D
7. WIP: Lagrangian MF-FEM-IDP-RD

THANK YOU!