

New perspective on time stepping techniques: Beyond strong stability.

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Collaborators and acknowledgments

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Support:



Outline



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Invariant domains

Problems with SSP time stepping

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Cauchy problem

► Cauchy problem

$$\begin{aligned}\partial_t \mathbf{u} + \nabla \cdot (\mathbf{f}(\mathbf{u}) + \mathbf{g}(\mathbf{u}, \nabla \mathbf{u})) &= \mathbf{S}(\mathbf{u}), & (\mathbf{x}, t) \in D \times \mathbb{R}_+. \\ u(\mathbf{x}, 0) &= \mathbf{u}_0(\mathbf{x}), & \mathbf{x} \in D.\end{aligned}$$



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- ▶ $\mathbf{S} \in \mathcal{C}^1(\mathbb{R}^m; \mathbb{R}^{m \times d})$, source.
- ▶ \mathbf{u}_0 , admissible initial data.
- ▶ Periodic BCs or \mathbf{u}_0 has compact support (to simplify BCs)



Example 0: Scalar advection-diffusion-reaction

- ▶ Find u so that

$$\partial_t u + \nabla \cdot (\mathbf{f}(\mathbf{x}, u) - \kappa(u) \nabla u) - \mathbf{S}(u) = 0, \quad u(\cdot, 0) = u_0(\cdot),$$



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- ▶ For instance

$$\mathbf{S}(u) := \mu \phi(u) u(1 - u), \quad \text{with } \phi(u) \in C^0([0, 1]; [-1, 1]), \quad \mu \geq 0.$$



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- ▶ Fluxes

$$\mathbb{f}(\mathbf{u}) := \begin{cases} \mathbf{f}(u) \\ \beta \mathbf{x} \end{cases} \quad \text{with } \nabla \cdot \beta = 0$$

$$\mathbb{g}(\mathbf{u}, \nabla \mathbf{u}) := \kappa(u) \nabla u.$$



Example 1: Navier-Stokes

- ▶ Find $\mathbf{u} := (\rho, \mathbf{m}, E)^\top$ so that

$$\partial_t \rho + \nabla \cdot (\mathbf{v} \rho) = 0,$$

$$\partial_t \mathbf{m} + \nabla \cdot (\mathbf{v} \otimes \mathbf{m} + \rho(\mathbf{u})\mathbb{I} - \mathbb{S}(\mathbf{v})) = \mathbf{0},$$

$$\partial_t E + \nabla \cdot (\mathbf{v}(E + \rho(\mathbf{u})) - \mathbb{S}(\mathbf{v}) \cdot \mathbf{v} + \mathbf{q}(\mathbf{u})) = 0,$$

with $\mathbf{v} := \mathbf{m}/\rho$: velocity; $\rho(\mathbf{u})$: pressure.



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$$\mathbf{f}(\mathbf{u}) := \begin{pmatrix} \mathbf{v} \rho \\ \mathbf{v} \otimes \mathbf{m} + p(\mathbf{u}) \mathbb{I} \\ \mathbf{v}(E + p(\mathbf{u})) \end{pmatrix}, \quad \mathbf{g}(\mathbf{u}, \nabla \mathbf{u}) := \begin{pmatrix} 0 \\ -\mathbb{S}(\mathbf{v}) \\ -\mathbb{S}(\mathbf{v}) \cdot \mathbf{v} + \mathbf{q}(\mathbf{u}) \end{pmatrix}.$$



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- ▶ Possible definitions for \mathfrak{s} and \mathbf{q} :

$$\mathfrak{s}(\mathbf{v}) = 2\mu \mathbf{e}(\mathbf{v}) + (\lambda - \frac{2}{3}\mu)(\nabla \cdot \mathbf{v}) \mathbb{I}, \quad \mathbf{q}(\mathbf{u}) = -\kappa \nabla e(\mathbf{u}).$$



Example 2: Gray radiation hydrodynamics

- Find $\mathbf{u} := (\rho, \mathbf{m}, E, \mathcal{E}_R)^T$ so that

$$\partial_t \rho + \nabla \cdot (\mathbf{v} \rho) = 0,$$

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$$\partial_t \mathcal{E}_R + \nabla \cdot (\mathbf{v}(\mathcal{E}_R + p_R(\mathcal{E}_R))) - \mathbf{v} \cdot \nabla p_R(\mathcal{E}_R) - \nabla \cdot \left(\frac{c}{3\sigma_t} \nabla \mathcal{E}_R\right) = \sigma_a c (a_R T^4 - \mathcal{E}_R),$$

with \mathcal{E}_R : radiation energy; $p_R(\mathcal{E}_R)$: radiation pressure; $T(\mathbf{u})$:
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c : speed of light; σ_a, σ_t : absorption and total cross sections; $a_R := \frac{4\sigma}{c}$
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c : speed of light; σ_a, σ_t : absorption and total cross sections; $a_R := \frac{4\sigma}{c}$ radiation constant; σ the Stefan–Boltzmann constant.

- Possible definitions:

$$p_R(\mathcal{E}_R) := \frac{1}{3} \mathcal{E}_R; \quad c_v T = e(\mathbf{u}) := \frac{1}{\rho} (E - \frac{1}{2} \rho \mathbf{v}^2).$$



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Key assumption: existence of an invariant domain

- ▶ Let $\mathbf{u}_0 \in \mathcal{D}$.
- ▶ There exists a set $\mathcal{A} \subsetneq \mathbb{R}^m$, **convex** and depending on \mathbf{u}_0 , so that the “entropy” solution takes values in \mathcal{A} for a.e. $\mathbf{x} \in D$ and $t > 0$.

$$(\mathbf{u}_0(\mathbf{x}) \in \mathcal{A}, \forall \mathbf{x} \in D) \implies (\mathbf{u}(\mathbf{x}, t) \in \mathcal{A}, \forall \mathbf{x} \in D, \forall t > 0).$$

- ▶ This is a generalization of the maximum principle.



Examples

- ▶ Scalar conservation equations without reaction

$\mathcal{A} := [\operatorname{ess\,inf}_{x \in \mathbb{R}} u_0(x), \operatorname{ess\,sup}_{x \in \mathbb{R}} u_0(x)]$ is a convex subset of \mathbb{R}



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- ▶ Scalar conservation equations with $\mathbf{S}(u) := \mu\phi(u)u(1-u)$,

$$\mathcal{A} := [0, 1] \quad \text{is a convex subset of } \mathbb{R}$$



Examples

- ▶ Euler equations with specific entropy s

$$\mathcal{A} := \{\mathbf{u} := (\rho, \mathbf{m}, E) \in \mathbb{R}^{d+2} \mid \rho > 0, E - \frac{1}{2} \frac{\mathbf{m}^2}{\rho} > 0, s(\mathbf{u}) \geq \operatorname{ess\,inf}_{\mathbf{x} \in D} s(\mathbf{u}_0)\}$$

- ▶ Euler equations with Nobel Abel stiffen gas equation of state

$$\mathcal{A} := \{\mathbf{u} := (\rho, \mathbf{m}, E) \in \mathbb{R}^{d+2} \mid \rho > 0, \\ \frac{1}{1 - b\rho} (E - \frac{1}{2} \frac{\mathbf{m}^2}{\rho} - q) - p_\infty > 0, s(\mathbf{u}) \geq \operatorname{ess\,inf}_{\mathbf{x} \in D} s(\mathbf{u}_0)\}$$



Examples

- ▶ Navier-Stokes equations

$$\mathcal{A} := \{(\rho, \mathbf{m}, E) \in \mathbb{R}^{d+2} \mid \rho > 0, E - \frac{1}{2} \frac{\mathbf{m}^2}{\rho} > 0\}$$

- ▶ \mathcal{A} is convex in both cases.
- ▶ Invariant domain for the Euler equations is smaller than that for the Navier-Stokes equations.



Questions

- ▶ Hyperbolic and parabolic operators may have conflicting constraints.



Questions

- ▶ **Example 1: Navier-Stokes**
 - ▶ Euler: Conserved variables are natural for solving the hyperbolic problem
 - ▶ Navier-Stokes: primitive variables (velocity, internal energy) are more appropriate for the parabolic part.
 - ▶ The invariant domain of the Euler part is smaller than the invariant domain of the parabolic part.



Questions

- ▶ **Example 2:** Gray radiation hydrodynamics
 - ▶ Euler: Conserved variables $(\rho, \mathbf{m}, E, \mathcal{E}_R^{\frac{3}{4}})^T$.
 - ▶ Parabolic part: $(T, \mathcal{E}_R)^T$.
 - ▶ The invariant domain of the Euler part is smaller than the invariant domain of the parabolic part.



Questions

- ▶ How can one reconcile all these constraints?
- ▶ How can one construct approximation techniques in time **and** space that preserve invariant domains?
- ▶ Terminology: approximation methods that preserve invariant domains are called **Invariant domain preserving** (IDP)



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SSP (strong stability preserving)

- ▶ Approximate $\mathbf{u}(\mathbf{x}, t)$ in **space** with dofs in $\mathbb{R}^{m \times I}$.
- ▶ I : dimension of the approximation vector space (Finite elements (C^0 or dG), Finite Volume, Finite Differences, etc.).
- ▶ Let $\mathbf{F} : \mathbb{R}^{m \times I} \rightarrow \mathbb{R}^{m \times I}$ be approximation in space of $-\nabla \cdot \mathbf{f}(\mathbf{u})$.
(The way this is done does not matter here.)
- ▶ Semi-discrete problem: Find $\mathbf{U} \in C^1([0, T]; \mathbb{R}^{m \times I})$ s.t.

$$\mathbb{M} \partial_t \mathbf{U} = \mathbf{F}(\mathbf{U}), \quad \mathbf{U}(0) = \mathbf{U}_0.$$

\mathbb{M} : mass matrix (invertible)



SSP (strong stability preserving)

- ▶ Assume $\mathbf{U}_0 \in \mathcal{A}'$.



SSP (strong stability preserving)

- ▶ Assume $\mathbf{U}_0 \in \mathcal{A}'$.
- ▶ How can one construct time-stepping technique that guarantee $\mathbf{U}^n \in \mathcal{A}'$, for all $n \geq 0$?



SSP (strong stability preserving)

- ▶ Key idea by **Shu&Osher (1988)**

Use explicit Runge-Kutta methods where the final update is a **convex combination** of updates computed with the forward Euler method.



SSP (strong stability preserving)

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Use explicit Runge-Kutta methods where the final update is a **convex combination** of updates computed with the forward Euler method.

- ▶ **Key assumption:** (Forward Euler with low-order flux is invariant-domain preserving.) $\exists \Delta t^* > 0$ s.t. $\forall \Delta t \in (0, \Delta t^*)$ and $\forall \mathbf{V} \in \mathbb{R}^{m \times l}$

$$(\mathbf{V} \in \mathcal{A}^l) \implies (\mathbf{V} + \Delta t(\mathbb{M})^{-1}\mathbf{F}(\mathbf{V}) \in \mathcal{A}^l).$$

$\Leftrightarrow \mathcal{A}^l$ is invariant by the forward Euler method under the CFL condition $\Delta t \in (0, \Delta t^*)$.



SSP (strong stability preserving)

- ▶ Theory well understood now:
 - ▶ **Kraaijevanger (1991),**
 - ▶ **Spiteri-Ruuth (2002),**
 - ▶ **Ferracina-Spijker (2005),**
 - ▶ **Higuera (2005).**



Examples (for $\partial_t u = L(t, u)$)

► SSPRK(2,2)

α	β	γ
1	1	0
$\frac{1}{2}$ $\frac{1}{2}$	0 $\frac{1}{2}$	1

$$w^{(1)} := u^n + \Delta t L(t_n, u^n),$$

$$w^{(2)} := \frac{1}{2} u^n + \frac{1}{2} (w^{(1)} + \Delta t L(t_n + \Delta t, w^{(1)})),$$



Examples (for $\partial_t u = L(t, u)$)

► SSPRK(3,3)

α			β			γ
1			1			0
$\frac{3}{4}$	$\frac{1}{4}$		0	$\frac{1}{4}$		1
$\frac{1}{3}$	0	$\frac{2}{3}$	0	0	$\frac{2}{3}$	$\frac{1}{2}$

$$w^{(1)} := u^n + \Delta t L(t_n, u^n),$$

$$w^{(2)} := \frac{3}{4}u^n + \frac{1}{4}(w^{(1)} + \Delta t L(t_n + \Delta t, w^{(1)})),$$

$$w^{(3)} := \frac{1}{3}u^n + \frac{2}{3}(w^{(2)} + \Delta t L(t_n + \frac{1}{2}\Delta t, w^{(2)})),$$



Examples (for $\partial_t u = L(t, u)$)

► SSPRK(4,3)

α				β			γ
1				$\frac{1}{2}$			0
0	1			0	$\frac{1}{2}$		$\frac{1}{2}$
$\frac{2}{3}$	0	$\frac{1}{3}$		0	0	$\frac{1}{6}$	1
0	0	0	1	0	0	0	$\frac{1}{2}$

$$w^{(1)} := u^n + \frac{1}{2}\Delta t L(t_n, u^n),$$

$$w^{(2)} := w^{(1)} + \frac{1}{2}\Delta t L(t_n + \frac{1}{2}\Delta t, w^{(1)}),$$

$$w^{(3)} := \frac{2}{3}u^n + \frac{1}{3}(w^{(2)} + \frac{1}{2}\Delta t L(t_n + \Delta t, w^{(2)})),$$

$$w^{(4)} := w^{(3)} + \frac{1}{2}\Delta t L(t_n + \frac{1}{2}\Delta t, w^{(3)}),$$



Problems with SSPRK: Efficiency

Definition (Efficiency ratio)

- ▶ Let τ^* maximal time step that makes the forward Euler method IDP.
- ▶ Let $\tilde{\tau}$ be the maximal time step that makes some s -stage ERK method IDP as well.
- ▶ We call *efficiency ratio* of the s -stage ERK method the ratio
$$c_{\text{eff}} := \frac{\tilde{\Delta}t}{s\Delta t^*}. \quad (\text{Usually } c_{\text{eff}} \leq 1.)$$

Proposition

Under the same CFL constraint, the number of flux evaluations of SSPRK(s, p) is equal to $\frac{1}{c_{\text{eff}}} \times$ that of the forward Euler method.



Problems with SSPRK: Efficiency

Examples

- ▶ $c_{\text{eff}} = \frac{1}{2}$ for SSPRK(2,2).
- ▶ $c_{\text{eff}} = \frac{1}{3}$ for SSPRK(3,3).
- ▶ $c_{\text{eff}} = \frac{1}{2}$ for SSPRK(4,3).



Problems with SPPRK: Efficiency

- ▶ *SSPRK* methods are usually **inefficient!**
- ▶ The most **popular method** *SSPRK*(3,3) is actually one of the most **inefficient!**



Some optimal methods

- ▶ Four-stages, third-order, **AE, JLG (2022)**.

$$\begin{array}{c|ccc} 0 & 0 & & \\ \frac{1}{4} & \frac{1}{4} & 0 & \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ \frac{3}{4} & 0 & \frac{1}{4} & \frac{1}{2} \\ \hline 1 & 0 & \frac{2}{3} & -\frac{1}{3} \quad \frac{2}{3} \end{array}$$

- ▶ Five-stages, fourth-order, **AE, JLG (2022)**.

0	0				
1/4	0.2				
1/2	0.2607558226955500	0.1392441773044501			
3/4	-0.2585651787257025	0.9113627416628056	-0.0527975629371033		
1	0.2162327643150383	0.5153422309960234	-0.8166279419926541	0.8850529466815924	
1	-0.1051167845469190	0.8788004715210083	-0.5890340406148447	0.4621338048543404	0.3532165487864



Problems with SPPRK: Accuracy

- ▶ Accuracy of *SSPRK* methods restricted to fourth-order if one insists on never stepping backward in time, **Ruuth, Spiteri (2002)**.



Problems with SSPRK: extensions to IMEX methods

- ▶ The *SSPRK* paradigm cannot be easily modified to accommodate implicit and explicit sub-steps.
- ▶ Implicit RK schemes of order 2 and above cannot be SSP, **Gottlieb, Shu, Tadmor (2001)**
- ▶ Some alternatives:
 - ▶ SSP Explicit methods \Rightarrow Parabolic time step restriction $\Delta t \leq ch^2$; see **Zhang & Shu (2017)**
 - ▶ Using two derivatives **Gottlieb, Grant, Hu, Shu (2022)**



Problems with SPPRK: extensions to IMEX methods

Example (Compressible Navier-Stokes)

- ▶ Difficulties: conflicting invariant sets and conflicting variables.
- ▶ Which invariant domain to preserve?
 - ▶ Minimum entropy principle is **true** for Euler.
 - ▶ Minimum entropy principle is **false** for NS.
- ▶ Which variable should be used?
 - ▶ “Right variable” for Euler is $\mathbf{u} = (\rho, \mathbf{m}, E)$ (conserved variables).
 - ▶ “Right variable” for NS is (ρ, \mathbf{v}, e) (primitive variables).
 - ▶ Some advocate “entropy variable” and “entropy stability”. Why?
- ▶ How to do the explicit-implicit time stepping?
- ▶ How linearization should be done in the implicit substeps?
 - ▶ Most “IMEX” methods cannot make the difference between conserved and primitive variables.
 - ▶ Most “IMEX” methods cannot be properly linearized and be conservative (no generic theory).



Problems with SPPRK: extensions to IMEX methods

- ▶ **Conclusion:** One needs a new paradigm.



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IDPERK

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Peep under the hood of SSPRK

- ▶ The beauty of SSPRK methods is that the forward Euler sub-step is a **black box**.
- ▶ The black box invokes **two** fluxes (not just one as one might think):
 - ▶ Low-order (in space) \mathbf{F}^L , low-order mass matrix \mathbf{M}^L
 - ▶ High-order (in space) \mathbf{F}^H , low-order mass matrix \mathbf{M}^H
- ▶ Ideally, one would like to solve

$$\mathbf{M}^H \partial_t \mathbf{U} = \mathbf{F}^H(\mathbf{U})$$

since the space approximation is accurate, but this method **violates** the invariant-domain property.



Peep under the hood of SSPRK

Key assumptions

- ▶ **Assumption 1:** (Forward Euler with low-order flux is invariant-domain preserving.) Assume $\exists \Delta t^* > 0$ so that for all $\Delta t \in (0, \Delta t^*)$ for all $\mathbf{V} \in \mathbb{R}^{m \times l}$

$$(\mathbf{V} \in \mathcal{A}^l) \implies (\mathbf{V} + \Delta t(\mathbb{M}^L)^{-1} \mathbf{F}^L(\mathbf{V}) \in \mathcal{A}^l).$$



Peep under the hood of SSPRK

Key assumptions

- ▶ **Assumption 2:** There exists a nonlinear limiting operator $\ell : \mathcal{A}' \times (\mathbb{R}^m)' \times (\mathbb{R}^m)' \rightarrow (\mathbb{R}^m)'$ such that for all $(\mathbf{V}, \boldsymbol{\Phi}^L, \boldsymbol{\Phi}^H)$

$$(\mathbf{V} + \Delta t(\mathbb{M}^L)^{-1}\boldsymbol{\Phi}^L \in \mathcal{A}') \implies (\ell(\mathbf{V}, \boldsymbol{\Phi}^L, \boldsymbol{\Phi}^H) \in \mathcal{A}').$$



Peep under the hood of SSPRK

Key assumptions

- ▶ **Assumption 2:** There exists a nonlinear limiting operator $\ell : \mathcal{A}' \times (\mathbb{R}^m)^l \times (\mathbb{R}^m)^l \rightarrow (\mathbb{R}^m)^l$ such that for all $(\mathbf{V}, \boldsymbol{\Phi}^L, \boldsymbol{\Phi}^H)$

$$(\mathbf{V} + \Delta t(\mathbb{M}^L)^{-1}\boldsymbol{\Phi}^L \in \mathcal{A}') \implies (\ell(\mathbf{V}, \boldsymbol{\Phi}^L, \boldsymbol{\Phi}^H) \in \mathcal{A}').$$

- ▶ Key idea: $\ell(\mathbf{V}, \boldsymbol{\Phi}^L, \boldsymbol{\Phi}^H)$ is defined as convex combination of $\mathbf{V} + \Delta t(\mathbb{M}^L)^{-1}\boldsymbol{\Phi}^H$ and $\mathbf{V} + \Delta t(\mathbb{M}^L)^{-1}\boldsymbol{\Phi}^L$.



Peep under the hood of SSPRK

- ▶ Given \mathbf{U}^n in the invariant set \mathcal{A}' (approximation at time t^n),
- ▶ The forward Euler step proceeds as follows:
 - ▶ Compute low-order flux $\mathbf{F}^L(\mathbf{U}^n)$
 - ▶ Compute high-order flux $\mathbf{F}^H(\mathbf{U}^n)$
 - ▶ Compute update \mathbf{U}^{n+1} by limiting

$$\mathbf{U}^{n+1} := \ell(\mathbf{U}^n, \mathbf{F}^L(\mathbf{U}^n), \mathbf{F}^H(\mathbf{U}^n)).$$

Theorem (IDP Explicit Euler)

Let Assumptions 1 and 2 be met. Assume $\mathbf{U}^n \in \mathcal{A}'$, then $\mathbf{U}^{n+1} \in \mathcal{A}'$ for all $\Delta t \in (0, \Delta t^*)$.



Key idea of invariant-domain-preserving ERK

- ▶ Externalize the limiting process at each RK sub-step.



Details for s -stage ERK method

- ▶ Consider Butcher tableau for s -stage method

$$\begin{array}{c|cccccc} c_1 & 0 & & & & \\ c_2 & a_{2,1} & 0 & & & \\ c_3 & a_{3,1} & a_{3,2} & 0 & & \\ \vdots & \vdots & & \ddots & \ddots & \\ c_s & a_{s,1} & a_{s,2} & \cdots & a_{s,s-1} & 0 \\ \hline & b_1 & b_2 & \cdots & b_{s-1} & b_s \end{array}$$

- ▶ Rename last line, set $c_1 = 0$ and $c_{s+1} = 1$.

$$\begin{array}{c|cccccc} 0 & 0 & & & & \\ c_2 & a_{2,1} & 0 & & & \\ c_3 & a_{3,1} & a_{3,2} & 0 & & \\ \vdots & \vdots & & \ddots & \ddots & \\ c_s & a_{s,1} & a_{s,2} & \cdots & a_{s,s-1} & 0 \\ 1 & a_{s+1,1} & a_{s+1,2} & \cdots & a_{s+1,s-1} & a_{s+1,s} \end{array}$$


Details

- ▶ Assume $c_k \geq 0$ for all $k \in \{1:s+1\}$.
- ▶ For sake of simplicity assume $c_{l-1} \leq c_l, \forall l \in \{2:s+1\}$, and set

$$l'(l) := l - 1.$$

(Otherwise set $l'(l) := \max\{k < l \mid c_l - c_k \geq 0\}$.)



Details

- ▶ Let $\mathbf{U}^n \in \mathcal{A}^l$.
- ▶ Set $\mathbf{U}^{n,1} := \mathbf{U}^n$.
- ▶ Loop over $l \in \{2:s+1\}$.
- ▶ Compute first-order update starting from $\mathbf{U}^{n,l'}$ (think of $l' = l-1$)

$$\mathbb{M}^L \mathbf{U}^{L,l} := \mathbb{M}^L \mathbf{U}^{n,l'} + \Delta t (c_l - c_{l'}) \mathbf{F}^L(\mathbf{U}^{n,l'}).$$

- ▶ Compute high-order ERK update starting from \mathbf{U}^n

$$\mathbb{M}^H \mathbf{U}^{H,l} := \mathbb{M}^H \mathbf{U}^n + \Delta t \sum_{k \in \{1:l-1\}} a_{l,k} \mathbf{F}^H(\mathbf{U}^{n,k}).$$



Details

- ▶ Let $\mathbf{U}^n \in \mathcal{A}^l$.
- ▶ Set $\mathbf{U}^{n,1} := \mathbf{U}^n$.
- ▶ Loop over $l \in \{2:s+1\}$.
- ▶ Compute first-order update starting from $\mathbf{U}^{n,l'}$ (think of $l' = l-1$)

$$\mathbb{M}^L \mathbf{U}^{L,l} := \mathbb{M}^L \mathbf{U}^{n,l'} + \Delta t (c_l - c_{l'}) \mathbf{F}^L(\mathbf{U}^{n,l'}).$$

- ▶ Compute high-order ERK update starting from \mathbf{U}^n

$$\mathbb{M}^H \mathbf{U}^{H,l} := \mathbb{M}^H \mathbf{U}^n + \Delta t \sum_{k \in \{1:l-1\}} a_{l,k} \mathbf{F}^H(\mathbf{U}^{n,k}).$$

- ▶ **Incompatibility** of the starting points ($\mathbf{U}^{n,l'} \neq \mathbf{U}^n$ in general).



Details

- ▶ Let $\mathbf{U}^n \in \mathcal{A}^l$.
- ▶ Set $\mathbf{U}^{n,1} := \mathbf{U}^n$.
- ▶ Loop over $l \in \{2:s+1\}$.
- ▶ Compute first-order update starting from $\mathbf{U}^{n,l'}$ (think of $l' = l-1$)

$$\mathbb{M}^L \mathbf{U}^{L,l} := \mathbb{M}^L \mathbf{U}^{n,l'} + \Delta t (c_l - c_{l'}) \mathbf{F}^L(\mathbf{U}^{n,l'}).$$

- ▶ Compute high-order ERK update starting from \mathbf{U}^n

$$\mathbb{M}^H \mathbf{U}^{H,l} := \mathbb{M}^H \mathbf{U}^n + \Delta t \sum_{k \in \{1:l-1\}} a_{l,k} \mathbf{F}^H(\mathbf{U}^{n,k}).$$

- ▶ **Incompatibility** of the starting points ($\mathbf{U}^{n,l'} \neq \mathbf{U}^n$ in general).
- ▶ Subtract ERK update at $t^n + c_l \Delta t$ from ERK update at $t^n + c_{l'} \Delta t$

$$\implies \boxed{\mathbb{M}^H \mathbf{U}^{H,l} = \mathbb{M}^H \mathbf{U}^{H,l'} + \Delta t \sum_{k \in \{1:l-1\}} (a_{l,k} - a_{l',k}) \mathbf{F}^H(\mathbf{U}^{n,k}).}$$



Details

- ▶ Replace $\mathbf{U}^{H,l'}$ (which is not IDP) by $\mathbf{U}^{n,l'}$ (which is IDP by induction assumption).
- ▶ Final scheme

$$\mathbb{M}^L \mathbf{U}^{L,l} := \mathbb{M}^L \mathbf{U}^{n,l'} + \Delta t \underbrace{(c_l - c_{l'})}_{\Phi^L} \mathbf{F}^L(\mathbf{U}^{n,l'}).$$

$$\mathbb{M}^H \mathbf{U}^{H,l} := \mathbb{M}^H \mathbf{U}^{n,l'} + \Delta t \underbrace{\sum_{k \in \{1:l-1\}} (a_{l,k} - a_{l',k}) \mathbf{F}^H(\mathbf{U}^{n,k})}_{\Phi^H}.$$

$$\mathbf{U}^{n,l} := \ell(\mathbf{U}^{n,l'}, \Phi^L, \Phi^H).$$

- ▶ Set $\mathbf{U}^{n+1} := \mathbf{U}^{n,s+1}$.



Details

Theorem

Assume that $\mathbf{U}^n \in \mathcal{A}^I$. Then $\mathbf{U}^{n+1} \in \mathcal{A}^I$ for all $\Delta t \in (0, \frac{\Delta t^*}{\max_{I \in \{2:s+1\}} (c_I - c_{I'})})$.

Corollary

- ▶ $c_{\text{ef}} = \frac{1}{s \max_{I \in \{2:s+1\}} (c_I - c_{I'})}$.
- ▶ The complexity of the ERK method is optimal if the points $\{c_I\}_{I \in \{1:s+1\}}$ are *equi-distributed* in $[0, 1]$.



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Examples (optimal methods)

$$\begin{array}{c|cc} 0 & 0 & \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline 1 & 0 & 1 \end{array}$$

RK(2,2;1)

$$\begin{array}{c|ccc} 0 & 0 & & \\ \frac{1}{3} & \frac{1}{3} & 0 & \\ \frac{2}{3} & 0 & \frac{2}{3} & 0 \\ \hline 1 & \frac{1}{4} & 0 & \frac{3}{4} \end{array}$$

RK(3,3;1)

$$\begin{array}{c|cccc} 0 & 0 & & & \\ \frac{1}{4} & \frac{1}{4} & 0 & & \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & \\ \frac{3}{4} & 0 & \frac{1}{4} & \frac{1}{2} & 0 \\ \hline 1 & 0 & \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \end{array}$$

RK(4,3;1)



Examples SSPRK (sub-optimal methods)

$$\begin{array}{c|cc} 0 & 0 & \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

SSPRK(2,2; $\frac{1}{2}$)

$$\begin{array}{c|ccc} 0 & 0 & & \\ 1 & 1 & 0 & \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{4} & 0 \\ \hline & \frac{1}{6} & \frac{1}{6} & \frac{2}{3} \end{array}$$

SSPRK(3,3; $\frac{1}{3}$)



Examples: popular RK4 (left) and 3/8 rule (right)

0		0			
$\frac{1}{2}$		$\frac{1}{2}$	0		
$\frac{1}{2}$		0	$\frac{1}{2}$	0	
1		0	0	1	0
<hr/>					
1		$\frac{1}{6}$	$\frac{2}{6}$	$\frac{2}{6}$	$\frac{1}{6}$

RK(4,4; $\frac{1}{2}$)

0		0			
$\frac{1}{3}$		$\frac{1}{3}$	0		
$\frac{2}{3}$		$-\frac{1}{3}$	1	0	
1		1	-1	1	0
<hr/>					
1		$\frac{1}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{1}{8}$

RK(4,4; $\frac{3}{4}$)



Examples RK5 methods: Equi-distributed (left), Butcher's method (right)

0	0					
$\frac{1}{5}$	$\frac{1}{5}$	0				
$\frac{2}{5}$	0	$\frac{2}{5}$	0			
$\frac{3}{5}$	$\frac{3}{20}$	0	$\frac{9}{20}$	0		
$\frac{4}{5}$	$\frac{4}{5}$	$-\frac{8}{5}$	$\frac{8}{5}$	0	0	
1	$-\frac{71}{4}$	40	$-\frac{75}{4}$	-10	$\frac{15}{2}$	0
1	$\frac{17}{144}$	0	$\frac{25}{36}$	$-\frac{25}{72}$	$\frac{25}{48}$	$\frac{1}{72}$

RK(6,5; $\frac{5}{6}$)

0	0					
$\frac{1}{4}$	$\frac{1}{4}$	0				
$\frac{1}{4}$	$\frac{1}{8}$	$\frac{1}{8}$	0			
$\frac{1}{2}$	0	$-\frac{1}{2}$	1	0		
$\frac{3}{4}$	$\frac{3}{16}$	0	0	$\frac{9}{16}$	0	
1	$-\frac{3}{7}$	$\frac{2}{7}$	$\frac{12}{7}$	$-\frac{12}{7}$	$\frac{8}{7}$	0
1	$\frac{7}{90}$	0	$\frac{32}{90}$	$\frac{12}{90}$	$\frac{32}{90}$	$\frac{7}{90}$

RK(6,5; $\frac{2}{3}$)



Convergence tests

- ▶ All the tests are done with

$$\Delta t := \text{CFL} \times s \times \Delta t^*,$$

- ▶ \Rightarrow All the methods perform exactly the same number of time steps independently of s (i.e., number of flux evaluations is constant).



1D linear transport, 4th-order FD

- ▶ 4th-order FD in space.
- ▶ Linear transport $D = (0, 1)$

$$\partial_t u + \partial_x u = 0, \quad u_0(x) := \begin{cases} \left(4 \frac{(x-x_0)(x_1-x)}{x_1-x_0}\right)^6 & x \in (x_0 := 0.1, x_1 := 0.4) \\ 0 & \textit{otherwise} \end{cases}$$

- ▶ **Local** maximum/minimum principle guaranteed **at every grid point**.
- ▶ Global maximum and minimum also **exactly enforced**.
- ▶ All errors computed in L^∞ -norm.



1D linear transport, 4th-order FD

Table: Second-order methods (SSPRK(2,2) behaves badly).

l	CFL = 0.2				CFL = 0.25			
	RK(2,2;1)	rate	RK(2,2; $\frac{1}{2}$)	rate	RK(2,2;1)	rate	RK(2,2; $\frac{1}{2}$)	rate
50	4.72E-02	–	1.23E-01	–	4.91E-02	–	1.30E-01	–
100	2.81E-03	4.07	1.50E-02	3.03	4.51E-03	3.44	4.32E-02	1.60
200	1.16E-03	1.28	1.24E-03	3.60	2.01E-03	1.17	2.14E-03	4.34
400	3.38E-04	1.78	3.47E-04	1.84	5.41E-04	1.89	5.67E-04	1.91
800	8.79E-05	1.94	9.28E-05	1.90	1.38E-04	1.97	1.48E-04	1.94
1600	2.22E-05	1.98	2.33E-05	1.99	3.47E-05	1.99	3.78E-05	1.97
3200	5.58E-06	1.99	5.92E-06	1.98	8.73E-06	1.99	5.36E-05	-5.0



1D linear transport, 4th-order FD

Table: Third-order methods (SSPRK(3,3) behaves badly).

l	CFL = 0.05						CFL = 0.25					
	RK(3,3;1) rate		RK(3,3; $\frac{1}{3}$) rate		RK(4,3;1) rate		RK(3,3;1) rate		RK(3,3; $\frac{1}{3}$) rate		RK(4,3;1) rate	
50	5.15E-02	-	4.76E-02	-	5.15E-02	-	5.48E-02	-	1.55E-01	-	6.08E-02	-
100	5.41E-03	3.25	5.41E-03	3.14	5.41E-03	3.25	5.15E-03	3.41	6.12E-02	1.35	6.15E-03	3.31
200	3.79E-04	3.83	3.79E-04	3.83	3.79E-04	3.83	3.92E-04	3.72	1.07E-03	5.84	3.83E-04	4.01
400	2.27E-05	4.06	2.27E-05	4.06	2.27E-05	4.06	2.89E-05	3.76	2.18E-04	2.29	2.30E-05	4.06
800	1.58E-06	3.85	1.58E-06	3.85	1.58E-06	3.85	3.20E-06	3.18	6.41E-05	1.77	1.59E-06	3.85
1600	9.12E-08	4.12	1.22E-07	3.69	8.13E-08	4.28	8.23E-07	1.96	1.83E-05	1.81	8.25E-08	4.27
3200	1.52E-08	2.58	6.84E-08	0.84	5.31E-09	3.94	2.40E-07	1.78	5.39E-06	1.76	5.39E-09	3.94



1D linear transport, 4th-order FD

Table: Fourth-order methods (SSPRK(5,4) behaves badly).

l	CFL = 0.05						CFL = 0.2					
	RK(4,4; $\frac{1}{2}$)	rate	RK ‡ (5,4; $\frac{1}{2}$)	rate	RK(5,4;1)	rate	RK(4,4; $\frac{1}{2}$)	rate	RK ‡ (5,4; $\frac{1}{2}$)	rate	RK(5,4;1)	rate
50	4.32E-02	-	5.37E-02	-	5.95E-02	-	1.26E-01	-	5.63E-02	-	5.55E-02	-
100	5.41E-03	3.00	5.09E-03	3.40	5.09E-03	3.54	1.65E-02	2.93	7.82E-03	2.85	5.72E-03	3.28
200	3.79E-04	3.84	3.04E-04	4.07	3.04E-04	4.07	4.10E-04	5.33	3.80E-04	4.36	3.82E-04	3.90
400	2.27E-05	4.06	1.91E-05	3.99	1.91E-05	3.99	5.02E-05	3.03	2.27E-05	4.06	2.29E-05	4.06
800	1.58E-06	3.85	1.19E-06	4.00	1.19E-06	4.00	1.10E-05	2.19	1.79E-06	3.67	1.60E-06	3.84
1600	8.13E-08	4.28	7.45E-08	4.00	7.45E-08	4.00	2.70E-06	2.03	3.66E-07	2.29	8.26E-08	4.28
3200	5.36E-09	3.92	4.65E-09	4.00	4.65E-09	4.00	7.69E-07	1.81	9.29E-08	1.98	5.38E-09	3.94



1D linear transport, 4th-order FD

Table: Fifth-order methods, error in the L^∞ -norm.

l	CFL = 0.02				CFL = 0.025			
	RK(6,5; $\frac{1}{3}$)	rate	RK(7,5;1)	rate	RK(6,5; $\frac{2}{3}$)	rate	RK(7,5;1)	rate
50	5.19E-02	–	5.19E-02	–	5.19E-02	–	5.19E-02	–
100	5.41E-03	3.26	5.41E-03	3.26	5.41E-03	3.26	5.41E-03	3.26
200	3.79E-04	3.83	3.79E-04	3.83	3.79E-04	3.84	3.79E-04	3.83
400	2.27E-05	4.06	2.27E-05	4.06	2.27E-05	4.06	2.27E-05	4.06
800	1.58E-06	3.85	1.58E-06	3.85	1.58E-06	3.85	1.58E-06	3.85
1600	8.48E-08	4.22	8.13E-08	4.28	8.71E-08	4.18	8.13E-08	4.28
3200	7.10E-09	3.58	5.92E-09	3.78	1.16E-08	2.91	5.56E-09	3.87



2D linear transport, \mathbb{P}_1 FE (3th-order super-convergent)

- ▶ \mathbb{P}_1 finite elements in space (4th-order super-convergence on uniform meshes).
- ▶ Linear transport $D := (0, 1)^2$ with $\beta := (0.9, 1)^T$

$$\partial_t u + \nabla \cdot (\beta u) = 0, \quad u_0(\mathbf{x}) := \begin{cases} \left(4 \frac{(x-x_0)(x_1-x)}{x_1-x_0}\right)^4 \times \left(4 \frac{(y-y_0)(y_1-y)}{y_1-y_0}\right)^4 & \mathbf{x} \in D_0 \\ 0 & \text{oth.} \end{cases}$$

with $D_0 = \{x_0 \leq x \leq x_1, y_0 \leq y \leq y_1\}$, $x_0 = y_0 = 0.1$, $x_1 = y_1 = 0.4$.

- ▶ Local maximum/minimum principle guaranteed at every grid point.
- ▶ Global maximum and minimum also exactly enforced.
- ▶ All errors computed at $T = 0.5$



2D linear transport, \mathbb{P}_1 FE (4th-order super-convergent)

Table: Relative error L^1 -norm, $T = 0.5$. CFL = 0.4, second-order; CFL = 0.7 third-order; CFL = 0.5 fourth-order; CFL = 0.4 fifth-order.

l	RK(2,1;1)	rate	RK ‡ (2,2; $\frac{1}{2}$)	rate
50	2.96E-02	-	3.91E-02	-
100	7.36E-03	2.01	7.47E-03	2.39
200	1.94E-03	1.93	1.94E-03	1.95
400	4.89E-04	1.99	4.89E-04	1.99
800	1.23E-04	1.99	1.26E-04	1.95

l	RK(3,3;1)	rate	RK ‡ (3,3; $\frac{1}{3}$)	rate	RK(4,3;1)	rate
50	2.80E-02	-	6.48E-02	-	2.40E-02	-
100	3.31E-03	3.08	6.81E-03	3.25	1.48E-03	4.02
200	4.11E-04	3.01	4.23E-04	4.01	8.48E-05	4.13
400	5.15E-05	3.00	5.33E-05	2.99	5.37E-06	3.98
800	6.42E-06	3.00	6.63E-06	3.01	3.57E-07	3.91

l	RK(4,4; $\frac{1}{5}$)	rate	RK(4,4; $\frac{3}{4}$)	rate	RK ‡ (5,4; $\frac{1}{5}$)	rate	RK(5,4;1)	rate	RK(6,4;1)	rate
50	3.79E-02	-	6.25E-02	-	2.32E-02	-	2.20E-02	-	3.32E-02	-
100	1.68E-03	4.49	5.85E-03	3.42	1.30E-03	4.16	1.27E-03	4.12	1.57E-03	4.40
200	6.45E-05	4.71	8.28E-05	6.14	6.43E-05	4.33	7.49E-05	4.08	5.05E-05	4.95
400	3.93E-06	4.04	7.21E-06	3.52	4.56E-06	3.82	4.92E-06	3.93	3.33E-06	3.92
800	2.82E-07	3.80	6.73E-07	3.42	3.59E-07	3.67	3.53E-07	3.80	2.33E-07	3.84

l	RK(6,5; $\frac{2}{3}$)	rate	RK(7,5;1)	rate
50	1.87E-02	-	1.66E-02	-
100	1.01E-03	4.21	9.26E-04	4.17
200	5.07E-05	4.31	4.95E-05	4.23
400	3.27E-06	3.95	3.01E-06	4.04
800	2.37E-07	3.79	1.92E-07	3.97



2D linear transport, \mathbb{P}_1 FE (3th-order super-convergent)

Table: Relative error in L^∞ -norm, $T = 0.5$ at CFL = 0.2.

l	RK(2,1;1)	rate	RK ‡ (2,2; $\frac{1}{2}$)	rate
50	1.81E-02	–	2.20E-02	–
100	1.76E-03	3.37	1.84E-03	3.58
200	3.20E-04	2.46	3.20E-04	2.52
400	7.90E-05	2.02	7.90E-05	2.02
800	1.99E-05	1.99	1.99E-05	1.99

l	RK(3,3;1)	rate	RK ‡ (3,3; $\frac{1}{3}$)	rate	RK(4,3;1)	rate
50	2.28E-02	–	3.87E-02	–	2.30E-02	–
100	1.13E-03	4.33	2.64E-03	3.87	1.14E-03	4.34
200	4.54E-05	4.64	6.85E-05	5.27	4.81E-05	4.56
400	2.49E-06	4.19	2.01E-05	1.77	2.10E-06	4.52
800	4.09E-07	2.60	5.29E-06	1.93	1.09E-07	4.27

l	RK(4,4; $\frac{1}{5}$)	rate	RK(4,4; $\frac{3}{4}$)	rate	RK ‡ (5,4; $\frac{1}{5}$)	rate	RK(5,4;1)	rate	RK(6,4;1)	rate
50	2.68E-02	–	2.39E-02	–	2.43E-02	–	2.30E-02	–	2.32E-02	–
100	1.55E-03	4.11	1.17E-03	4.35	1.33E-03	4.19	1.14E-03	4.33	1.13E-03	4.36
200	4.98E-05	4.96	5.51E-05	4.41	5.18E-05	4.68	4.80E-05	4.57	4.70E-05	4.59
400	2.61E-06	4.25	1.37E-05	2.01	2.45E-06	4.40	2.30E-06	4.39	2.74E-06	4.10
800	4.37E-07	2.58	3.56E-06	1.94	2.78E-07	3.14	1.77E-07	3.70	7.04E-07	1.96

l	RK(6,5; $\frac{2}{3}$)	rate	RK(7,5;1)	rate
50	2.41E-02	–	2.29E-02	–
100	1.14E-03	4.40	1.14E-03	4.34
200	4.65E-05	4.62	4.73E-05	4.59
400	3.37E-06	3.78	2.51E-06	4.24
800	9.76E-07	1.79	5.31E-07	2.24



Linear transport with non-smooth solutions

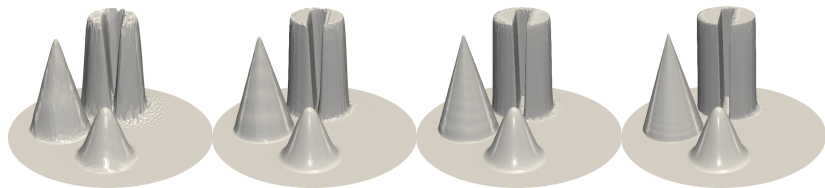


Figure: Three solids problem at $T = 1$, using RK(2,2;1) at CFL = 0.25. 2D \mathbb{P}_1 finite elements on non-uniform meshes. From left to right: $I = 6561$; $I = 24917$; $I = 98648$; $I = 389860$.



Linear transport with non-smooth solutions

Table: Three solids problem at $T = 1$ and $\text{CFL} = 0.25$. 2D \mathbb{P}_1 finite elements on non-uniform meshes. Relative error in the L^1 -norm for methods RK(2,2;1) and RK(4,3;1).

l	RK(2,2;1)	rate	RK(4,3;1)	rate
1605	2.45E-01	–	2.49E-01	–
6561	1.28E-01	0.93	1.31E-01	0.92
24917	7.34E-02	0.81	7.49E-02	0.84
98648	4.26E-02	0.78	4.44E-02	0.76
389860	2.44E-02	0.81	2.56E-02	0.80



2D Burgers' equation

2D Burgers' equation in $D := (-.25, 1.75)^2$:

$$\partial_t u + \nabla \cdot (\mathbf{f}(u)) = 0, \quad \mathbf{f}(u) := \frac{1}{2}(u^2, u^2)^\top, \quad u(\mathbf{x}, 0) = u_0(\mathbf{x}) \text{ a.e. } \mathbf{x} \in D,$$

with the initial data

$$u_0(\mathbf{x}) := \begin{cases} 1 & \text{if } |x_1 - \frac{1}{2}| \leq 1 \text{ and } |x_2 - \frac{1}{2}| \leq 1 \\ -a & \text{otherwise.} \end{cases}$$



2D Burgers' equation

Table: Burgers' equation. 2D \mathbb{P}_1 finite elements on uniform meshes. $T = 0.65$ at CFL = 0.25. Relative error in the L^1 -norm for all the methods.

I	RK(2,2;1)	rate	RK(2,2; $\frac{1}{2}$)	rate	RK(3,3;1)	rate	RK(3,3; $\frac{1}{3}$)	rate	RK(4,3;1)	rate
51^2	7.71E-02	-	7.79E-02	-	7.71E-02	-	8.03E-02	-	7.71E-02	-
101^2	3.69E-02	1.06	3.73E-02	1.06	3.69E-02	1.06	3.85E-02	1.06	3.69E-02	1.06
201^2	2.30E-02	0.68	2.32E-02	0.68	2.30E-02	0.68	2.38E-02	0.70	2.30E-02	0.68
401^2	1.24E-02	0.90	1.24E-02	0.90	1.24E-02	0.90	1.27E-02	0.90	1.24E-02	0.90
801^2	6.47E-03	0.93	6.52E-03	0.93	6.48E-03	0.93	6.65E-03	0.93	6.47E-03	0.93

I	RK(4,4; $\frac{1}{2}$)	rate	RK(4,4; $\frac{3}{4}$)	rate	RK(5,4;0.51)	rate	RK(6,5; $\frac{5}{6}$)	rate	RK(6,5; $\frac{2}{3}$)	rate
51^2	7.94E-02	-	8.15E-02	-	7.79E-02	-	1.81E-01	-	9.29E-02	-
101^2	3.80E-02	1.06	3.89E-02	1.07	3.89E-02	1.00	8.56E-02	1.08	4.39E-02	1.08
201^2	2.36E-02	0.69	2.40E-02	0.70	2.47E-02	0.66	4.78E-02	0.84	2.72E-02	0.69
401^2	1.26E-02	0.90	1.28E-02	0.90	1.36E-02	0.86	2.38E-02	1.00	1.41E-02	0.95
801^2	6.61E-03	0.93	6.72E-03	0.94	7.11E-03	0.93	1.22E-02	0.97	7.24E-03	0.96

- ▶ Non-SSP methods converge as well as the SSP methods.



Outline



IDPMEX

Introduction
Invariant domains
Problems with SSP time stepping
Invariant-domain-preserving Explicit Runge-Kutta
Numerical illustrations
Invariant-domain-preserving IMEX



The low-order, linearized update

- ▶ Let \mathbf{F}^L be low-order approximation of hyperbolic flux.



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- ▶ Let $\mathbf{G}^{L,\text{lin}}$ be Low-order **quasi-linearized** approximation of parabolic flux plus sources (i.e., approximation of $-\nabla \cdot (\mathbf{g}(\mathbf{u}, \nabla \mathbf{u})) + \mathbf{S}(\mathbf{u})$).



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- ▶ Let $\mathbf{G}^{L,\text{lin}}$ be Low-order **quasi-linearized** approximation of parabolic flux plus sources (i.e., approximation of $-\nabla \cdot (\mathbf{g}(\mathbf{u}, \nabla \mathbf{u})) + \mathbf{S}(\mathbf{u})$).
- ▶ Consider the low-order update (IMEX Euler)

$$\mathbb{M}^L \mathbf{U}^{L,n+1} = \mathbb{M}^L \mathbf{U}^n + \Delta t \mathbf{F}^L(\mathbf{U}^n) + \Delta t \mathbf{G}^{L,\text{lin}}(\mathbf{U}^n; \mathbf{U}^{L,n+1}).$$



The low-order, linearized update

- ▶ **Assumption 1:** (Forward Euler with low-order hyperbolic flux is invariant-domain preserving.) There exists $\Delta t^* > 0$ such that:
 - ▶ For every $\Delta t \in (0, \Delta t^*]$, the low-order hyperbolic flux satisfies

$$(\mathbf{V} \in \mathcal{A}') \implies (\mathbf{U} := \mathbf{V} + \Delta t(\mathbb{M}^L)^{-1}\mathbf{F}^L(\mathbf{V}) \in \mathcal{A}').$$

- ▶ (Backward Euler with low-order, linearized, parabolic flux is invariant-domain preserving.) For all $\Delta t \in (0, \Delta t^*]$ and all $\mathbf{W} \in \mathcal{A}'$, the operator $\mathbb{I} - \Delta t(\mathbb{M}^L)^{-1}\mathbf{G}^{L,\text{lin}}(\mathbf{W}; \cdot) : (\mathbb{R}^m)^I \rightarrow (\mathbb{R}^m)^I$ is bijective and

$$(\mathbf{V} \in \mathcal{A}') \implies \left((\mathbb{I} - \Delta t(\mathbb{M}^L)^{-1}\mathbf{G}^{L,\text{lin}}(\mathbf{W}; \cdot))^{-1}\mathbf{V} \in \mathcal{A}' \right).$$



The low-order, linearized update

- ▶ **Assumption 1:** (Forward Euler with low-order hyperbolic flux is invariant-domain preserving.) There exists $\Delta t^* > 0$ such that:
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- ▶ (Backward Euler with low-order, linearized, parabolic flux is invariant-domain preserving.) For all $\Delta t \in (0, \Delta t^*]$ and all $\mathbf{W} \in \mathcal{A}'$, the operator $\mathbb{I} - \Delta t(\mathbb{M}^L)^{-1}\mathbf{G}^{L,\text{lin}}(\mathbf{W}; \cdot) : (\mathbb{R}^m)^I \rightarrow (\mathbb{R}^m)^I$ is bijective and

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Lemma (Low-order IDP Euler IMEX)

Let Assumption 1 hold. Assume that $\mathbf{U}^n \in \mathcal{A}'$ and $\Delta t \in (0, \Delta t^*]$. Then, $\mathbf{U}^{L,n+1} \in \mathcal{A}'$.



The high-order, linearized update (one Euler step)

- **Assumption 2:** There exists two nonlinear limiting operators ℓ^{hyp} , $\ell^{\text{par}} : \mathcal{A}' \times (\mathbb{R}^m)' \times (\mathbb{R}^m)' \rightarrow (\mathbb{R}^m)'$ s.t. for all $(\mathbf{V}, \boldsymbol{\Phi}^{\text{L}}, \boldsymbol{\Phi}^{\text{H}}) \in \mathcal{A}' \times (\mathbb{R}^m)' \times (\mathbb{R}^m)'$,

$$(\mathbf{V} + \Delta t(\mathbb{M}^{\text{L}})^{-1}\boldsymbol{\Phi}^{\text{L}} \in \mathcal{A}') \implies (\ell^{\text{hyp}}(\mathbf{V}, \boldsymbol{\Phi}^{\text{L}}, \boldsymbol{\Phi}^{\text{H}}) \in \mathcal{A}'),$$

$$(\mathbf{V} + \Delta t(\mathbb{M}^{\text{L}})^{-1}\boldsymbol{\Phi}^{\text{L}} \in \mathcal{A}') \implies (\ell^{\text{par}}(\mathbf{V}, \boldsymbol{\Phi}^{\text{L}}, \boldsymbol{\Phi}^{\text{H}}) \in \mathcal{A}').$$



Important remark

- ▶ The invariant domain enforced by the hyperbolic limiting operator **can be smaller** than that enforced the parabolic limiting operator.



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- ▶ The invariant domain enforced by the hyperbolic limiting operator **can be smaller** than that enforced the parabolic limiting operator.
- ▶ Bounds for limiting are deduced from the low-order updates (hyperbolic and parabolic bounds can be different).
- ▶ \Rightarrow the method is naturally asymptotic preserving.



The high-order update (one Euler step)

- ▶ Given $\mathbf{U}^n \in \mathcal{A}^I$, the high-order update \mathbf{U}^{n+1} is constructed as follows:



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- ▶ **Step 1:** Compute the low-order and high-order hyperbolic updates defined by

$$\begin{aligned}\mathbb{M}^L \mathbf{W}^{L,n+1} &:= \mathbb{M}^L \mathbf{U}^n + \Delta t \mathbf{F}^L(\mathbf{U}^n), \\ \mathbb{M}^H \mathbf{W}^{H,n+1} &:= \mathbb{M}^H \mathbf{U}^n + \Delta t \mathbf{F}^H(\mathbf{U}^n).\end{aligned}$$



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- ▶ **Step 2:** Compute the hyperbolic fluxes Φ^L, Φ^H (details given later) and limit

$$\mathbf{W}^{n+1} := \ell^{\text{hyp}}(\mathbf{U}^n, \Phi^L, \Phi^H).$$



The high-order update (one Euler step)

- ▶ **Step 3:** Compute the low-order and high-order parabolic updates defined by

$$\begin{aligned}\mathbb{M}^L \mathbf{U}^{L,n+1} - \Delta t \mathbf{G}^{L,\text{lin}}(\mathbf{U}^n; \mathbf{U}^{L,n+1}) &:= \mathbb{M}^L \mathbf{W}^{n+1}, \\ \mathbb{M}^H \mathbf{U}^{H,n+1} - \Delta t \mathbf{G}^{H,\text{lin}}(\mathbf{U}^n; \mathbf{U}^{H,n+1}) &:= \mathbb{M}^H \mathbf{W}^{n+1},\end{aligned}$$



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- ▶ **Step 4:** Compute the parabolic fluxes $\boldsymbol{\Psi}^L$, $\boldsymbol{\Psi}^H$ (details given later) and limit

$$\mathbf{U}^{n+1} := \ell^{\text{par}}(\mathbf{W}^{n+1}, \boldsymbol{\Psi}^L, \boldsymbol{\Psi}^H).$$



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$$\mathbf{U}^{n+1} := \ell^{\text{par}}(\mathbf{W}^{n+1}, \boldsymbol{\Psi}^L, \boldsymbol{\Psi}^H).$$

Lemma (High-order IDP Euler IMEX)

Assume Assumptions 1 and 2. Assume that $\mathbf{U}^n \in \mathcal{A}^I$ and $\Delta t \in (0, \Delta t^*]$. Let \mathbf{U}^{n+1} be defined as above. Then $\mathbf{U}^{n+1} \in \mathcal{A}^I$.



The high-order update (IMEX)

- ▶ Key idea: Consider low-order and high-order updates and limit.



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- ▶ Set $\mathbf{U}(t^n) = \mathbf{U}^n$ (with the induction assumption $\mathbf{U}^n \in \mathcal{A}$)



The high-order update (IMEX)

- ▶ Key idea: Consider low-order and high-order updates and limit.
- ▶ Set $\mathbf{U}(t^n) = \mathbf{U}^n$ (with the induction assumption $\mathbf{U}^n \in \mathcal{A}$)
- ▶ For $t \in (t^n, t^{n+1})$ solve

$$\mathbb{M}^L \partial_t \mathbf{U} = \underbrace{\mathbf{F}^L(\mathbf{U})}_{\text{Explicit}} + \underbrace{\mathbf{G}^{\text{H,lin}}(\mathbf{U}^n; \mathbf{U})}_{\text{Implicit}},$$

$$\mathbb{M}^H \partial_t \mathbf{U} = \underbrace{\mathbf{F}^H(\mathbf{U}) + \mathbf{G}^H(\mathbf{U}) - \mathbf{G}^{\text{H,lin}}(\mathbf{U}^n; \mathbf{U})}_{\text{Explicit}} + \underbrace{\mathbf{G}^{\text{H,lin}}(\mathbf{U}^n; \mathbf{U})}_{\text{Implicit}}.$$



The high-order update (IMEX)

► Explicit Butcher tableau

0	0				
c_2	$a_{2,1}^e$	0			
c_3	$a_{3,1}^e$	$a_{3,2}^e$	0		
\vdots	\vdots	\ddots	\ddots	\ddots	
c_s	$a_{s,1}^e$	$a_{s,2}^e$	\cdots	$a_{s,s-1}^e$	0
1	$a_{s+1,1}^e$	$a_{s+1,2}^e$	\cdots	$a_{s+1,s-1}^e$	$a_{s+1,s}^e$

► Implicit Butcher tableau

0	0				
c_2	$a_{2,1}^i$	$a_{2,2}^i$			
c_3	$a_{3,1}^i$	$a_{3,2}^i$	$a_{3,3}^i$		
\vdots	\vdots	\ddots	\ddots	\ddots	
c_s	$a_{s,1}^i$	$a_{s,2}^i$	\cdots	$a_{s,s-1}^i$	$a_{s,s}^i$
1	$a_{s+1,1}^i$	$a_{s+1,2}^i$	\cdots	$a_{s+1,s-1}^i$	$a_{s+1,s}^i$



Hyperbolic update

- ▶ For all $l \in \{2:s+1\}$



Hyperbolic update

- ▶ For all $l \in \{2:s+1\}$
- ▶ Compute $\mathbf{W}^{L,l}$ and $\mathbf{W}^{H,l}$

$$\mathbb{M}^L \mathbf{W}^{L,l} := \mathbb{M}^L \mathbf{U}^{n,l'} + \Delta t (c_l - c_{l'}) \mathbf{F}^L(\mathbf{U}^{n,l'}),$$

$$\mathbb{M}^H \mathbf{W}^{H,l} := \mathbb{M}^H \mathbf{U}^{n,l'} + \Delta t \sum_{k \in \{1:l-1\}} (a_{l,k}^e - a_{l',k}^e) \mathbf{F}^H(\mathbf{U}^{n,k}).$$



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- ▶ Use hyperbolic limiter

$$\mathbf{W}^{n,l} := \ell^{\text{hyp}}(\mathbf{U}^{L,l}, \Phi^L, \Phi^H), \quad \forall l \in \{2:s+1\}.$$



Parabolic update

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- ▶ Compute $\mathbf{U}^{L,l}$ and $\mathbf{U}^{H,l}$

$$\mathbf{M}^L \mathbf{U}^{L,l} := \mathbf{M}^L \mathbf{W}^{n,l'} + \Delta t (c_l - c_{l'}) \mathbf{G}^{L,\text{lin}}(\mathbf{W}^{n,l'}; \mathbf{U}^{L,l}),$$

$$\mathbf{M}^H \mathbf{U}^{H,l} := \mathbf{M}^H \mathbf{W}^{n,l'} + \Delta t a_{l,l}^i \mathbf{G}^{H,\text{lin}}(\mathbf{U}^n; \mathbf{U}^{H,l})$$

$$+ \sum_{k \in \{1:l-1\}} \Delta t \left\{ (a_{l,k}^e - a_{l',k}^e) \mathbf{G}^H(\mathbf{U}^{n,k}) + (a_{l,k}^i - a_{l',k}^i - a_{l,k}^e + a_{l',k}^e) \mathbf{G}^{H,\text{lin}}(\mathbf{U}^n; \mathbf{U}^{n,k}) \right\}.$$

- ▶ Notice $\Delta t (c_l - c_{l'}) > 0$, but $\Delta t a_{l,l}^i \geq 0$ (i.e., $a_{s+1,s+1}^i = 0$).



Parabolic update

- ▶ For all $l \in \{2:s+1\}$
- ▶ Compute $\mathbf{U}^{L,l}$ and $\mathbf{U}^{H,l}$

$$\mathbf{M}^L \mathbf{U}^{L,l} := \mathbf{M}^L \mathbf{W}^{n,l'} + \Delta t (c_l - c_{l'}) \mathbf{G}^{L,\text{lin}}(\mathbf{W}^{n,l'}; \mathbf{U}^{L,l}),$$

$$\mathbf{M}^H \mathbf{U}^{H,l} := \mathbf{M}^H \mathbf{W}^{n,l'} + \Delta t a_{l,l}^i \mathbf{G}^{H,\text{lin}}(\mathbf{U}^n; \mathbf{U}^{H,l})$$

$$+ \sum_{k \in \{1:l-1\}} \Delta t \left\{ (a_{l,k}^e - a_{l',k}^e) \mathbf{G}^H(\mathbf{U}^{n,k}) + (a_{l,k}^i - a_{l',k}^i - a_{l,k}^e + a_{l',k}^e) \mathbf{G}^{H,\text{lin}}(\mathbf{U}^n; \mathbf{U}^{n,k}) \right\}.$$

- ▶ Notice $\Delta t (c_l - c_{l'}) > 0$, but $\Delta t a_{l,l}^i \geq 0$ (i.e., $a_{s+1,s+1}^i = 0$).
- ▶ Use hyperbolic limiter

$$\mathbf{U}^{n+1} := \ell^{\text{hyp}}(\mathbf{W}^{L,l}, \Psi^L, \Psi^H), \quad \forall l \in \{2:s+1\}.$$



Key result

Theorem (*s*-stage IDP-IMEX)

Assume Assumptions 1 and 2 and

$$\Delta t_{\text{eff}} \leq \Delta t^*, \quad c_{\text{eff}} := \max_{l \in \{2:s+1\}} (c_l - c_l')$$

If $\mathbf{U}^n \in \mathcal{A}^l$, then $\mathbf{U}^{n+1} \in \mathcal{A}^l$.



Example: Second-order

- ▶ Heun's method + Crank-Nicolson:

$$\begin{array}{c|cc} 0 & 0 & \\ 1 & 1 & 0 \\ \hline 1 & \frac{1}{2} & \frac{1}{2} \end{array} \quad \begin{array}{c|cc} 0 & 0 & \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline 1 & \frac{1}{2} & \frac{1}{2} \end{array}$$

- ▶ $l' = l - 1$ for all $l \in \{2:3\}$, and the efficiency ratio is $\frac{1}{2}$.



Example: Second-order

- ▶ Explicit and implicit midpoint rules.

$$\begin{array}{c|cc} 0 & 0 & \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline 1 & 0 & 1 \end{array} \quad \begin{array}{c|cc} 0 & 0 & \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \hline 1 & 0 & 1 \end{array}$$

- ▶ $l' = l - 1$ for all $l \in \{2:3\}$, and the efficiency ratio is 1.



Example: Second-order, Strang splitting

- ▶ Strang's splitting



Example: Second-order, Strang splitting

- ▶ Strang's splitting
- ▶ Explicit midpoint rule for the two hyperbolic solves and implicit midpoint rule for the parabolic solve.



Example: Second-order, Strang splitting

- ▶ Strang's splitting
- ▶ Explicit midpoint rule for the two hyperbolic solves and implicit midpoint rule for the parabolic solve.
- ▶ The whole process can be rewritten as a five-stage IMEX scheme with the following Butcher tableaux

$$\begin{array}{c|cccc} 0 & 0 & & & & \\ \frac{1}{4} & \frac{1}{4} & 0 & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & & \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & \\ \frac{3}{4} & 0 & \frac{1}{2} & 0 & \frac{1}{4} & 0 \\ \hline 1 & 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{array}$$
$$\begin{array}{c|cccc} 0 & 0 & & & & \\ \frac{1}{4} & 0 & 0 & & & \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} & & \\ \frac{1}{2} & 0 & 0 & 1 & 0 & \\ \frac{3}{4} & 0 & 0 & 1 & 0 & 0 \\ \hline 1 & 0 & 0 & 1 & 0 & 0 \end{array}$$


Example: Second-order, Strang splitting

- ▶ Strang's splitting
- ▶ Explicit midpoint rule for the two hyperbolic solves and implicit midpoint rule for the parabolic solve.
- ▶ The whole process can be rewritten as a five-stage IMEX scheme with the following Butcher tableaux

$$\begin{array}{c|ccccc} 0 & 0 & & & & \\ \frac{1}{4} & \frac{1}{4} & 0 & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & & \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & \\ \frac{3}{4} & 0 & \frac{1}{2} & 0 & \frac{1}{4} & 0 \\ \hline 1 & 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{array} \quad \begin{array}{c|cccc} 0 & 0 & & & \\ \frac{1}{4} & 0 & 0 & & \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} & \\ \frac{1}{2} & 0 & 0 & 1 & 0 \\ \frac{3}{4} & 0 & 0 & 1 & 0 & 0 \\ \hline 1 & 0 & 0 & 1 & 0 & 0 \end{array}$$

- ▶ $I' = (1, 2, 2, 4, 5)$ but the efficiency ratio is 1 because stages 3 and 4 do not require new function evaluations.



Example: Third-order

- ▶ Two-stage, third-order (A-stable) SDIRK method **Crouzeix (1975), Norsett (1974)**

$$\begin{array}{c|ccc} 0 & 0 & & \\ \gamma & \gamma & 0 & \\ 1-\gamma & \gamma-1 & 2-2\gamma & 0 \\ \hline 1 & 0 & \frac{1}{2} & \frac{1}{2} \end{array} \quad \begin{array}{c|ccc} 0 & 0 & & \\ \gamma & 0 & \gamma & \\ 1-\gamma & 0 & 1-2\gamma & \gamma \\ \hline 1 & 0 & \frac{1}{2} & \frac{1}{2} \end{array}$$

- ▶ with $\gamma := \frac{1}{2} + \frac{1}{2\sqrt{3}} \approx 0.78867$.
- ▶ The values for l' are $(1, 1, 2)$. The efficiency ratio is $\frac{1}{3}\gamma \approx 0.26$.
- ▶ The implicit method is A-stable.



Example: New Third-order **AE,JLG** (2022)

- ▶ Three-stage, third-order

$$\begin{array}{c|ccc} 0 & 0 & & \\ \frac{1}{3} & \frac{1}{3} & 0 & \\ \frac{2}{3} & 0 & \frac{2}{3} & 0 \\ \hline 1 & \frac{1}{4} & 0 & \frac{3}{4} \end{array} \quad \begin{array}{c|ccc} 0 & 0 & & \\ \frac{1}{3} & \frac{1}{3} - \gamma & \gamma & \\ \frac{2}{3} & \gamma & \frac{2}{3} - 2\gamma & \gamma \\ \hline 1 & \frac{1}{4} & 0 & \frac{3}{4} \end{array}$$

- ▶ With $\gamma := \frac{1}{2} + \frac{1}{2\sqrt{3}} \approx 0.78867$.
- ▶ We have $l' = l - 1$ for all $l \in \{2:4\}$, and the method is **optimal** (efficiency is **1**).



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Lemma

- ▶ *The amplification function for Crouzeix's method and the new method are identical.*
- ▶ *The implicit method is A-stable.*



Example: New four stages, third-order, **AE,JLG (2022)**

- ▶ Four-stages, third-order.

$$\begin{array}{c|ccc} 0 & 0 & & \\ \frac{1}{4} & \frac{1}{4} & 0 & \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ \frac{3}{4} & 0 & \frac{1}{4} & \frac{1}{2} \\ \hline 1 & 0 & \frac{2}{3} & -\frac{1}{3} \quad \frac{2}{3} \end{array}$$



Example: New four stages, third-order, **AE,JLG (2022)**

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 \frac{3}{4} & 0 & \frac{1}{4} & \frac{1}{2} \\
 \hline
 1 & 0 & \frac{2}{3} & -\frac{1}{3} \quad \frac{2}{3}
 \end{array}$$

$$\begin{array}{c|cccc}
 0 & 0 & & & \\
 \frac{1}{4} & -0.1858665215084591 & 0.4358665215084591 & & \\
 \frac{1}{2} & -0.4367256409878701 & 0.5008591194794110 & 0.4358665215084591 & \\
 \frac{3}{4} & -0.0423391342724147 & 0.7701152303135821 & -0.4136426175496265 & 0.4358665215084591 \\
 \hline
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- ▶ Implicit part is L-stable.
- ▶ We have $l' = l - 1$ for all $l \in \{2:5\}$, and the method is **optimal** (efficiency is **1**).



Example: New five stages, fourth-order, **AE,JLG (2022)**

► Five-stages, fourth-order.

$$a_{2,1}^e = 0.2$$

$$a_{3,1}^e = 0.2607558226955500 \quad a_{3,2}^e = 0.1392441773044501$$

$$a_{4,1}^e = -0.2585651787257025 \quad a_{4,2}^e = 0.9113627416628056 \quad a_{4,3}^e = -0.0527975629371033$$

$$a_{5,1}^e = 0.2162327643150383 \quad a_{5,2}^e = 0.5153422309960234 \quad a_{5,3}^e = -0.8166279419926541$$

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Important omitted details

- ▶ The definition of $\mathbf{G}^{\text{L,lin}}$ is **problem-dependent**.
 - ▶ For scalar equation with source $\mathbf{S}(u) = \mu\phi(u)u(1-u)$, the following low-order linearization is **explicit and IDP for all $\mu \geq 0$**

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- ▶ Limiting done with **convex limiting (Guermont, Popov, Tomas (2019))** if the constraints are not affine.



Conclusions

- ▶ Every ERK and IMEX methods can be made invariant-domain preserving.

