Invariant-domain preserving Runge-Kutta methods

Alexandre Ern

ENPC and INRIA, Paris, France joint work with Jean-Luc Guermond (TAMU)

FORTH Workshop, 09/2023

Outline

- Setting
- Beyond strong stability preserving (SSP) RK schemes
- New perspective on explicit RK schemes
- New perspective on implicit-explicit (IMEX) schemes

Outline

- Setting
- Beyond strong stability preserving (SSP) RK schemes
- New perspective on explicit RK schemes
- New perspective on implicit-explicit (IMEX) schemes

Warning: space discretization is hidden in the background, but is important!

Outline

- Setting
- Beyond strong stability preserving (SSP) RK schemes
- New perspective on explicit RK schemes
- New perspective on implicit-explicit (IMEX) schemes

Warning: space discretization is hidden in the background, but is important!

Main references:

- [AE & JLG, SISC 22] for ERK
- [AE & JLG, SISC 23] for IMEX

Setting

Cauchy problem

Cauchy problem

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

 $D \subset \mathbb{R}^d$ (open Lipschitz polytope)

Cauchy problem

Cauchy problem

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

 $D \subset \mathbb{R}^d$ (open Lipschitz polytope)

- Field u takes values in \mathbb{R}^m , i.e., $u: D \times \mathbb{R}_+ \to \mathbb{R}^m$
- $f \in C^1(\mathbb{R}^m; \mathbb{R}^{m \times d})$: hyperbolic flux
- $\mathbf{g} \in C^1(\mathbb{R}^m \times \mathbb{R}^{m \times d}; \mathbb{R}^{m \times d})$: parabolic/diffusive flux
- $S \in C^1(\mathbb{R}^m; \mathbb{R}^m)$: source/relaxation term

Cauchy problem

Cauchy problem

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

 $D \subset \mathbb{R}^d$ (open Lipschitz polytope)

- Field u takes values in \mathbb{R}^m , i.e., $u: D \times \mathbb{R}_+ \to \mathbb{R}^m$
- $f \in C^1(\mathbb{R}^m; \mathbb{R}^{m \times d})$: hyperbolic flux
- $g \in C^1(\mathbb{R}^m \times \mathbb{R}^{m \times d}; \mathbb{R}^{m \times d})$: parabolic/diffusive flux
- $S \in C^1(\mathbb{R}^m; \mathbb{R}^m)$: source/relaxation term
- u_0 : admissible initial data
- BCs not discussed herein

Exemple 1: Scalar advection-diffusion-reaction

• Find $u: D \times \mathbb{R}_+ \to \mathbb{R}$ such that

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

Hyperbolic and parabolic fluxes

$$f(x, u) := \begin{cases} (f_1(u), \dots, f_d(u)) \\ \beta(x)u \text{ with } \nabla \cdot \beta = 0 \end{cases} \qquad g(u, \nabla u) := \kappa(u) \nabla u$$

• Source term, for instance

$$S(u) := \mu \phi(u) u(1-u), \qquad \phi \in C^0(\mathbb{R}; [-1, 1]), \qquad \mu \ge 0$$

Exemple 2: compressible Navier-Stokes

• Find $\mathbf{u} := (\rho, \mathbf{m}^{\mathsf{T}}, E)^{\mathsf{T}} : D \times \mathbb{R}_+ \to \mathbb{R}^{d+2}$ such that

$$\begin{cases} \partial_t \rho + \nabla \cdot (v\rho) = 0 \\ \partial_t \mathbf{m} + \nabla \cdot (v \otimes \mathbf{m} + p(\mathbf{u}) \mathbb{I} - s(v)) = \mathbf{0} \\ \partial_t E + \nabla \cdot (v(E + p(\mathbf{u})) - v \cdot s(v) + q(\mathbf{u})) = 0 \end{cases}$$

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

Exemple 2: compressible Navier–Stokes

• Find $\mathbf{u} := (\rho, \mathbf{m}^\mathsf{T}, E)^\mathsf{T} : D \times \mathbb{R}_+ \to \mathbb{R}^{d+2}$ such that

$$\begin{cases} \partial_t \rho + \nabla \cdot (\mathbf{v}\rho) = 0 \\ \partial_t \mathbf{m} + \nabla \cdot (\mathbf{v} \otimes \mathbf{m} + p(\mathbf{u})\mathbb{I} - s(\mathbf{v})) = \mathbf{0} \\ \partial_t E + \nabla \cdot (\mathbf{v}(E + p(\mathbf{u})) - \mathbf{v} \cdot s(\mathbf{v}) + q(\mathbf{u})) = 0 \end{cases}$$

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

• Hyperbolic (Euler) and parabolic fluxes

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

with viscous stress tensor and heat flux such that

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

with (linearized) strain tensor $e(v) := \frac{1}{2}(\nabla v + \nabla v^{\mathsf{T}})$ and temperature T(u) (from specific internal energy $e(u) := E/\rho - \frac{1}{2}||v||_{\ell^2}^2$)

• μ , λ , κ constant for simplicity

• Key assumption: There exists a convex subset $\mathcal{A} \subseteq \mathbb{R}^m$ (depending on the initial data u_0) s.t. the entropy/admissible solution to the Cauchy problem takes values in \mathcal{A} for a.e. $(x,t) \in D \times \mathbb{R}_+$

$$\left\{ \boldsymbol{u}_0(\boldsymbol{x}) \in \mathcal{A} \text{ for a.e. } \boldsymbol{x} \in D \right\} \implies \left\{ \boldsymbol{u}(\boldsymbol{x},t) \in \mathcal{A} \text{ for a.e. } (\boldsymbol{x},t) \in D \in \mathbb{R}_+ \right\}$$

• Key assumption: There exists a convex subset $\mathcal{A} \subseteq \mathbb{R}^m$ (depending on the initial data u_0) s.t. the entropy/admissible solution to the Cauchy problem takes values in \mathcal{A} for a.e. $(x,t) \in D \times \mathbb{R}_+$

$$\left\{ u_0(x) \in \mathcal{A} \text{ for a.e. } x \in D \right\} \implies \left\{ u(x,t) \in \mathcal{A} \text{ for a.e. } (x,t) \in D \in \mathbb{R}_+ \right\}$$

• This is a generalization of the maximum principle

• Key assumption: There exists a convex subset $\mathcal{A} \subseteq \mathbb{R}^m$ (depending on the initial data u_0) s.t. the entropy/admissible solution to the Cauchy problem takes values in \mathcal{A} for a.e. $(x,t) \in D \times \mathbb{R}_+$

$$\left\{ \boldsymbol{u}_0(\boldsymbol{x}) \in \mathcal{A} \text{ for a.e. } \boldsymbol{x} \in D \right\} \implies \left\{ \boldsymbol{u}(\boldsymbol{x},t) \in \mathcal{A} \text{ for a.e. } (\boldsymbol{x},t) \in D \in \mathbb{R}_+ \right\}$$

- This is a generalization of the maximum principle
- Scalar conservation equations without reaction

$$\mathcal{A} := [\operatorname{ess\,inf} u_0, \operatorname{ess\,sup} u_0]$$

• Scalar conservation equations with $S(u) := \mu \phi(u) u (1 - u)$

$$\mathcal{A} := [0, 1]$$

• Key assumption: There exists a convex subset $\mathcal{A} \subseteq \mathbb{R}^m$ (depending on the initial data u_0) s.t. the entropy/admissible solution to the Cauchy problem takes values in \mathcal{A} for a.e. $(x,t) \in D \times \mathbb{R}_+$

$$\left\{ u_0(x) \in \mathcal{A} \text{ for a.e. } x \in D \right\} \implies \left\{ u(x,t) \in \mathcal{A} \text{ for a.e. } (x,t) \in D \in \mathbb{R}_+ \right\}$$

- This is a generalization of the maximum principle
- Scalar conservation equations without reaction

$$\mathcal{A} := [\operatorname{ess\,inf} u_0, \operatorname{ess\,sup} u_0]$$

• Scalar conservation equations with $S(u) := \mu \phi(u) u (1 - u)$

$$\mathcal{A} := [0, 1]$$

• Navier–Stokes and Euler equations (s(u): specific entropy)

$$\mathcal{A}_{\text{NS}} := \{ (\rho, \boldsymbol{m}^{\mathsf{T}}, E)^{\mathsf{T}} \in \mathbb{R}^m \mid 0 < \rho, \ 0 < T(\boldsymbol{u}) \}$$

$$\mathcal{A}_{\text{Eu}} := \{ (\rho, \boldsymbol{m}^{\mathsf{T}}, E)^{\mathsf{T}} \in \mathbb{R}^m \mid 0 < \rho, \ 0 < T(\boldsymbol{u}), \text{ ess inf } s(\boldsymbol{u}_0) \le s(\boldsymbol{u}) \}$$

Invariant-domain preserving (IDP) approximation methods

 Approximation methods that preserve invariant domains are called Invariant domain preserving (IDP)

Invariant-domain preserving (IDP) approximation methods

- Approximation methods that preserve invariant domains are called Invariant domain preserving (IDP)
- Space semi-discrete problem: Find $\mathbf{U} \in C^1(\mathbb{R}_+; (\mathbb{R}^m)^I)$ s.t.

$$\mathbb{M}\partial_t \mathbf{U} = \mathbf{F}(\mathbf{U}) + \mathbf{G}(\mathbf{U}), \qquad \mathbf{U}(0) = \mathbf{U}_0$$

- *I*: #dofs for space approximation (C^0 -FEM, dG, FV, FD, ...)
- M: mass matrix (invertible)
- $F: (\mathbb{R}^m)^I \to (\mathbb{R}^m)^I$: space approximation of $-\nabla \cdot f(u)$
- $G: (\mathbb{R}^m)^I \to (\mathbb{R}^m)^I$: space approximation of $-\nabla \cdot g(u, \nabla u) + S(u)$
- U_i approximates u at some point $x_i \in D \Longrightarrow$ natural requirement is $U \in \mathcal{A}^I$

Invariant-domain preserving (IDP) approximation methods

- Approximation methods that preserve invariant domains are called Invariant domain preserving (IDP)
- Space semi-discrete problem: Find $\mathbf{U} \in C^1(\mathbb{R}_+; (\mathbb{R}^m)^I)$ s.t.

$$\mathbb{M}\partial_t \mathbf{U} = \mathbf{F}(\mathbf{U}) + \mathbf{G}(\mathbf{U}), \qquad \mathbf{U}(0) = \mathbf{U}_0$$

- 1: #dofs for space approximation (C⁰-FEM, dG, FV, FD, ...)
- M: mass matrix (invertible)
- $F: (\mathbb{R}^m)^I \to (\mathbb{R}^m)^I$: space approximation of $-\nabla \cdot f(u)$
- $G: (\mathbb{R}^m)^I \to (\mathbb{R}^m)^I$: space approximation of $-\nabla \cdot g(u, \nabla u) + S(u)$
- U_i approximates u at some point $x_i \in D \Longrightarrow$ natural requirement is $U \in \mathcal{A}^I$
- Time-stepping scheme produces a sequence $\mathbf{U}^0, \mathbf{U}^1, \dots, \mathbf{U}^n, \dots$
- Time-stepping scheme is IDP if

$$\left\{ \mathbf{U}_{0}\in\mathcal{A}^{I}\right\} \implies \left\{ \mathbf{U}^{n}\in\mathcal{A}^{I}\;\forall n\geq0\right\}$$

How to achieve this goal?

SSP paradigm for hyperbolic problems

- Let us focus first on hyperbolic problems
- Key idea: [Shu & Osher 88] SSPRK are ERK methods where all updates are convex combinations of previous updates computed with forward Euler method (recall ## convex)

SSP paradigm for hyperbolic problems

- Let us focus first on hyperbolic problems
- Key idea: [Shu & Osher 88] SSPRK are ERK methods where all updates are convex combinations of previous updates computed with forward Euler method (recall ## convex)
- Key assumption: $\exists \tau^* > 0 \text{ s.t. } \forall \tau \in (0, \tau^*],$

$$\left\{ \mathbf{V} \in \mathcal{A}^{I} \right\} \implies \left\{ \mathbf{V} + \tau(\mathbb{M})^{-1} \mathbf{F}(\mathbf{V}) \in \mathcal{A}^{I} \right\}$$

In other words, \mathcal{A}^I is invariant under the forward Euler method with CFL condition $\tau \in (0,\tau^*]$

SSP paradigm for hyperbolic problems

- Let us focus first on hyperbolic problems
- Key idea: [Shu & Osher 88] SSPRK are ERK methods where all updates are convex combinations of previous updates computed with forward Euler method (recall ## convex)
- Key assumption: $\exists \tau^* > 0 \text{ s.t. } \forall \tau \in (0, \tau^*],$

$$\left\{ \mathbf{V} \in \mathcal{A}^{I} \right\} \implies \left\{ \mathbf{V} + \tau(\mathbb{M})^{-1} \mathbf{F}(\mathbf{V}) \in \mathcal{A}^{I} \right\}$$

In other words, \mathcal{A}^I is invariant under the forward Euler method with CFL condition $\tau \in (0, \tau^*]$

• Theory of SSP methods applied to ODEs is well understood [Kraaijevanger 91;S Ruuth & Spiteri 02; Ferracina & Spijker 05; Higueras 05]

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

- Notation: SSPRK(s, p) for s-stage, pth-order method
- SSPRK(2,2) (two-stage, second-order) [Heun's second-order method]

$$\begin{split} w^{(1)} &= u^n + \tau L(t^n, u^n) \\ u^{n+1} &= \frac{1}{2}u^n + \frac{1}{2} \left(w^{(1)} + \tau L(t^{n+1}, w^{(1)}) \right) \end{split}$$

 $\bullet \ SSPRK(3,3) \ (three-stage, \ third-order) \ [\texttt{Fehlberg's method}]$

$$\begin{split} w^{(1)} &= u^n + \tau L(t^n, u^n) \\ w^{(2)} &= \frac{3}{4}u^n + \frac{1}{4} \left(w^{(1)} + \tau L(t^{n+1}, w^{(1)}) \right) \\ u^{n+1} &= \frac{1}{3}u^n + \frac{2}{3} \left(w^{(2)} + \tau L(t^{n+\frac{1}{2}}, w^{(2)}) \right) \end{split}$$

• SSPRK(4,3) and SSPRK(5,4) also available

Why (and how to) go beyond SSP?

• Restriction in accuracy: SSPRK are restricted to fourth-order (if one insists on never stepping backward in time) [Ruuth & Spiteri 02]

- Restriction in accuracy: SSPRK are restricted to fourth-order (if one insists on never stepping backward in time) [Ruuth & Spiteri 02]
- Difficult to accommodate implicit and explicit substeps
 - implicit RK schemes of order ≥ 2 cannot be SSP [Gottlieb, Shu, Tadmor 01]
 - explicit methods suffer from parabolic CFL restriction $\tau \le ch^2$

- **Definition:** efficiency ratio of any s-stage ERK method
 - τ^* : maximal time step that makes forward Euler method IDP
 - $\tilde{\tau}$: maximal time step that makes s-stage ERK method IDP

$$c_{\text{eff}} := \frac{\tilde{\tau}}{s\tau^*}$$
 (usually, $c_{\text{eff}} \le 1$)

- **Definition:** efficiency ratio of any s-stage ERK method
 - τ^* : maximal time step that makes forward Euler method IDP
 - $\tilde{\tau}$: maximal time step that makes s-stage ERK method IDP

$$c_{\text{eff}} := \frac{\tilde{\tau}}{s\tau^*}$$
 (usually, $c_{\text{eff}} \le 1$)

• Do we care? Under the same CFL constraint, # flux evaluations to reach some T for s-stage ERK is $\frac{1}{C_{off}} \times$ that for forward Euler method

- **Definition:** efficiency ratio of any s-stage ERK method
 - ullet au^* : maximal time step that makes forward Euler method IDP
 - \bullet $\tilde{\tau}$: maximal time step that makes s-stage ERK method IDP

$$c_{\text{eff}} := \frac{\tilde{\tau}}{s\tau^*}$$
 (usually, $c_{\text{eff}} \le 1$)

- Do we care? Under the same CFL constraint, # flux evaluations to reach some T for s-stage ERK is $\frac{1}{c_{\text{eff}}} \times$ that for forward Euler method
- SSPRK methods are usually inefficient!
 - $c_{\text{eff}} = \frac{1}{2} \text{ for SSPRK}(2,2)$
 - $c_{\text{eff}} = \frac{1}{3} \text{ for SSPRK}(3,3)$
 - $c_{\text{eff}} = \frac{3}{2} \text{ for SSPRK}(4,3)$

- **Definition:** efficiency ratio of any s-stage ERK method
 - τ^* : maximal time step that makes forward Euler method IDP
 - $\tilde{\tau}$: maximal time step that makes s-stage ERK method IDP

$$c_{\text{eff}} := \frac{\bar{\tau}}{s\tau^*}$$
 (usually, $c_{\text{eff}} \le 1$)

- Do we care? Under the same CFL constraint, # flux evaluations to reach some T for s-stage ERK is $\frac{1}{C_{\text{eff}}} \times$ that for forward Euler method
- SSPRK methods are usually inefficient!
 - $c_{\text{eff}} = \frac{1}{2} \text{ for SSPRK}(2,2)$
 - $c_{\text{eff}} = \frac{1}{3}$ for SSPRK(3,3)
 - $c_{\text{eff}} = \frac{1}{2} \text{ for SSPRK}(4,3)$
- **Notation:** RK(s, p; e) for s-stage, pth-order method, efficiency ratio e SSPRK($2, 2; \frac{1}{2}$) SSPRK($3, 3; \frac{1}{3}$) SSPRK($4, 3; \frac{1}{2}$)

Our contribution

• Introduce a new methodology that makes any ERK scheme IDP

Our contribution

- Introduce a new methodology that makes any ERK scheme IDP
- Introduce a new methodology that makes any IMEX scheme IDP

Our contribution

- Introduce a new methodology that makes any ERK scheme IDP
- Introduce a new methodology that makes any IMEX scheme IDP
- Benefits
 - · employ optimally efficient methods
 - break order barriers
 - introduce IDP-IMEX schemes of order $p \ge 2$

Examples of optimally efficient ERK methods

• We will see that for an ERK-IDP scheme, maximal efficiency with $c_{\text{eff}} = 1$ is reached for equi-distributed sub-stages

Examples of optimally efficient ERK methods

- We will see that for an ERK-IDP scheme, maximal efficiency with $c_{\text{eff}} = 1$ is reached for equi-distributed sub-stages
- RK(2,2;1) (midpoint), RK(3,3;1) (Heun), RK(4,3;1) [fourth-order on linear pb.]

• RK(5,4;1), RK(6,4;1) [fifth-order on linear pb.] and RK(7,5;1) [AE & JLG 22]

IDP ERK schemes

Peep under the hood of SSP (1/3)

• The beauty of SSP is that the forward Euler substep is a black box

Peep under the hood of SSP (1/3)

- The beauty of SSP is that the forward Euler substep is a black box
- This black box involves two fluxes (not just one as one might think)
 - \bullet low-order in space: flux \textbf{F}^L and mass matrix \mathbb{M}^L
 - \bullet high-order in space: flux \textbf{F}^H and mass matrix \mathbb{M}^H

Peep under the hood of SSP (1/3)

- The beauty of SSP is that the forward Euler substep is a black box
- This black box involves two fluxes (not just one as one might think)
 - \bullet low-order in space: flux \textbf{F}^L and mass matrix \mathbb{M}^L
 - high-order in space: flux \mathbf{F}^H and mass matrix \mathbb{M}^H
- Some details

$$\begin{split} \mathbb{M}^{L}\mathbf{U}^{L,n+1} &:= \mathbb{M}^{L}\mathbf{U}^{n} + \tau \mathbf{F}^{L}(\mathbf{U}^{n}) \\ \mathbb{M}^{H}\mathbf{U}^{H,n+1} &:= \mathbb{M}^{H}\mathbf{U}^{n} + \tau \mathbf{F}^{H}(\mathbf{U}^{n}) \end{split}$$

Peep under the hood of SSP (1/3)

- The beauty of SSP is that the forward Euler substep is a black box
- This black box involves two fluxes (not just one as one might think)
 - \bullet low-order in space: flux \textbf{F}^L and mass matrix \mathbb{M}^L
 - high-order in space: flux \mathbf{F}^H and mass matrix \mathbb{M}^H
- Some details

$$\begin{split} \mathbb{M}^{L}\mathbf{U}^{L,n+1} &:= \mathbb{M}^{L}\mathbf{U}^{n} + \tau \mathbf{F}^{L}(\mathbf{U}^{n}) \\ \mathbb{M}^{H}\mathbf{U}^{H,n+1} &:= \mathbb{M}^{H}\mathbf{U}^{n} + \tau \mathbf{F}^{H}(\mathbf{U}^{n}) \end{split}$$

Starting from $\mathbf{U}^n \in \mathcal{A}^I$,

- $U^{L,n+1} \in \mathcal{A}^I$ under CFL, but is low-order accurate ...
- $U^{H,n+1}$ departs from \mathcal{A}^I but is high-order accurate ...

 \implies employ a limiter to construct new update $\mathbf{U}^{n+1} \in \mathcal{A}^I$ as close as possible to $\mathbf{U}^{H,n+1}$

Peep under the hood of SSP (2/3)

- Let us formalize a little bit
- Assumption 1. [forward Euler with low-order flux is IDP under CFL condition] $\exists \tau^* \text{ s.t. } \forall \tau \in (0, \tau^*] \text{ and all } \mathbf{V} \in (\mathbb{R}^m)^I,$

$$\left\{ \mathbf{V} \in \mathcal{A}^I \right\} \implies \left\{ \mathbf{V} + \tau (\mathbb{M}^{\mathrm{L}})^{-1} \mathbf{F}^{\mathrm{L}}(\mathbf{V}) \in \mathcal{A}^I \right\}$$

Peep under the hood of SSP (2/3)

- Let us formalize a little bit
- Assumption 1. [forward Euler with low-order flux is IDP under CFL condition] $\exists \tau^* \text{ s.t. } \forall \tau \in (0, \tau^*] \text{ and all } \mathbf{V} \in (\mathbb{R}^m)^I$,

$$\left\{\mathbf{V} \in \mathcal{A}^I\right\} \implies \left\{\mathbf{V} + \tau(\mathbb{M}^{\mathrm{L}})^{-1}\mathbf{F}^{\mathrm{L}}(\mathbf{V}) \in \mathcal{A}^I\right\}$$

• Assumption 2. [nonlinear limiting operator] $\ell : \mathcal{A}^I \times (\mathbb{R}^m)^I \times (\mathbb{R}^m)^I \to (\mathbb{R}^m)^I$ s.t. for all $(V, \mathbf{F}^L, \mathbf{F}^H)$,

$$\left\{ \mathbf{V} + \tau(\mathbf{M}^{\mathrm{L}})^{-1} \mathbf{F}^{\mathrm{L}}(\mathbf{V}) \in \mathcal{A}^{I} \right\} \implies \left\{ \ell(\mathbf{V}, \mathbf{F}^{\mathrm{L}}, \mathbf{F}^{\mathrm{H}}) \in \mathcal{A}^{I} \right\}$$

Key idea: $\ell(\mathbf{V}, \mathbf{F}^L, \mathbf{F}^H)$ is built as a convex combination of $\mathbf{V} + \tau(\mathbb{M}^L)^{-1}\mathbf{F}^L$ and $\mathbf{V} + \tau(\mathbb{M}^L)^{-1}\mathbf{F}^H$

Peep under the hood of SSP (2/3)

- Let us formalize a little bit
- Assumption 1. [forward Euler with low-order flux is IDP under CFL condition] $\exists \tau^* \text{ s.t. } \forall \tau \in (0, \tau^*] \text{ and all } \mathbf{V} \in (\mathbb{R}^m)^I,$

$$\left\{ \mathbf{V} \in \mathcal{A}^I \right\} \implies \left\{ \mathbf{V} + \tau (\mathbb{M}^{\mathrm{L}})^{-1} \mathbf{F}^{\mathrm{L}} (\mathbf{V}) \in \mathcal{A}^I \right\}$$

• Assumption 2. [nonlinear limiting operator] $\ell: \mathcal{A}^I \times (\mathbb{R}^m)^I \times (\mathbb{R}^m)^I \to (\mathbb{R}^m)^I$ s.t. for all $(\mathbf{V}, \mathbf{F}^L, \mathbf{F}^H)$,

$$\left\{ \mathbf{V} + \tau(\mathbb{M}^{\mathrm{L}})^{-1}\mathbf{F}^{\mathrm{L}}(\mathbf{V}) \in \mathcal{A}^{I} \right\} \implies \left\{ \ell(\mathbf{V}, \mathbf{F}^{\mathrm{L}}, \mathbf{F}^{\mathrm{H}}) \in \mathcal{A}^{I} \right\}$$

Key idea: $\ell(V, F^L, F^H)$ is built as a convex combination of $V + \tau(\mathbb{M}^L)^{-1}F^L$ and $V + \tau(\mathbb{M}^L)^{-1}F^H$

• Notice that both low/high-order updates start from the same vector **V**

Peep under the hood of SSP (3/3)

- Given \mathbf{U}^n in the invariant set \mathcal{A}^I
- The forward Euler step proceeds as follows:
 - compute low-order flux $\mathbf{F}^{L}(\mathbf{U}^{n})$
 - compute high-order flux $\mathbf{F}^{\mathbf{H}}(\mathbf{U}^n)$
 - compute update by limiting

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

Peep under the hood of SSP (3/3)

- Given \mathbf{U}^n in the invariant set \mathcal{A}^I
- The forward Euler step proceeds as follows:
 - compute low-order flux $\mathbf{F}^{\mathbf{L}}(\mathbf{U}^n)$
 - compute high-order flux $\mathbf{F}^{\mathbf{H}}(\mathbf{U}^n)$
 - compute update by limiting

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

• (Well-known) Proposition. [Forward Euler is IDP] Let Assumptions 1 and 2 be met. Assume $\mathbf{U}^n \in \mathcal{A}^I$. Then, $\mathbf{U}^{n+1} \in \mathcal{A}^I$ for all $\tau \in (0, \tau^*]$

• We are now ready to go high-order in time!

- We are now ready to go high-order in time!
- Externalize the limiting process at each ERK stage

- We are now ready to go high-order in time!
- Externalize the limiting process at each ERK stage
- Rewrite ERK scheme in incremental form: at each stage,
 - compute low/high-order updates using a common previous IDP-update
 - apply limiter

- We are now ready to go high-order in time!
- Externalize the limiting process at each ERK stage
- Rewrite ERK scheme in incremental form: at each stage,
 - compute low/high-order updates using a common previous IDP-update
 - apply limiter

• Literature:

- idea of externalizing the limiter proposed independently in [Kuzmin, Quezada de Luna, Ketcheson, Grüll, 22] for ERK and in [Quezada de Luna, Ketcheson 22] for DIRK
- central idea of writing scheme in incremental form and maximizing efficiency only in [AE, JLG 22]
- schemes with two time-derivatives [Gottlieb, Grant, Hu, Shu 22]

Butcher tableau of s-stage ERK method

• Generic form of Butcher tableau

Butcher tableau of s-stage ERK method

• Generic form of Butcher tableau

• Rename last line, set $c_1 := 0$ and $c_{s+1} := 1$

Butcher tableau of s-stage ERK method

Generic form of Butcher tableau

• Rename last line, set $c_1 := 0$ and $c_{s+1} := 1$

- Assume $c_k \ge 0$ for all $k \in \{1:s+1\}$
- For all $l \in \{2:s+1\}$, set

$$l'(l) := \max\{k < l \mid c_k \le c_l\}$$

Think of l'(l) := l - 1 if sequence $(c_l)_{l \in \{1:s+1\}}$ is increasing

• Let $\mathbf{U}^n \in \mathcal{A}^I$ and set $\mathbf{U}^{n,1} := \mathbf{U}^n$

- Let $\mathbf{U}^n \in \mathcal{A}^I$ and set $\mathbf{U}^{n,1} := \mathbf{U}^n$
- Loop over $l \in \{2:s+1\}$ (stage index)

- Let $\mathbf{U}^n \in \mathcal{A}^I$ and set $\mathbf{U}^{n,1} := \mathbf{U}^n$
- Loop over $l \in \{2:s+1\}$ (stage index)
- Compute low-order update starting from $\mathbf{U}^{n,l'}$ (think of l' = l 1)

$$\mathbb{M}^{\mathsf{L}}\mathbf{U}^{\mathsf{L},l} := \mathbb{M}^{\mathsf{L}}\mathbf{U}^{n,l'} + \tau \underbrace{(c_l - c_{l'})\mathbf{F}^{\mathsf{L}}(\mathbf{U}^{n,l'})}_{:=\mathbf{\Phi}^{\mathsf{L}}}$$

- Let $\mathbf{U}^n \in \mathcal{A}^I$ and set $\mathbf{U}^{n,1} := \mathbf{U}^n$
- Loop over $l \in \{2:s+1\}$ (stage index)
- Compute low-order update starting from $\mathbf{U}^{n,l'}$ (think of l' = l 1)

$$\mathbb{M}^{L}\mathbf{U}^{L,l} := \mathbb{M}^{L}\mathbf{U}^{n,l'} + \tau \underbrace{(c_{l} - c_{l'})\mathbf{F}^{L}(\mathbf{U}^{n,l'})}_{:=\mathbf{\Phi}^{L}}$$

• Compute high-order update using same starting point $\mathbf{U}^{n,l'}$ (incremental form)

$$\mathbb{M}^{\mathbf{H}}\mathbf{U}^{\mathbf{H},l} := \mathbb{M}^{\mathbf{H}}\mathbf{U}^{n,l'} + \tau \sum_{\substack{k \in \{1:l-1\}\\ := \mathbf{\Phi}^{\mathbf{H}}}} (a_{l,k} - a_{l',k}) \mathbf{F}^{\mathbf{H}}(\mathbf{U}^{n,k})$$

- Let $\mathbf{U}^n \in \mathcal{A}^I$ and set $\mathbf{U}^{n,1} := \mathbf{U}^n$
- Loop over $l \in \{2:s+1\}$ (stage index)
- Compute low-order update starting from $\mathbf{U}^{n,l'}$ (think of l' = l 1)

$$\mathbb{M}^{L}\mathbf{U}^{L,l} := \mathbb{M}^{L}\mathbf{U}^{n,l'} + \tau \underbrace{(c_{l} - c_{l'})\mathbf{F}^{L}(\mathbf{U}^{n,l'})}_{:=\mathbf{\Phi}^{L}}$$

• Compute high-order update using same starting point $\mathbf{U}^{n,l'}$ (incremental form)

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

$$:= \mathbf{\Phi}^{\mathbf{H}}$$

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

- Let $\mathbf{U}^n \in \mathcal{A}^I$ and set $\mathbf{U}^{n,1} := \mathbf{U}^n$
- Loop over $l \in \{2:s+1\}$ (stage index)
- Compute low-order update starting from $\mathbf{U}^{n,l'}$ (think of l' = l 1)

$$\mathbb{M}^{\mathbf{L}}\mathbf{U}^{\mathbf{L},l} := \mathbb{M}^{\mathbf{L}}\mathbf{U}^{n,l'} + \tau \underbrace{\left(c_{l} - c_{l'}\right)}_{:=\mathbf{\Phi}^{\mathbf{L}}}$$

• Compute high-order update using same starting point $\mathbf{U}^{n,l'}$ (incremental form)

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

$$:= \mathbf{\Phi}^{\mathbf{H}}$$

- Apply limiter: $\mathbf{U}^{n,l} := \ell(\mathbf{U}^{n,l'}, \mathbf{\Phi}^{L}, \mathbf{\Phi}^{H})$
- End of loop: return $\mathbf{U}^{n+1} := \mathbf{U}^{n,s+1}$

Main results

• Theorem. [IDP-ERK scheme] Let Assumptions 1 and 2 be met. Assume $\mathbf{U}^n \in \mathcal{A}^I$. Then, $\mathbf{U}^{n+1} \in \mathcal{A}^I$ (as well as all intermediate stages) for all

$$\tau \in (0, \tau^* / \max_{l \in \{2:s+1\}} (c_l - c_{l'})]$$

Main results

• **Theorem.** [IDP-ERK scheme] Let Assumptions 1 and 2 be met. Assume $\mathbf{U}^n \in \mathcal{A}^I$. Then, $\mathbf{U}^{n+1} \in \mathcal{A}^I$ (as well as all intermediate stages) for all

$$\tau \in (0, \tau^* / \max_{l \in \{2:s+1\}} (c_l - c_{l'})]$$

- Corollary. [Optimal efficiency]
 - $c_{\text{eff}} = 1/(s \max_{l \in \{2:s+1\}} (c_l c_{l'}))$
 - optimal efficiency (with $c_{\text{eff}} = 1$) reached when points $(c_l)_{l \in \{1:s+1\}}$ are equi-distributed in [0, 1]

Examples: second- and third-order methods

• Some optimal methods: RK(2,2;1), RK(3,3;1), RK(4,3;1)

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

Examples: second- and third-order methods

• Some optimal methods: RK(2,2;1), RK(3,3;1), RK(4,3;1)

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

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

• Some non-optimal methods: $SSPRK(2,2;\frac{1}{2})$, $SSPRK(3,3;\frac{1}{3})$

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

Examples: fourth-order methods

• Two popular but sub-optimal methods: $RK(4,4;\frac{1}{2})$ and $RK(4,4;\frac{3}{4})$

Examples: fourth-order methods

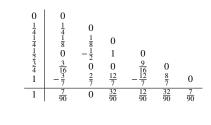
• Two popular but sub-optimal methods: $RK(4,4;\frac{1}{2})$ and $RK(4,4;\frac{3}{4})$

• Optimal RK(5,4;1) and RK(6,4;1) devised in [AE & JLG 22] [both can be used within an IMEX scheme]

RK(6,4;1) is fifth-order accurate on linear problems

Examples: fifth-order methods

• Butcher's method RK(6,5; $\frac{2}{3}$) (requires $c_6 = 1$)



Examples: fifth-order methods

• Butcher's method RK(6,5; $\frac{2}{3}$) (requires $c_6 = 1$)

• Novel RK(7,5;1) method [AE & JLG 22]

| 0 | 0 | | | | |
|----------------|--------------------|---------------------|---------------------|---------------------|---|
| 1 7 | 0.1428571428571428 | 0 | | | |
| 2 7 | 0.0107112392440216 | 0.2750030464702641 | 0 | | |
| 37 | 0.4812641640977338 | -0.9634955610240432 | 0.9108028254977381 | 0 | |
| 4 7 | 0.3718168921589701 | -0.5615016072648120 | 0.5590150320681445 | 0.2020982544662687 | 0 |
| <u>5</u> | 0.2210152091353413 | 0.3526985345185138 | -0.8940286416537777 | 0.8097519357352928 | |
| <u>6</u> | 0.2038005573304709 | -0.4759394836772968 | 1.0938423462712870 | -0.2853403360392873 | |
| 1 | 0.0979996468518433 | -0.0044680013474903 | 0.3592897484042552 | 0.0225280828210172 | |

Methodology for numerical tests

• All the tests are done by fixing $CFL \in (0, 1]$ and setting

$$\tau := \mathrm{CFL} \times s \times \tau^*$$

 \implies all the methods perform the same number of flux evaluations and limiting operations independently of s

 \implies each method is IDP at least up to CFL $\leq c_{\text{eff}}$

Methodology for numerical tests

• All the tests are done by fixing $CFL \in (0, 1]$ and setting

$$\tau := \mathrm{CFL} \times s \times \tau^*$$

 \implies all the methods perform the same number of flux evaluations and limiting operations independently of s

 \implies each method is IDP at least up to CFL $\leq c_{\text{eff}}$

- Local maximum/minimum principle enforced at every dof (relaxation performed as in [Guermond, Popov, Tomas, 19])
- Global maximum/minimum principle strictly enforced

Methodology for numerical tests

• All the tests are done by fixing $CFL \in (0, 1]$ and setting

$$\tau := \mathrm{CFL} \times s \times \tau^*$$

 \implies all the methods perform the same number of flux evaluations and limiting operations independently of s

 \implies each method is IDP at least up to CFL $\leq c_{\text{eff}}$

- Local maximum/minimum principle enforced at every dof (relaxation performed as in [Guermond, Popov, Tomas, 19])
- Global maximum/minimum principle strictly enforced
- Affine constraints defining \mathcal{A} : Flux-Corrected Transport (FCT) [Boris & Book 73; Zalesak 79; Kuzmin, Löhner, Turek 12]
- Non-affine constraints: some nonlinear technique
 [Sanders 88; Coquel & LeFloch 91; Liu & Osher 96; Zhang & Shu 11; Lohman & Kuzmin 16; Guermond, Nazarov, Popov, Tomas 18]

1D linear transport, 4th-order FD (1/3)

• Linear transport, D := (0, 1), periodic BCs

$$\partial_t u + \partial_x u = 0, \qquad u_0(x) := \begin{cases} (4 \frac{(x - x_0)(x_1 - x)}{(x_1 - x_0)^2})^6 & x \in (x_0, x_1) := (0.1, 0.4) \\ 0 & \text{otherwise} \end{cases}$$

• 4th order Finite Differences in space

1D linear transport, 4th-order FD (1/3)

• Linear transport, D := (0, 1), periodic BCs

$$\partial_t u + \partial_x u = 0, \qquad u_0(x) := \begin{cases} (4 \frac{(x - x_0)(x_1 - x)}{(x_1 - x_0)^2})^6 & x \in (x_0, x_1) := (0.1, 0.4) \\ 0 & \text{otherwise} \end{cases}$$

- 4th order Finite Differences in space
- In the *L*¹-norm, all the methods achieve the expected convergence order with CFL of the order of 0.5
- Let us look at the more challenging L^{∞} -error measure

1D linear transport, 4th-order FD (2/3)

• Second-order methods: RK(2,2;1) outperforms SSPRK(2,2; $\frac{1}{2}$)

| | | CF | L = 0.2 | | CFL = 0.25 | | | | | |
|------|-------------|------|----------------------------|--------|-------------|------|----------------------------|------|--|--|
| I | RK(2, 2; 1) | rate | $SSPRK(2, 2; \frac{1}{2})$ |) rate | RK(2, 2; 1) | rate | $SSPRK(2, 2; \frac{1}{2})$ | 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 | 50 | | |

1D linear transport, 4th-order FD (2/3)

• Second-order methods: RK(2,2;1) outperforms SSPRK(2,2; $\frac{1}{2}$)

| | | CF | L = 0.2 | CFL = 0.25 | | | | | |
|------|-------------|------|----------------------------|------------|-------------|------|----------------------------|------|--|
| I | RK(2, 2; 1) | rate | $SSPRK(2, 2; \frac{1}{2})$ | rate | RK(2, 2; 1) | rate | $SSPRK(2, 2; \frac{1}{2})$ | 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 | 50 | |

• Third-order methods: SSPRK $(3,3;\frac{1}{3})$ behaves poorly, RK(4,3;1) performs best

| | | CFL = 0.0 | | CFL = 0.25 | | | | | | | | |
|------|-----------|-----------|----------------------------|------------|-----------|------|-----------|------|----------------------------|------|-----------|------|
| I | RK(3,3;1) | rate | SSPRK(3,3; $\frac{1}{3}$) | rate | RK(4,3;1) | rate | RK(3,3;1) | rate | SSPRK(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 (3/3)

• Fourth-order methods: RK(5,4;1) outperforms SSPRK(5,4; $\frac{1}{2}$)

| | | CFL = 0.0 | | CFL = 0.2 | | | | | | | | |
|------|-----------------------|-----------|--------------------------|-----------|-----------|------|-----------------------|--------|----------------------------|------|-----------|------|
| I | $RK(4,4;\frac{1}{2})$ | rate | SSPRK(5,4; $\frac{1}{2}$ |) rate | RK(5,4;1) | rate | $RK(4,4;\frac{1}{2})$ |) rate | SSPRK(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 (3/3)

• Fourth-order methods: RK(5,4;1) outperforms SSPRK(5,4; $\frac{1}{2}$)

| | | CFL = 0.05 | | CFL = 0.2 | | | | | | | | |
|------|-----------------------|------------|--------------------------|-----------|-----------|------|-----------------------|------|----------------------------|------|-----------|------|
| I | $RK(4,4;\frac{1}{2})$ | rate | $SSPRK(5,4;\frac{1}{2})$ | rate | RK(5,4;1) | rate | $RK(4,4;\frac{1}{2})$ | rate | SSPRK(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 |

• Fifth-order methods: no SSP competitor!

| | C | CFL = | 0.02 | CFL = 0.025 | | | | | |
|------|-----------------------|-------|-----------|-------------|-----------------------|------|-----------|------|--|
| I | $RK(6,5;\frac{1}{3})$ | 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 | |

Linear transport with non-smooth solution

- Three-solid problem with rotating advection field [Zalesak 79]
- Continuous \mathbb{P}^1 -FEM on unstructured non-nested Delaunay meshes
- Solutions at T = 1 using RK(2,2;1) (midpoint rule) at CFL = 0.25 [From left to right: I = 6561; I = 24917; I = 98648; I = 389860 dofs]



• Relative error in L^1 -norm for RK(2,2;1) and RK(4,3;1)

| I | 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 (1/3)

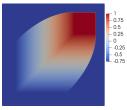
• 2D Burgers' equation in $D := (-.25, 1.75)^2$

$$\partial_t u + \nabla \cdot \mathbf{f}(u) = 0, \qquad \mathbf{f}(u) := \frac{1}{2}(u^2, u^2)^\mathsf{T}$$

with initial data

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

- This problem exhibits many sonic points, which makes methods with too little low/high-order viscosity to fail [Guermond, Popov 17]
- Solution at T = 0.65 computed with RK(4,3;1) at CFL = 0.25 using 801^2 grid points



2D Burgers' equation (2/3)

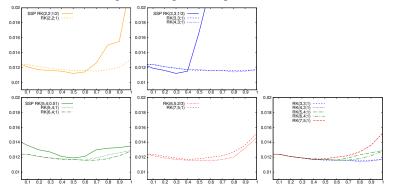
• T = 0.65, CFL = 0.25, relative L^1 -error for all the methods

| I | RK(2,1;1) | rate | SSPRK(2,2 | $(\frac{1}{2})$ | rate | I | RK | (3,3;1) | rate | SSPRK(| $3,3;\frac{1}{3}$) | rate | R | K(4,3;1) | rate |
|-----|-----------------------|------|-----------------------|-----------------|------|---------|-----------------|---------|-----------|--------|---------------------|------|------|----------|------|
| 50 | 6.61E-02 | - | 6.70E-02 | 2 | - | 50 | 6.6 | 1E-02 | - | 6.74E | -02 | - | 6 | .62E-02 | - |
| 100 | 3.31E-02 | 1.00 | 3.34E-02 | 2 | 1.00 | 100 | 3.3 | 1E-02 | 1.00 | 3.35E | -02 | 1.01 | 3 | .31E-02 | 1.00 |
| 200 | 2.12E-02 | 0.65 | 2.12E-02 | 2 | 0.66 | 200 | 2.1 | 2E-02 | 0.65 | 2.13E | -02 | 0.66 | 2 | .12E-02 | 0.65 |
| 400 | 1.20E-02 | 0.82 | 1.16E-02 | 2 | 0.87 | 400 | 1.2 | 0E-02 | 0.82 | 1.15E | -02 | 0.89 | 1 | .20E-02 | 0.82 |
| 800 | 6.04E-03 | 0.99 | 5.73E-03 | 3 | 1.02 | 800 | 6.0 | 04E-03 | 0.99 | 5.72E | -03 | 1.01 | 6 | .04E-03 | 0.99 |
| I | $RK(4,4;\frac{1}{2})$ | rate | $RK(4,4;\frac{3}{4})$ | rate | SSPI | RK(5,4; | $\frac{1}{2}$) | rate | RK(5,4;1) | rate | RK(6,4 | 1) | rate | | |
| 50 | 6.74E-02 | - | 6.63E-02 | - | 6 | .72E-02 | | - | 6.63E-02 | - | 6.60E-0 |)2 | - | 1 | |
| 100 | 3.35E-02 | 1.01 | 3.31E-02 | 1.00 | 3 | 43E-02 | | 0.97 | 3.32E-02 | 1.00 | 3.30E-0 |)2 | 1.00 | | |
| 200 | 2.13E-02 | 0.66 | 2.11E-02 | 0.65 | 2 | .26E-02 | | 0.60 | 2.12E-02 | 0.64 | 2.11E-0 |)2 | 0.64 | | |
| 400 | 1.17E-02 | 0.87 | 1.18E-02 | 0.84 | 1. | 28E-02 | | 0.82 | 1.20E-02 | 0.82 | 1.20E-0 |)2 | 0.82 | | |
| 800 | 5.75E-03 | 1.02 | 5.84E-03 | 1.02 | 6 | .20E-03 | | 1.05 | 6.06E-03 | 0.99 | 6.03E-0 |)3 (| 0.99 | | |
| I | $RK(6,5;\frac{2}{3})$ | rate | RK(7,5;1) | rate | | | | | | | | | | | |
| 50 | 6.65E-02 | - | 6.62E-02 | - | | | | | | | | | | | |
| 100 | 3.32E-02 | 1.00 | 3.31E-02 | 1.00 | | | | | | | | | | | |
| 200 | 2.11E-02 | 0.65 | 2.12E-02 | 0.65 | | | | | | | | | | | |
| 400 | 1.18E-02 | 0.84 | 1.20E-02 | 0.82 | | | | | | | | | | | |
| 800 | 5.79E-03 | 1.02 | 6.06E-03 | 0.99 | | | | | | | | | | | |
| | | | | | | | | | | | | | | | |

• \Longrightarrow at moderate CFL, all the methods converge equally well (all at order one)

2D Burgers' equation (3/3)

- Challenge methods by increasing CFL
- Results for second- and third-order methods (top), fourth-order, fifth-order methods plus a recap for all optimal methods



• \Longrightarrow SSPRK (2,2) and SSPRK(3,3) start loosing accuracy at CFL \approx 0.5, whereas IDP-ERK methods behave well over whole CFL range

 All IDP-ERK methods perform as well, and often better, than SSPRK methods of the same order

- All IDP-ERK methods perform as well, and often better, than SSPRK methods of the same order
- RK(2,2;1) (midpoint rule) outperforms popular SSPRK(2,2; $\frac{1}{2}$)
- RK(4,3;1) (vastly) outperforms popular SSPRK(3,3; $\frac{1}{3}$)

- All IDP-ERK methods perform as well, and often better, than SSPRK methods of the same order
- RK(2,2;1) (midpoint rule) outperforms popular SSPRK(2,2; $\frac{1}{2}$)
- RK(4,3;1) (vastly) outperforms popular SSPRK(3,3; $\frac{1}{3}$)
- The considered fourth-order methods provide comparable results

- All IDP-ERK methods perform as well, and often better, than SSPRK methods of the same order
- RK(2,2;1) (midpoint rule) outperforms popular SSPRK(2,2; $\frac{1}{2}$)
- RK(4,3;1) (vastly) outperforms popular SSPRK(3,3; $\frac{1}{3}$)
- The considered fourth-order methods provide comparable results
- Novel fifth-order IDP-ERK method with no SSP competitor

IDP IMEX schemes

- Consider low-order and high-order fluxes for
 - hyperbolic terms
 - parabolic (diffusion/relaxation) terms

- Consider low-order and high-order fluxes for
 - hyperbolic terms
 - parabolic (diffusion/relaxation) terms
- Quasi-linearization of parabolic fluxes (both low- and high-order)

- Consider low-order and high-order fluxes for
 - hyperbolic terms
 - parabolic (diffusion/relaxation) terms
- Quasi-linearization of parabolic fluxes (both low- and high-order)
- Key assumption: Under CFL condition, we have two IDP steps
 - forward Euler with low-order hyperbolic flux
 - backward Euler with low-order quasi-linear parabolic flux

- Consider low-order and high-order fluxes for
 - hyperbolic terms
 - parabolic (diffusion/relaxation) terms
- Quasi-linearization of parabolic fluxes (both low- and high-order)
- Key assumption: Under CFL condition, we have two IDP steps
 - forward Euler with low-order hyperbolic flux
 - backward Euler with low-order quasi-linear parabolic flux
- Rewrite IMEX scheme in incremental form

- Consider low-order and high-order fluxes for
 - hyperbolic terms
 - parabolic (diffusion/relaxation) terms
- Quasi-linearization of parabolic fluxes (both low- and high-order)
- Key assumption: Under CFL condition, we have two IDP steps
 - forward Euler with low-order hyperbolic flux
 - backward Euler with low-order quasi-linear parabolic flux
- Rewrite IMEX scheme in incremental form
- Apply (possibly distinct) limiters to hyperbolic and parabolic substeps

Butcher tableaux

• Explicit Butcher tableau

Butcher tableaux

• Explicit Butcher tableau

• Implicit Butcher tableau

Butcher tableaux

• Explicit Butcher tableau

• Implicit Butcher tableau

• Both tableaux share the same coefficients $(c_l)_{l \in \{1:s+1\}}$

Examples: second-order IMEX

• Heun + Crank–Nicolson: efficiency ratio is $\frac{1}{2}$

Examples: second-order IMEX

• Heun + Crank–Nicolson: efficiency ratio is $\frac{1}{2}$

• Explicit + implicit midpoint rules: efficiency ratio is 1

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

Examples: third-order IMEX (1/2)

• Three-stage, third-order method [Nørsett 74, Crouzeix 75] $(\gamma := \frac{1}{2} + \frac{1}{2\sqrt{3}} \approx 0.78867)$

• Implicit method is A-stable, but efficiency ratio is only $\frac{1}{3}\gamma \approx 0.26$

Examples: third-order IMEX (1/2)

• Three-stage, third-order method [Nørsett 74, Crouzeix 75] $(\gamma := \frac{1}{2} + \frac{1}{2\sqrt{3}} \approx 0.78867)$

- Implicit method is A-stable, but efficiency ratio is only $\frac{1}{3}\gamma \approx 0.26$
- New scheme with optimal efficiency 1 [AE & JLG 22]

 Implicit method has the same amplification function as above (and hence is A-stable)

Examples: third-order IMEX (2/2)

- Novel four-stage, third-order IMEX scheme with optimal efficiency 1 and implicit method is L-stable
- Explicit scheme is ERK(4,3;1) (already considered!)

• Implicit scheme as follows:

| 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 |
| 1 | 0 | 2/3 | $-\frac{1}{3}$ | 2/3 |

Examples: fourth-order IMEX

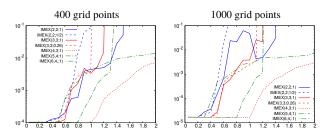
- Five- and six-stage schemes reviewed in [Carpenter & Kennedy 19]
- Novel five-stage scheme devised in [AE & JLG 22]
 - optimal efficiency 1
 - implicit scheme is singly diagonal and L-stable
- Novel six-stage scheme devised in [AE & JLG 22] with similar properties
 - the scheme is of linear order 5

Compressible Navier-Stokes equations, 1D

- Travelling viscous wave [Becker, 1922; Johnson, 13], $\Omega := [-0.5, 1]$, T = 3
- Ideal gas law, constant properties ($\mu = 0.01, Pr = 0.75$)
- \bullet Cumulated relative L^1 -error on density, momentum and total energy
- Challenge all IMEX methods by increasing CFL

Compressible Navier-Stokes equations, 1D

- Travelling viscous wave [Becker, 1922; Johnson, 13], $\Omega := [-0.5, 1], T = 3$
- Ideal gas law, constant properties ($\mu = 0.01, Pr = 0.75$)
- \bullet Cumulated relative L^1 -error on density, momentum and total energy
- Challenge all IMEX methods by increasing CFL



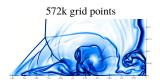
- Main conclusions:
 - IMEX(2, 2; 1) always outperforms IMEX(2, 2; $\frac{1}{2}$)
 - IMEX(4, 3; 1) outperforms the other two third-order methods
 - IMEX(6, 4; 1) slightly more robust than IMEX(5, 4; 1)

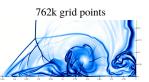
Compressible Navier-Stokes equations, 2D

- Viscous shock tube problem [Daru & Tenaud, 01, 09]
- $\Omega := [0, 1] \times [0, \frac{1}{2}], T = 1$
- Ideal gas law, constant properties ($\mu = 0.001, Pr = 0.73$)
- \mathbb{P}_1 Lagrange FEM, IMEX(4, 3; 1) at CFL = 1.5

Compressible Navier-Stokes equations, 2D

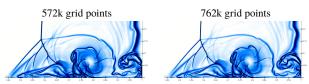
- Viscous shock tube problem [Daru & Tenaud, 01, 09]
- $\Omega := [0, 1] \times [0, \frac{1}{2}], T = 1$
- Ideal gas law, constant properties ($\mu = 0.001, Pr = 0.73$)
- \mathbb{P}_1 Lagrange FEM, IMEX(4, 3; 1) at CFL = 1.5
- Density isocontours





Compressible Navier-Stokes equations, 2D

- Viscous shock tube problem [Daru & Tenaud, 01, 09]
- $\Omega := [0, 1] \times [0, \frac{1}{2}], T = 1$
- Ideal gas law, constant properties ($\mu = 0.001, Pr = 0.73$)
- \mathbb{P}_1 Lagrange FEM, IMEX(4, 3; 1) at CFL = 1.5
- Density isocontours



• Numerical tests using non-ideal gas laws in progress

Thank you for your attention!

• Gentle introduce ideas on Euler IDP-IMEX scheme

- Gentle introduce ideas on Euler IDP-IMEX scheme
- \mathbf{F}^{L} : Low-order approx. of hyperbolic flux $-\nabla \cdot f(\mathbf{u})$
- $G^{L,lin}(W^n;\cdot)$: Low-order quasi-linear approx. of parabolic flux $-\nabla \cdot g(u,\nabla u) + S(u)$

- Gentle introduce ideas on Euler IDP-IMEX scheme
- \mathbf{F}^{L} : Low-order approx. of hyperbolic flux $-\nabla \cdot f(\mathbf{u})$
- $G^{L,lin}(W^n;\cdot)$: Low-order quasi-linear approx. of parabolic flux $-\nabla \cdot g(u,\nabla u) + S(u)$
- Consider low-order quasi-linear update

$$\mathbb{M}^{L}\mathbf{U}^{L,n+1} = \underbrace{\mathbb{M}^{L}\mathbf{U}^{n} + \tau\mathbf{F}^{L}(\mathbf{U}^{n})}_{=:\mathbb{M}^{L}\mathbf{W}^{L,n}} + \tau\mathbf{G}^{L,\mathrm{lin}}(\mathbf{W}^{L,n};\mathbf{U}^{L,n+1})$$

- Gentle introduce ideas on Euler IDP-IMEX scheme
- \mathbf{F}^{L} : Low-order approx. of hyperbolic flux $-\nabla \cdot f(\mathbf{u})$
- $G^{L,lin}(W^n;\cdot)$: Low-order quasi-linear approx. of parabolic flux $-\nabla \cdot g(u,\nabla u) + S(u)$
- Consider low-order quasi-linear update

$$\mathbb{M}^L \mathbf{U}^{L,n+1} = \underbrace{\mathbb{M}^L \mathbf{U}^n + \tau \mathbf{F}^L(\mathbf{U}^n)}_{=:\mathbb{M}^L \mathbf{W}^{L,n}} + \tau \mathbf{G}^{L,\mathrm{lin}}(\mathbf{W}^{L,n};\mathbf{U}^{L,n+1})$$

- This can be decomposed as
 - hyperbolic sub-step (explicit update):

$$\mathbf{W}^{\mathbf{L},n} := \mathbf{U}^n + \tau(\mathbb{M}^{\mathbf{L}})^{-1}\mathbf{F}^{\mathbf{L}}(\mathbf{U}^n)$$

• parabolic sub-step (quasi-linear solve):

$$\mathbf{U}^{L,n+1} := \left(\mathbb{I} - \tau(\mathbb{M}^L)^{-1}\mathbf{G}^{L,\operatorname{lin}}(\mathbf{W}^{L,n};\cdot)\right)^{-1}(\mathbf{W}^{L,n})$$

Key assumption on low-order fluxes

- Assumption 1. There exists $\tau^* > 0$ s.t. for all $\tau \in (0, \tau^*]$,
 - forward Euler with low-order hyperbolic flux is IDP:

$$\left\{ \mathbf{V} \in \mathcal{A}^I \right\} \implies \left\{ \mathbf{V} + \tau (\mathbb{M}^{\mathrm{L}})^{-1} \mathbf{F}^{\mathrm{L}} (\mathbf{V}) \in \mathcal{A}^I \right\}$$

Key assumption on low-order fluxes

- Assumption 1. There exists $\tau^* > 0$ s.t. for all $\tau \in (0, \tau^*]$,
 - forward Euler with low-order hyperbolic flux is IDP:

$$\left\{ \mathbf{V} \in \mathcal{A}^{I} \right\} \implies \left\{ \mathbf{V} + \tau (\mathbb{M}^{L})^{-1} \mathbf{F}^{L} (\mathbf{V}) \in \mathcal{A}^{I} \right\}$$

• backward Euler with low-order quasi-linear parabolic flux is IDP: For all $\mathbf{W} \in \mathcal{A}^I$, $\mathbb{I} - \tau(\mathbb{M}^L)^{-1}\mathbf{G}^{\mathrm{L},\mathrm{lin}}(\mathbf{W};\cdot): (\mathbb{R}^m)^I \to (\mathbb{R}^m)^I$ is bijective and

$$\left\{\mathbf{V} \in \mathcal{A}^I\right\} \implies \left\{\left(\mathbb{I} - \tau(\mathbb{M}^L)^{-1}\mathbf{G}^{L,\mathrm{lin}}(\mathbf{V};\cdot)\right)^{-1}(\mathbf{V}) \in \mathcal{A}^I\right\}$$

Notice that quasi-linearization is performed at ${\bf V}$

Key assumption on low-order fluxes

- Assumption 1. There exists $\tau^* > 0$ s.t. for all $\tau \in (0, \tau^*]$,
 - forward Euler with low-order hyperbolic flux is IDP:

$$\left\{ \mathbf{V} \in \mathcal{A}^{I} \right\} \implies \left\{ \mathbf{V} + \tau (\mathbb{M}^{L})^{-1} \mathbf{F}^{L} (\mathbf{V}) \in \mathcal{A}^{I} \right\}$$

• backward Euler with low-order quasi-linear parabolic flux is IDP: For all $\mathbf{W} \in \mathcal{A}^I$, $\mathbb{I} - \tau(\mathbb{M}^L)^{-1}\mathbf{G}^{L,\mathrm{lin}}(\mathbf{W};\cdot): (\mathbb{R}^m)^I \to (\mathbb{R}^m)^I$ is bijective and

$$\left\{\mathbf{V} \in \mathcal{A}^I\right\} \implies \left\{\left(\mathbb{I} - \tau(\mathbb{M}^L)^{-1}\mathbf{G}^{L,\mathrm{lin}}(\mathbf{V};\cdot)\right)^{-1}(\mathbf{V}) \in \mathcal{A}^I\right\}$$

Notice that quasi-linearization is performed at V

• (Well-known) Proposition. [Low-order Euler IDP-IMEX] Let Assumption 1 hold. Assume that $\mathbf{U}^n \in \mathcal{A}^I$ and $\tau \in (0, \tau^*]$. Then, $\mathbf{U}^{\mathbf{L}, n+1} \in \mathcal{A}^I$

• We want to use high-order fluxes in space!

- We want to use high-order fluxes in space!
- Assumption 2. There exist two nonlinear limiting operators

$$\ell^{\text{hyp}}, \ell^{\text{par}}: \mathcal{A}^I \times (\mathbb{R}^m)^I \times (\mathbb{R}^m)^I \to (\mathbb{R}^m)^I$$

such that

• for all $(\mathbf{V}, \mathbf{\Phi}^{\mathbb{L}}, \mathbf{\Phi}^{\mathbb{H}}) \in \mathcal{A}^I \times (\mathbb{R}^m)^I \times (\mathbb{R}^m)^I$,

$$\left\{ \mathbf{V} + \tau(\mathbb{M}^L)^{-1}\mathbf{\Phi}^L \in \mathcal{A}^I \right\} \implies \left\{ \ell^{\text{hyp}}(\mathbf{V}, \mathbf{\Phi}^L, \mathbf{\Phi}^H) \in \mathcal{A}^I \right\}$$

• for all $(\mathbf{W}, \mathbf{\Psi}^{\mathbf{L}}, \mathbf{\Psi}^{\mathbf{H}}) \in \mathcal{A}^I \times (\mathbb{R}^m)^I \times (\mathbb{R}^m)^I$,

$$\left\{\mathbf{W} + \tau(\mathbb{M}^{L})^{-1}\mathbf{\Psi}^{L} \in \mathcal{A}^{I}\right\} \implies \left\{\ell^{\mathrm{par}}(\mathbf{W}, \mathbf{\Psi}^{L}, \mathbf{\Psi}^{\mathrm{H}}) \in \mathcal{A}^{I}\right\}$$

- We want to use high-order fluxes in space!
- Assumption 2. There exist two nonlinear limiting operators

$$\ell^{\text{hyp}}, \ell^{\text{par}}: \mathcal{A}^I \times (\mathbb{R}^m)^I \times (\mathbb{R}^m)^I \to (\mathbb{R}^m)^I$$

such that

• for all $(\mathbf{V}, \mathbf{\Phi}^{\mathbf{L}}, \mathbf{\Phi}^{\mathbf{H}}) \in \mathcal{A}^I \times (\mathbb{R}^m)^I \times (\mathbb{R}^m)^I$,

$$\left\{ \mathbf{V} + \tau(\mathbb{M}^L)^{-1}\mathbf{\Phi}^L \in \mathcal{A}^I \right\} \implies \left\{ \ell^{\text{hyp}}(\mathbf{V}, \mathbf{\Phi}^L, \mathbf{\Phi}^H) \in \mathcal{A}^I \right\}$$

 $\bullet \ \, \text{for all} \, (\mathbf{W}, \mathbf{\Psi}^{\mathbb{L}}, \mathbf{\Psi}^{\mathbb{H}}) \in \mathcal{A}^I \times (\mathbb{R}^m)^I \times (\mathbb{R}^m)^I,$

$$\left\{\mathbf{W} + \tau(\mathbb{M}^{L})^{-1}\mathbf{\Psi}^{L} \in \mathcal{A}^{I}\right\} \implies \left\{\ell^{\mathrm{par}}(\mathbf{W}, \mathbf{\Psi}^{L}, \mathbf{\Psi}^{\mathrm{H}}) \in \mathcal{A}^{I}\right\}$$

- Important remarks
 - the invariant domains enforced by the two limiters can be different
 - bounds for limiting are deduced from the low-order updates

• Given $\mathbf{U}^n \in \mathcal{A}^l$, high-order Euler IDP-IMEX proceeds as follows:

$$\mathbf{U}^{n} \underbrace{\overset{(1)}{\longrightarrow} (\mathbf{W}^{L,n+1}, \mathbf{W}^{H,n+1}) \overset{(2)}{\longrightarrow} \mathbf{W}^{n+1}}_{\text{hyperbolic step}} \mathbf{W}^{n+1} \underbrace{\overset{(3)}{\longrightarrow} (\mathbf{U}^{L,n+1}, \mathbf{U}^{H,n+1}) \overset{(4)}{\longrightarrow} \mathbf{U}^{n+1}}_{\text{parabolic step}}$$

• Given $\mathbf{U}^n \in \mathcal{A}^I$, high-order Euler IDP-IMEX proceeds as follows:

$$\mathbf{U}^{n} \xrightarrow{(1)} (\mathbf{W}^{L,n+1}, \mathbf{W}^{H,n+1}) \xrightarrow{(2)} \mathbf{W}^{n+1} \xrightarrow{(3)} (\mathbf{U}^{L,n+1}, \mathbf{U}^{H,n+1}) \xrightarrow{(4)} \mathbf{U}^{n+1}$$
hyperbolic step

• Hyperbolic steps (1) and (2): compute low/high-order updates and limit

$$\begin{split} & \mathbb{M}^L \mathbf{W}^{L,n+1} := \mathbb{M}^L \mathbf{U}^n + \tau \mathbf{F}^L (\mathbf{U}^n), \\ & \mathbb{M}^H \mathbf{W}^{H,n+1} := \mathbb{M}^H \mathbf{U}^n + \tau \mathbf{F}^H (\mathbf{U}^n). \end{split} \qquad \qquad \mathbf{W}^{n+1} := \ell^{hyp} (\mathbf{U}^n, \mathbf{\Phi}^L, \mathbf{\Phi}^H) \end{split}$$

• Given $\mathbf{U}^n \in \mathcal{A}^I$, high-order Euler IDP-IMEX proceeds as follows:

$$\mathbf{U}^{n} \underbrace{\overset{(1)}{\longrightarrow} (\mathbf{W}^{L,n+1}, \mathbf{W}^{H,n+1}) \overset{(2)}{\longrightarrow} \mathbf{W}^{n+1}}_{\text{hyperbolic step}} \mathbf{W}^{n+1} \underbrace{\overset{(3)}{\longrightarrow} (\mathbf{U}^{L,n+1}, \mathbf{U}^{H,n+1}) \overset{(4)}{\longrightarrow} \mathbf{U}^{n+1}}_{\text{parabolic step}}$$

• Hyperbolic steps (1) and (2): compute low/high-order updates and limit

$$\begin{split} & \mathbb{M}^L \textbf{W}^{L,n+1} := \mathbb{M}^L \textbf{U}^n + \tau \textbf{F}^L(\textbf{U}^n), \\ & \mathbb{M}^H \textbf{W}^{H,n+1} := \mathbb{M}^H \textbf{U}^n + \tau \textbf{F}^H(\textbf{U}^n), \end{split} \qquad & \textbf{W}^{n+1} := \ell^{hyp}(\textbf{U}^n, \boldsymbol{\Phi}^L, \boldsymbol{\Phi}^H) \end{split}$$

 Parabolic steps (3) and (4): compute low/high-order updates (quasi-linear solves) and limit

$$\begin{split} & \mathbb{M}^L \textbf{U}^{L,n+1} - \tau \textbf{G}^{L,\text{lin}}(\textbf{W}^{n+1};\textbf{U}^{L,n+1}) := \mathbb{M}^L \textbf{W}^{n+1}, \\ & \mathbb{M}^H \textbf{U}^{H,n+1} - \tau \textbf{G}^{H,\text{lin}}(\textbf{U}^n;\textbf{U}^{H,n+1}) := \mathbb{M}^H \textbf{W}^{n+1}, \end{split} \\ & \textbf{U}^{n+1} := \ell^{par}(\textbf{W}^{n+1}, \boldsymbol{\Psi}^L, \boldsymbol{\Psi}^H) \end{split}$$

• Given $\mathbf{U}^n \in \mathcal{A}^I$, high-order Euler IDP-IMEX proceeds as follows:

$$\mathbf{U}^{n} \underbrace{\overset{(1)}{\longrightarrow} (\mathbf{W}^{L,n+1}, \mathbf{W}^{H,n+1}) \overset{(2)}{\longrightarrow} \mathbf{W}^{n+1}}_{\text{hyperbolic step}} \mathbf{W}^{n+1} \underbrace{\overset{(3)}{\longrightarrow} (\mathbf{U}^{L,n+1}, \mathbf{U}^{H,n+1}) \overset{(4)}{\longrightarrow} \mathbf{U}^{n+1}}_{\text{parabolic step}}$$

• Hyperbolic steps (1) and (2): compute low/high-order updates and limit

$$\begin{split} & \mathbb{M}^L \textbf{W}^{L,n+1} := \mathbb{M}^L \textbf{U}^n + \tau \textbf{F}^L(\textbf{U}^n), \\ & \mathbb{M}^H \textbf{W}^{H,n+1} := \mathbb{M}^H \textbf{U}^n + \tau \textbf{F}^H(\textbf{U}^n), \end{split} \qquad & \textbf{W}^{n+1} := \ell^{hyp}(\textbf{U}^n, \boldsymbol{\Phi}^L, \boldsymbol{\Phi}^H) \end{split}$$

 Parabolic steps (3) and (4): compute low/high-order updates (quasi-linear solves) and limit

$$\begin{split} & \mathbb{M}^L \textbf{U}^{L,n+1} - \tau \textbf{G}^{L,\text{lin}}(\textbf{W}^{n+1};\textbf{U}^{L,n+1}) \coloneqq \mathbb{M}^L \textbf{W}^{n+1}, \\ & \mathbb{M}^H \textbf{U}^{H,n+1} - \tau \textbf{G}^{H,\text{lin}}(\textbf{U}^n;\textbf{U}^{H,n+1}) \coloneqq \mathbb{M}^H \textbf{W}^{n+1}, \end{split} \\ & := \ell^{par}(\textbf{W}^{n+1}, \boldsymbol{\Psi}^L, \boldsymbol{\Psi}^H) \end{split}$$

• (Well-known) Proposition. [High-order Euler IDP-IMEX] Let Assumptions 1 and 2 hold. Assume that $\mathbf{U}^n \in \mathcal{A}^I$ and $\tau \in (0, \tau^*]$. Then, $\mathbf{U}^{n+1} \in \mathcal{A}^I$

High-order IDP-IMEX

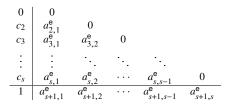
- We are now ready to go high-order in time!
- Key idea. Consider the following two ODE systems on (t^n, t^{n+1}) :

$$\mathbb{M}^{L} \partial_{t} \mathbf{U} = \underbrace{\mathbf{F}^{L}(\mathbf{U})}_{\text{explicit}} + \underbrace{\mathbf{G}^{L,\text{lin}}(\mathbf{W}^{n,l}; \mathbf{U})}_{\text{implicit}} \qquad \text{(at each stage } l)$$

$$\mathbb{M}^{H} \partial_{t} \mathbf{U} = \underbrace{\mathbf{F}^{H}(\mathbf{U}) + \mathbf{G}^{H}(\mathbf{U}) - \mathbf{G}^{H,\text{lin}}(\mathbf{U}^{n}; \mathbf{U})}_{\text{explicit}} + \underbrace{\mathbf{G}^{H,\text{lin}}(\mathbf{U}^{n}; \mathbf{U})}_{\text{implicit}}$$

Butcher tableaux

• Explicit Butcher tableau



Butcher tableaux

• Explicit Butcher tableau

• Implicit Butcher tableau

Butcher tableaux

Explicit Butcher tableau

• Implicit Butcher tableau

• Both tableaux share the same coefficients $(c_l)_{l \in \{1:s+1\}}$; recall the notation $l'(l) := \max\{k < l \mid c_k \le c_l\}$ (think of l'(l) = l - 1)

Details (1/2)

- Given $\mathbf{U}^n \in \mathcal{A}^I$, set $\mathbf{U}^{n,1} := \mathbf{U}^n$
- At each stage $l \in \{2: s+1\}$, one performs the following steps:

$$\underbrace{\mathbf{U}^{n,l'}}_{\text{hyperbolic step}}\underbrace{\overset{(1)}{\underbrace{}}}_{\text{hyperbolic step}}(\mathbf{W}^{\mathrm{L},l},\mathbf{W}^{\mathrm{H},l}) \xrightarrow{(2)}_{\text{parabolic step}}\mathbf{U}^{n,l}$$

Details (1/2)

- Given $\mathbf{U}^n \in \mathcal{A}^I$, set $\mathbf{U}^{n,1} := \mathbf{U}^n$
- At each stage $l \in \{2: s+1\}$, one performs the following steps:

$$\underbrace{ \mathbf{U}^{n,l'} \underbrace{\overset{(1)}{\longrightarrow} (\mathbf{W}^{\mathrm{L},l},\mathbf{W}^{\mathrm{H},l}) \overset{(2)}{\longrightarrow} }_{\text{hyperbolic step}} \mathbf{W}^{n,l} \underbrace{\overset{(3)}{\longrightarrow} (\mathbf{U}^{\mathrm{L},l},\mathbf{U}^{\mathrm{H},l}) \overset{(4)}{\longrightarrow} }_{\text{parabolic step}} \mathbf{U}^{n,l}$$

• Hyperbolic steps (1) and (2): compute low/high-order updates

$$\begin{split} \mathbb{M}^{\mathbf{L}}\mathbf{W}^{\mathbf{L},l} &:= \mathbb{M}^{\mathbf{L}}\mathbf{U}^{n,l'} + \tau(c_l - c_{l'})\mathbf{F}^{\mathbf{L}}(\mathbf{U}^{n,l'}) \\ \mathbb{M}^{\mathbf{H}}\mathbf{W}^{\mathbf{H},l} &:= \mathbb{M}^{\mathbf{H}}\mathbf{U}^{n,l'} + \tau \sum_{k \in \{1:l-1\}} (a_{l,k}^{\mathbf{e}} - a_{l',k}^{\mathbf{e}})\mathbf{F}^{\mathbf{H}}(\mathbf{U}^{n,k}) \end{split}$$

and limit

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

Details (2/2)

• Recall $\mathbf{W}^{n,l}$ just computed from hyperbolic steps (1) and (2)

Details (2/2)

- Recall $\mathbf{W}^{n,l}$ just computed from hyperbolic steps (1) and (2)
- Parabolic steps (3) and (4): compute low/high-order updates

$$\begin{split} \mathbb{M}^{\mathbf{L}}\mathbf{U}^{\mathbf{L},l} - \tau(c_{l} - c_{l'})\mathbf{G}^{\mathbf{L},\mathrm{lin}}(\mathbf{W}^{n,l};\mathbf{U}^{\mathbf{L},l}) &:= \mathbb{M}^{\mathbf{L}}\mathbf{W}^{n,l} \\ \mathbb{M}^{\mathbf{H}}\mathbf{U}^{\mathbf{H},l} - \tau a_{l,l}^{\mathbf{i}}\mathbf{G}^{\mathbf{H},\mathrm{lin}}(\mathbf{U}^{n};\mathbf{U}^{\mathbf{H},l}) &:= \mathbb{M}^{\mathbf{H}}\mathbf{W}^{n,l} + \tau \Delta_{l} \end{split}$$

$$\left(\Delta_{l} := \sum_{k \in \{1:l-1\}} (a_{l,k}^{\mathbf{i}} - a_{l',k}^{\mathbf{i}})\mathbf{G}^{\mathbf{H},\mathrm{lin}}(\mathbf{U}^{n};\mathbf{U}^{n,k}) + \sum_{k \in \{1:l-1\}} (a_{l,k}^{\mathbf{e}} - a_{l',k}^{\mathbf{e}})(\mathbf{G}^{\mathbf{H}}(\mathbf{U}^{n,k}) - \mathbf{G}^{\mathbf{H},\mathrm{lin}}(\mathbf{U}^{n};\mathbf{U}^{n,k}))\right) \end{split}$$

- Notice that $a_{l,l}^i = 0$ for l = s + 1 (final high-order stage is explicit)
- Limit: $\mathbf{U}^{n+1} := \ell^{\text{par}}(\mathbf{W}^{n,l}, \mathbf{\Psi}^{\text{L}}, \mathbf{\Psi}^{\text{H}})$

Details (2/2)

- Recall $\mathbf{W}^{n,l}$ just computed from hyperbolic steps (1) and (2)
- Parabolic steps (3) and (4): compute low/high-order updates

$$\begin{split} \mathbb{M}^{L}\mathbf{U}^{L,l} - \tau(c_{l} - c_{l'})\mathbf{G}^{L,\mathrm{lin}}(\mathbf{W}^{n,l};\mathbf{U}^{L,l}) &:= \mathbb{M}^{L}\mathbf{W}^{n,l} \\ \mathbb{M}^{H}\mathbf{U}^{H,l} - \tau a_{l,l}^{i}\mathbf{G}^{H,\mathrm{lin}}(\mathbf{U}^{n};\mathbf{U}^{H,l}) &:= \mathbb{M}^{H}\mathbf{W}^{n,l} + \tau \Delta_{l} \end{split}$$

$$\left(\Delta_{l} := \sum_{k \in \{1:l-1\}} (a_{l,k}^{i} - a_{l',k}^{i})\mathbf{G}^{H,\mathrm{lin}}(\mathbf{U}^{n};\mathbf{U}^{n,k}) + \sum_{k \in \{1:l-1\}} (a_{l,k}^{e} - a_{l',k}^{e}) (\mathbf{G}^{H}(\mathbf{U}^{n,k}) - \mathbf{G}^{H,\mathrm{lin}}(\mathbf{U}^{n};\mathbf{U}^{n,k}))\right) \end{split}$$

- Notice that $a_{l,l}^i = 0$ for l = s + 1 (final high-order stage is explicit)
- Limit: $\mathbf{U}^{n+1} := \ell^{\mathrm{par}}(\mathbf{W}^{n,l}, \mathbf{\Psi}^{\mathrm{L}}, \mathbf{\Psi}^{\mathrm{H}})$
- Theorem. [High-order IDP-IMEX] Let Assumptions 1 and 2 hold. Assume that $\mathbf{U}^n \in \mathcal{A}^I$. Then, $\mathbf{U}^{n+1} \in \mathcal{A}^I$ (as well as all intermediate stages) $\forall \tau \in (0, \tau^*/\max_{l \in \{2:s+1\}} (c_l c_{l'})]$

Important omitted details

 The design of low-order linearized parabolic flux G^{L,lin} is problem-dependent

Important omitted details

- The design of low-order linearized parabolic flux G^{L,lin} is problem-dependent
- The whole scheme can be rewritten using conservative limiters

Important omitted details

- The design of low-order linearized parabolic flux G^{L,lin} is problem-dependent
- The whole scheme can be rewritten using conservative limiters
- The setting allows for the hyperbolic and parabolic problems to be solved each with its own natural set of variables
 - conservative for Euler, primitive for Navier–Stokes