Optimal strong stability preserving time-stepping methods with upwind- and downwind-biased operators

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# Outline



Background

- Spatial and temporal discretizations
- SSP LMMs and RK methods



- Perturbed and additive linear multistep methods
   Perturbed linear multistep methods
  - Linear multistep methods for additive problems
  - Perturbed Runge–Kutta methodsImplicit methods

### Conclusion

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- SSP LMMs and RK methods
- 2 SSP methods with downwind-biased operators
- 3 Perturbed and additive linear multistep methods
- Perturbed Runge–Kutta methods



### Nonlinear Stability for hyperbolic problems

Hyperbolic conservation laws:

$$\frac{\partial \boldsymbol{U}(\boldsymbol{x},t)}{\partial t} + \nabla \cdot \boldsymbol{\mathcal{F}} \left( \boldsymbol{U}(\boldsymbol{x},t) \right) = 0$$

Semi-discrete problem (IVP):

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Exact solution usually satisfies nonlinear or strong stability properties:

- monotonicity:  $\|\boldsymbol{u}(t)\| \leq \|\boldsymbol{u}(t-h)\|$ ;
- contractivity:  $\|\boldsymbol{u}(t) \tilde{\boldsymbol{u}}(t)\| \le \|\boldsymbol{u}(t-h) \tilde{\boldsymbol{u}}(t-h)\|;$
- positivity:  $\boldsymbol{u}(t) \geq 0$  if  $\boldsymbol{u}(t_0) \geq 0$ ;

# These qualitative properties should be also maintained by the numerical solution.

### **Spatial discretizations**

One way to guarantee that the numerical solution is strongly stable is to require stability in the total variation (TV) semi-norm:

 $\left\|\boldsymbol{u}^{n}\right\|_{\mathrm{TV}} \leq \left\|\boldsymbol{u}^{n-1}\right\|_{\mathrm{TV}},$ 

where  $\|\boldsymbol{u}\|_{\mathsf{TV}} = \sum_{j} |\boldsymbol{u}_{j+1} - \boldsymbol{u}_{j}|.$ 

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**Total variation diminishing (TVD)** methods introduced by Harten (1983) and further analyzed by many others (Hirsch, van Leer, Roe, Sweby, Laney, Toro).

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Weighted essentially nonoscillatory (WENO) spatial discretizations provide good resolution around discontinuities and higher order of accuracy at smooth regions (Zhang & Shu, 2011).

### Finite volume methods

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Finite volume integration over a cell  $C_i = (x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}})$ :

$$\frac{d}{dt}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\boldsymbol{U}(x,t)dx = -\left(\boldsymbol{\mathcal{F}}\left(\boldsymbol{U}(x_{i+\frac{1}{2}},t)\right) - \boldsymbol{\mathcal{F}}\left(\boldsymbol{U}(x_{i-\frac{1}{2}},t)\right)\right)$$

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Semi-discrete system of ODEs:

$$\boldsymbol{u}_{i}'(t) = -\frac{1}{\Delta x} \left( \boldsymbol{F}_{i+\frac{1}{2}} - \boldsymbol{F}_{i-\frac{1}{2}} \right),$$
$$\boldsymbol{u}_{i}(t) \approx \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \boldsymbol{U}(x,t) dx, \qquad \boldsymbol{F}_{i\pm\frac{1}{2}} \approx \boldsymbol{\mathcal{F}} \left( \boldsymbol{U}(x_{i\pm\frac{1}{2}},t) \right)$$

Let  $u_{i-1}$  and  $u_i$  be the left and right cell averages across interface  $x_{i-\frac{1}{2}}$ . Solving the local Riemann problem gives a solution  $\bar{u}(u_{i-1}, u_i)$ , hence

$$\boldsymbol{F}_{i-\frac{1}{2}} \coloneqq \boldsymbol{\mathcal{F}}(\boldsymbol{u}(\boldsymbol{u}_{i-1}, \boldsymbol{u}_i)).$$

### Finite volume methods (cont.)

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**TVD**<sup>1</sup>: 
$$\bar{\boldsymbol{u}}\left(\boldsymbol{u}_{i-\frac{1}{2}}^{L}, \boldsymbol{u}_{i-\frac{1}{2}}^{R}\right); \quad \boldsymbol{u}_{i-\frac{1}{2}}^{L} = \boldsymbol{u}_{i-1} + \frac{\Delta x}{2}\boldsymbol{\sigma}_{i-1}, \quad \boldsymbol{u}_{i-\frac{1}{2}}^{R} = \boldsymbol{u}_{i} - \frac{\Delta x}{2}\boldsymbol{\sigma}_{i}.$$

WENO<sup>2</sup>:  $\bar{\boldsymbol{u}}\left(\boldsymbol{u}_{i-\frac{1}{2}}^{-}, \boldsymbol{u}_{i-\frac{1}{2}}^{+}\right); \quad \boldsymbol{u}_{i-\frac{1}{2}}^{-}, \quad \boldsymbol{u}_{i-\frac{1}{2}}^{+} \text{ are WENO reconstructions,}$ e.g.,  $\boldsymbol{u}_{i-\frac{1}{2}}^{-} = \omega_1 \boldsymbol{u}_{i-\frac{1}{2}}^{(1)} + \omega_2 \boldsymbol{u}_{i-\frac{1}{2}}^{(2)} + \omega_3 \boldsymbol{u}_{i-\frac{1}{2}}^{(3)} \text{ over } \{\boldsymbol{l}_{i-3}, \boldsymbol{l}_{i-2}, \boldsymbol{l}_{i-1}, \boldsymbol{l}_{i}, \boldsymbol{l}_{i+1}\}.$ 

<sup>1</sup>Sweby, P. K., *High resolution schemes using flux limiters for hyperbolic conservation laws, SIAM J. Numer. Anal.* 21.5 (1984), pp. 995–1011. <sup>2</sup>Shu, C.-W., *High order weighted essentially nonoscillatory schemes for convection dominated problems, SIAM Rev.* 51.1 (2009), pp. 82–126. **Strong-stability-preserving (SSP) time discretization methods** ensure strong stability properties will be preserved, when spatial discretization is coupled with high-order temporal integration.

# Need for SSP methods

**Strong-stability-preserving (SSP) time discretization methods** ensure strong stability properties will be preserved, when spatial discretization is coupled with high-order temporal integration.

Principal idea behind SSP methods is:

• First use the method of lines to obtain a semi-discretization that is strongly stable in a certain norm (or semi-norm or convex functional) with forward Euler under a time-step  $h \leq h_{FE}$ .

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- Then try to find a higher order time discretization that maintains the strong stability in the same norm but under a different (relaxed) time-step restriction

#### $\mathsf{h} \leq \mathcal{C} \; \mathsf{h}_{\mathsf{FE}}.$

# Example 1



Usually first-order methods are non-oscillatory and satisfy those properties; however, high-order time integrators can lead to spurious overshots.

### Example 2



Buckley–Leverett equation, T = 0.5, CFL number  $\nu = 1.2$ .

Maximum rise in total variation.

# Historical background

#### ODEs

### u' = Lu

- positivity (Bolley & Crouzeix, 1978)
- contractivity (Spijker, 1983)
- absolute monotonicity, optimal RK methods (Kraaijevanger, 1986)
- contractive LMMs (Sand, 1986)

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- RK positivity (Horváth, 1997,1998)

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- TVD (Shu, 1988)
- ENO/WENO (Shu & Osher, 1988,1998)

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### **Optimal SSP methods**

- RK methods & bounds (Gottlieb et.al, 1988-2003, Ruuth & Spiteri, 2002-2006)
- TVB RK methods (Ferracina & Spijker, 2005)
- TVD/TVB LMMs (Hundsdorfer & Ruuth, 2005-2007)

#### absolute monotonicity $\Leftrightarrow$ optimal Shu–Osher representation

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#### More recently:

Implicit SSP RK methods, low storage, IMEX SSP methods, multirate, methods, spectral deferred correction methods, multistep multistage methods, multistage multiderivative methods, effective order methods, etc.

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### Monotonicity of linear multistep methods

$$\boldsymbol{u}'(t) = \boldsymbol{F}(\boldsymbol{u}(t), t)$$

Assume the upwind-biased operator *F* approximates  $-\nabla \cdot \mathcal{F}(U)$  and satisfies the forward Euler (FE) condition

 $\|\boldsymbol{u} + h\boldsymbol{F}(\boldsymbol{u})\| \le \|\boldsymbol{u}\|, \quad \forall \boldsymbol{u} \in \mathbb{R}^m, \ 0 \le h \le h_{\mathsf{FE}}.$ 

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A k-step linear multistep method (LMM) with non-negative coefficients

$$\boldsymbol{u}^{n} = \sum_{j=0}^{k-1} \alpha_{j} \boldsymbol{u}^{n-k+j} + h \sum_{j=0}^{k} \beta_{j} \boldsymbol{F}(\boldsymbol{u}^{n-k+j}),$$

is SSP, if it satisfies

$$\|\boldsymbol{u}^n\| \leq \max\left\{\|\boldsymbol{u}^{n-1}\|,\|\boldsymbol{u}^{n-2}\|,\ldots,\|\boldsymbol{u}^{n-k}\|\right\},$$

whenever  $h \leq Ch_{FE}$ .

The SSP coefficient of the method is  $C = \min_j \frac{\alpha_j}{\beta_j}$ .

### Monotonicity of Runge–Kutta methods

Again, the main assumption is

$$\|\boldsymbol{u} + h\boldsymbol{F}(\boldsymbol{u})\| \le \|\boldsymbol{u}\|, \quad \forall \boldsymbol{u} \in \mathbb{R}^m, \ 0 \le h \le h_{\mathsf{FE}}.$$

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Butcher form of Runge–Kutta method RK(2,2):

$$u^* = u^{n-1} + hF(u^{n-1}),$$
  
 $u^n = u^{n-1} + \frac{1}{2}hF(u^{n-1}) + \frac{1}{2}hF(u^*).$ 

Optimal Shu-Osher representation:

$$u^{*} = u^{n-1} + hF(u^{n-1}),$$
  
$$u^{n} = \frac{1}{2}u^{n-1} + \frac{1}{2}(u^{*} + hF(u^{*})).$$

### Monotonicity of Runge–Kutta methods (cont.)

Canonical Shu-Osher form of Runge-Kutta (RK) methods:

$$oldsymbol{y} = oldsymbol{v}_r oldsymbol{u}^{n-1} + oldsymbol{lpha}_r \left(oldsymbol{y} + rac{h}{r}oldsymbol{F}(oldsymbol{y})
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 $oldsymbol{u}^n = oldsymbol{y}_{s+1},$ 

where  $v_r = (I + rK)^{-1}e$  and  $\alpha_r = r(I + rK)^{-1}K$ . (K: Butcher array) We call

$$\mathcal{C}(\mathbf{K}) = \sup\{r \mid \exists (\mathbf{I} + r\mathbf{K})^{-1} \text{ and } \mathbf{v}_r \geq 0, \alpha_r \geq 0\}$$

the **SSP coefficient** of a given method with coefficients **K**.

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the **SSP coefficient** of a given method with coefficients **K**.

A RK with C > 0 is SSP, if it satisfies  $\|\boldsymbol{u}^n\| \le \|\boldsymbol{u}^{n-1}\|$  whenever  $h \le Ch_{\mathsf{FE}}$ .

### **Bounds and Barriers**

Let 
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 for RK methods ( $s : \#$  of stages).

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#### SSP explicit methods:

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- Linear multistep methods have no order barrier on order but  $\mathcal{C} \leq 1$ .

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#### SSP implicit methods:

- Unconditional monotonicity only for implicit Euler method.
- Runge–Kutta methods have order  $p \leq 6$  and  $C_{eff} \leq 2$ .
- Linear multistep methods have no order barrier on order but  $\mathcal{C} \leq 2$ .

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#### Conclusion

### Motivation: Why downwinding is important?

• For a given method downwinding allows a representation with augmented SSP coefficient.
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## Motivation: Why downwinding is important?

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- Optimal methods with downwind-biased operators attain larger SSP coefficient compared to classical SSP methods.
- Optimal implicit perturbed Runge-Kutta methods can attain arbitrarily large SSP coefficients.
- Extends monotonicity analysis for methods applied to additive problems, i.e.  $\mathbf{F}$  and  $\tilde{\mathbf{F}}$  approximate different parts of the PDE.

## Example

Consider the LeVeque and Yee problem

$$U_t + f(U)_x = s(U), \quad U(x,0) = U_0(x), \quad x \in \mathbb{R}, t \ge 0,$$

where  $s(U) = -\mu U(U-1)(U-0.5)$ ,  $\mu > 0$ .

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**Semi-discretization:** Let  $u_i \approx U(x_i, t)$  and define

$$D_i(u) = -\frac{f(u_i) - f(u_{i-1})}{\Delta x}, \qquad \widetilde{D}_i(u) = -\frac{f(u_{i+1}) - f(u_i)}{\Delta x},$$
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Consider the initial value problems (IVPs):

$$\begin{aligned} u'(t) &= F(u(t)), \quad F = D + S, \qquad u'(t) = \widetilde{F}(u(t)), \quad \widetilde{F} = \widetilde{D} + \widetilde{S}, \\ u(0) &= u_0. \qquad \qquad u(0) = u_0. \end{aligned}$$

# Example (cont.)

It can be shown that if  $u \in [0, 1]$ , then

$$0 \le u + h F(u) \le 1 \quad \text{for } 0 \le h \le h_{\mathsf{FE}} = \frac{2\tau}{2 + \mu\tau},$$
  
$$0 \le u - h \widetilde{F}(u) \le 1 \quad \text{for } 0 \le h \le \widetilde{h}_{\mathsf{FE}} = \frac{16\tau}{16 + \mu\tau},$$

where  $\tau > 0$  is such that

$$\begin{aligned} 0 &\leq u + h \, D(u) \leq 1 \quad \text{for } 0 \leq h \leq \tau, \\ 0 &\leq u - h \, \widetilde{D}(u) \leq 1 \quad \text{for } 0 \leq h \leq \tau. \end{aligned}$$

# Example (cont.)

Let 
$$\xi = \frac{h_{\mathsf{FE}}}{\tilde{h}_{\mathsf{FE}}} = \frac{16 + \mu \tau}{8(2 + \mu \tau)}$$

and apply an optimal explicit perturbed SSP LMM to u' = F(u).

# Example (cont.)

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Then, the numerical solution lies in [0, 1] under a step-size restriction

 $h \leq \mathcal{C}(\xi) h_{\mathsf{FE}}.$ 

This is less strict compared to the "classical" optimal SSP LMM (without downwinding), for all  $\xi \in \mathbb{R}^+$ .

e.g., choose SSP LMM(3,2) and  $\mu\tau = 8/3$ . Then,  $\xi = 1/2$  and

$$h \leq C(1/2) h_{\mathsf{FE}} = 0.3044\tau.$$

On the other hand, without downwinding:  $h \leq 0.2143\tau$ .

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#### Conclusion

## LMMs with downwind-biased operators

In addition to the operator F, consider the associated **downwind-biased** operator  $\tilde{F} \approx -\nabla \cdot \mathcal{F}(U)$  such that

$$\begin{split} \|\boldsymbol{u} + h\boldsymbol{F}(\boldsymbol{u})\| &\leq \|\boldsymbol{u}\|, \quad \forall \boldsymbol{u} \in \mathbb{R}^{m}, \ 0 \leq h \leq \mathbf{h}_{\mathsf{FE}}, \\ \|\boldsymbol{u} - h\widetilde{\boldsymbol{F}}(\boldsymbol{u})\| &\leq \|\boldsymbol{u}\|, \quad \forall \boldsymbol{u} \in \mathbb{R}^{m}, \ 0 \leq h \leq \widetilde{\mathbf{h}}_{\mathsf{FE}}. \end{split}$$

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By using both upwind and downwind operators, a k-step linear multistep method (LMM) applied to a semi-discrete problem

$$oldsymbol{u}'(t) = oldsymbol{F}(oldsymbol{u}(t)), \quad t \geq t_0, \ oldsymbol{u}(t_0) = oldsymbol{u}_0,$$

takes the form

$$\boldsymbol{u}^{n} = \sum_{j=0}^{k-1} \alpha_{j} \boldsymbol{u}^{n-k+j} + h \sum_{j=0}^{k} \left( \overline{\beta}_{j} \boldsymbol{F}(\boldsymbol{u}^{n-k+j}) + \widetilde{\beta}_{j} \left( \boldsymbol{F}(\boldsymbol{u}^{n-k+j}) - \widetilde{\boldsymbol{F}}(\boldsymbol{u}^{n-k+j}) \right) \right).$$

#### Perturbed LMMs

Let  $\bar{\beta}_j = \beta_j - \tilde{\beta}_j$ , then LMMs can be also written in the form

$$\boldsymbol{u}^{n} = \sum_{j=0}^{k-1} \alpha_{j} \boldsymbol{u}^{n-k+j} + \sum_{j=0}^{k} \left( \beta_{j} h \boldsymbol{F}(\boldsymbol{u}^{n-k+j}) - \tilde{\beta}_{j} h \widetilde{\boldsymbol{F}}(\boldsymbol{u}^{n-k+j}) \right).$$

The above LMMs are referred to as **perturbed LMMs** when applied to u'(t) = F(u(t)), where F and  $\tilde{F}$  satisfy the FE condition with different step-size restrictions.

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The above LMMs are referred to as **perturbed LMMs** when applied to u'(t) = F(u(t)), where F and  $\tilde{F}$  satisfy the FE condition with different step-size restrictions.

Next:

- Monotonicity properties
- Step-size bounds for monotonicity
- Optimal SSP perturbed methods

# Perturbed SSP LMMs

A perturbed LMM is SSP with threshold factor  $(\mathcal{C},\widetilde{\mathcal{C}}),$  if the monotonicity conditions hold

$$egin{aligned} eta_j &\geq 0, \, ilde{eta}_j \geq 0, \quad j \in \{0, \dots, k\}, \ lpha_j &- r eta_j - ilde{r} ilde{eta}_j \geq 0, \quad j \in \{0, \dots, k-1\}, \end{aligned}$$

for all  $0 \leq r \leq C$ ,  $0 \leq \tilde{r} \leq \widetilde{C}$ .

# Perturbed SSP LMMs

A perturbed LMM is SSP with threshold factor  $(C, \tilde{C})$ , if the monotonicity conditions hold

$$egin{aligned} eta_j \geq 0, \, ilde{eta}_j \geq 0, & j \in \{0, \dots, k\}, \ lpha_j - reta_j - ilde{r}eta_j \geq 0, & j \in \{0, \dots, k-1\}, \end{aligned}$$

for all  $0 \leq r \leq C$ ,  $0 \leq \tilde{r} \leq \widetilde{C}$ .

#### Theorem

Consider an IVP problem for which **F** and  $\tilde{F}$  satisfy the forward Euler condition for some  $h_{FE} > 0$ ,  $\tilde{h}_{FE} > 0$ . Apply a perturbed SSP LMM with threshold factor  $(C, \tilde{C})$ . Then the numerical solution satisfies

$$\|u^n\| \le \max\{\|u^{n-1}\|, \|u^{n-2}\|, \dots, \|u^{n-k}\|\},\$$

under a time-step restriction  $h \leq \min\{\mathcal{C} h_{\mathsf{FE}}, \widetilde{\mathcal{C}} \tilde{h}_{\mathsf{FE}}\}.$ 

# Perturbed SSP LMMs (cont.)

Since C,  $\widetilde{C}$  are continuous functions of the method's coefficients, the maximum step size is achieved when  $C = \widetilde{C} \ \tilde{h}_{\mathsf{FE}} / h_{\mathsf{FE}}$ .

For a given number of steps k, order of accuracy p and  $\xi := h_{\text{FE}}/\tilde{h}_{\text{FE}}$ , we want to find the largest possible value  $r(\xi)$  for which the monotonicity conditions are satisfied when  $\tilde{r} = \xi r(\xi)$ .

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Combining the order conditions and monotonicity constraints we have:

$$\sum_{j=0}^{k-1} (\gamma_j + r(\beta_j + \xi \tilde{\beta}_j)) j^i + \sum_{j=0}^k (\beta_j - \tilde{\beta}_j) i j^{i-1} = k^i, \quad i \in \{0, \dots, p\},$$
$$\beta_j \ge 0, \quad \tilde{\beta}_j \ge 0, \quad j \in \{0, \dots, k\},$$
$$\gamma_j \ge 0, \quad j \in \{0, \dots, k-1\}.$$

Since the conditions are non-linear only in r we can use bisection and solve a sequence of feasibility linear problems.

In contrast with other optimal SSP methods, now the SSP coefficient depends on the problem, not just the number of steps k and order of accuracy p.

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Optimal perturbed SSP LMMs have been found for  $k \in \{1, ..., 40\}$ ,  $p \in \{1, ..., 15\}$  and for different values of  $\xi$ .

• There exist optimal methods that satisfy  $\beta_j \tilde{\beta}_j = 0$  for each *j*.

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- Any second order perturbed LMM has SSP coefficient  $C(\xi) \leq 2$ .
- Optimal *p*th-order SSP methods have at most *p* non-zero coefficients.
- Given k, p, then for any value of ξ the optimal perturbed SSP LMMs attain larger step sizes for monotonicity when compared with other LMMs.

# Outline

#### Background

SSP methods with downwind-biased operators

Perturbed and additive linear multistep methods
 Perturbed linear multistep methods

• Linear multistep methods for additive problems

Perturbed Runge–Kutta methods



#### Additive linear multistep methods

Now, lets consider linear multistep methods applied to the additive problem

$$oldsymbol{u}'(t) = oldsymbol{F}(oldsymbol{u}(t)) + oldsymbol{\widehat{F}}(oldsymbol{u}(t)), \quad t \geq t_0$$
  
 $oldsymbol{u}(t_0) = oldsymbol{u}_0,$ 

and assume that  $\boldsymbol{F}$ ,  $\widehat{\boldsymbol{F}}$  satisfy

$$\begin{aligned} \|\boldsymbol{u} + h\boldsymbol{F}(\boldsymbol{u})\| &\leq \|\boldsymbol{u}\|, \quad \forall \boldsymbol{u} \in \mathbb{R}^{m}, \ 0 \leq h \leq h_{\mathsf{FE}} \\ \|\boldsymbol{u} + h\widehat{\boldsymbol{F}}(\boldsymbol{u})\| &\leq \|\boldsymbol{u}\|, \quad \forall \boldsymbol{u} \in \mathbb{R}^{m}, \ 0 \leq h \leq \hat{h}_{\mathsf{FE}}. \end{aligned}$$

$$\boldsymbol{u}^{n} = \sum_{j=0}^{k-1} \alpha_{j} \boldsymbol{u}^{n-k+j} + \sum_{j=0}^{k} \left( \beta_{j} h \boldsymbol{F}(\boldsymbol{u}^{n-k+j}) + \hat{\beta}_{j} h \widehat{\boldsymbol{F}}(\boldsymbol{u}^{n-k+j}) \right)$$

## SSP additive LMM methods

An additive linear multistep method has order of accuracy p if

$$\sum_{j=0}^{k-1} \alpha_j j^j + \sum_{j=0}^k \beta_j i j^{i-1} = k^i, \quad \sum_{j=0}^{k-1} \alpha_j j^j + \sum_{j=0}^k \hat{\beta}_j i j^{i-1} = k^i, \quad i \in \{0, \dots, p\}.$$

Combining the order conditions and monotonicity constraints we can formulate the feasibility problem:

$$\sum_{j=0}^{k-1} (\gamma_j + r(\beta_j + \xi \hat{\beta}_j)) j^i + \sum_{j=0}^k \beta_j i j^{i-1} = k^i, \quad i \in \{0, \dots, p\},$$
$$\sum_{j=0}^k (\beta_j - \hat{\beta}_j) j^{i-1} = 0, \quad i \in \{0, \dots, p\},$$
$$\beta_j \ge 0, \ \hat{\beta}_j \ge 0, \quad j \in \{0, \dots, k\},$$
$$\gamma_j \ge 0, \quad j \in \{0, \dots, k-1\}.$$

#### Theorem

For a given  $k \ge 1$ ,  $p \ge 1$  consider the optimal k-step, pth-order **additive** (explicit or implicit) LMM with threshold factor  $(\mathcal{C}, \widehat{\mathcal{C}})$ . Then this method is equivalent to the optimal **non-additive** k-step, pth-order SSP LMM with SSP coefficient  $\mathcal{C} + \widehat{\mathcal{C}}$ .

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It is interesting to consider only SSP IMEX linear multistep methods.

Optimal methods have been found for a range of k,p and for different values of  $\xi$ .

But, have small threshold factors; not practically useful.

Instead impose SSP conditions only on the explicit method and maximize  $A(\alpha)$  stability region of the implicit method.

# Outline

#### Background

- 2 SSP methods with downwind-biased operators
- 3 Perturbed and additive linear multistep methods
- Perturbed Runge–Kutta methods
  - Implicit methods

#### 5 Conclusion

## Perturbed Runge-Kutta methods

Assume that

$$\|\boldsymbol{u} + h\boldsymbol{F}(\boldsymbol{u})\| \le \|\boldsymbol{u}\|, \|\boldsymbol{u} - h\widetilde{\boldsymbol{F}}(\boldsymbol{u})\| \le \|\boldsymbol{u}\| \quad \forall \boldsymbol{u} \in \mathbb{R}^{m}, \ 0 \le h \le h_{\mathsf{FE}}.$$

A downwind-biased (or perturbed) Runge-Kutta method takes the form

$$\mathbf{y} = \mathbf{v}_r \mathbf{u}^{n-1} + h\mathbf{K}\mathbf{F} + h\widetilde{\mathbf{K}}(\mathbf{F} - \widetilde{\mathbf{F}}), \quad \widetilde{\mathbf{K}} = \begin{pmatrix} \widetilde{\mathbf{A}} & 0\\ \widetilde{\mathbf{b}}^{\mathsf{T}} & 0 \end{pmatrix}$$

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For example:

$$y_1 = u^{n-1} + \frac{2}{3}hF(u^{n-1}),$$
  
$$u^n = \frac{5}{8}u^{n-1} + \frac{3}{8}y_1 + \frac{3}{4}hF(y_1).$$

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$$\begin{aligned} \mathbf{y}_1 &= \frac{5}{6} \big( \mathbf{u}^{n-1} + h \mathbf{F}(\mathbf{u}^{n-1}) \big) + \frac{1}{6} \big( \mathbf{u}^{n-1} - h \widetilde{\mathbf{F}}(\mathbf{u}^{n-1}) \big), \\ \mathbf{u}^n &= \frac{3}{4} \big( \mathbf{y}_1 + h \mathbf{F}(\mathbf{y}_1) \big) + \frac{1}{4} \big( \mathbf{u}^{n-1} - h \widetilde{\mathbf{F}}(\mathbf{u}^{n-1}) \big). \end{aligned}$$

# Monotonicity and optimality of perturbed RK

Perturbed Runge-Kutta methods:

- Introduced by Shu & Osher (1988) and further studied by Gottlieb, Ruuth, Spiteri and others.
- Analysis of monotonicity conditions, Shu-Osher representations, and extension to additive problems investigated by Higueras (2005, 2006).
- Algorithms to obtained optimal perturbations and upper bounds on SSP coefficient were developed by Higueras/Ketcheson/Kocsis (2016).
- Formulae for second-order implicit methods with unbounded SSP coefficient (Ketcheson, 2012).

# Outline

#### Background

- 2 SSP methods with downwind-biased operators
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- Perturbed Runge–Kutta methods
  Implicit methods

#### Conclusion

## Implicit perturbed Runge–Kutta methods

A new three-step, third-order class of implicit perturbed Runge–Kutta methods, with arbitrarily large SSP coefficient C = r:

$$\begin{aligned} \mathbf{y}_1 &= \mathbf{v}_1 \mathbf{u}^{n-1} + \alpha_{11} \left( \mathbf{y}_1 + \frac{h}{r} \mathbf{F}(\mathbf{y}_1) \right) \\ &+ \alpha_{21} \left( \mathbf{y}_2 + \frac{h}{r} \mathbf{F}(\mathbf{y}_2) \right) + \tilde{\alpha}_{13} \left( \mathbf{y}_3 - \frac{h}{r} \tilde{\mathbf{F}}(\mathbf{y}_3) \right) \\ \mathbf{y}_2 &= \alpha_{21} \left( \mathbf{y}_1 + \frac{h}{r} \mathbf{F}(\mathbf{y}_1) \right) + \alpha_{22} \left( \mathbf{y}_2 + \frac{h}{r} \mathbf{F}(\mathbf{y}_2) \right) \\ \mathbf{y}_3 &= \mathbf{y}_1 + \frac{h}{r} \mathbf{F}(\mathbf{y}_1) \\ \mathbf{u}^n &= \mathbf{y}_2 + \frac{h}{r} \mathbf{F}(\mathbf{y}_2). \end{aligned}$$

Stability analysis of the underlying method (i.e. when  $\tilde{F} = F$ ) reveals that:

- if r = 6 then the method is A-stable;
- if r > 6 then the method is A( $\alpha$ )-stable with  $\alpha \ge 88.2302$ .

#### **Stability regions**



Stability regions and  $A(\alpha)$ -stability wedges.
## **Stability regions**



Stability regions and  $A(\alpha)$ -stability wedges.

Solution of Burgers' equation with 2nd-order TVD spatial discretization.

Time integrators:

- explicit SSP RK(3, 3) (SSPRK33)
- implicit perturbed SSPRK(3, 3)
  with r = 8 (PRK33)



2.5exact SSP33,  $\nu = 0.5$ Solution of Burgers' equation with PRK33.  $\nu = 4.0$ 2.02nd-order TVD spatial discretization. u 1.5Time integrators: explicit SSP RK(3, 3) (SSPRK33) 1.0 implicit perturbed SSPRK(3, 3) with r = 8 (PRK33) 0.50.70 0.720.74 0.76 0.78 x

Closeup view of the shock

# Outline

### Background

- 2 SSP methods with downwind-biased operators
- 3 Perturbed and additive linear multistep methods
- 4 Perturbed Runge–Kutta methods



#### Additive SSP linear multistep methods:

- Extended SSP theory of LMMs to problems where upwind and downwind operators have different stiffness properties.
- Analyzed monotonicity properties of perturbed SSP LMMs and construct optimal methods.
- Investigated monotonicity properties of additive linear multistep methods: SSP IMEX methods.

Future work:

- Study asymptotic behavior of SSP coefficient for perturbed methods.
- Perturbed SSP LMMs with variable step size.
- Find optimal IMEX methods: (explicit perturbed SSP LMM +  $A(\alpha)$ -stable implicit LMM).

#### Implicit perturbed SSP Runge–Kutta methods:

- Obtained a third-order implicit RK method with arbitrarily large SSP coefficient.
- Analyzed stability properties.
- Showed good performance with large CFL numbers.

Future work:

- Efficient implementation in relation to Newton iterations required at each step.
- Search for other families of higher order implicit perturbed RK methods.

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Expert in SSP time discretization methods with a huge contribution to the development of TVD/TVB LMMs and RK methods, IMEX methods, monotone multirate and partitioned RK methods, splitting methods, etc.

Among other research interests he worked on

- Stiff ODEs,
- Time-dependent PDEs,
- Streamer simulations for multiscale dynamical problems





https://www.cwi.nl/news/2017/in-memoriam-willem-hundsdorfer