On positive explicit peer methods of high order

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Outline

1. Strong stability preserving time discretizations
2. Explicit Runge–Kutta methods
3. Linear Multistep methods
4. Explicit Peer methods

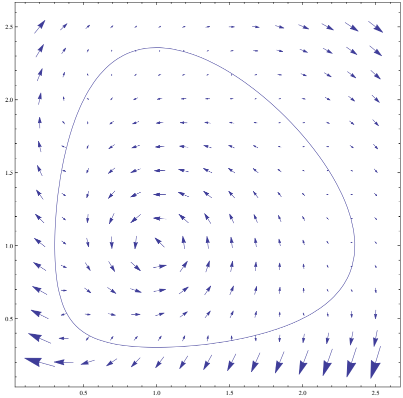
Strong stability preserving (SSP) time discretizations

A convex set S (e.g. $S = \mathbb{R}^n_+$) is preserved by the explicit Euler method for h_{E} sufficiently small if for $y \in S$ holds

$$y + h_E f(y) \in S.$$

A method X shall preserve the same set with $h = \mathcal{C} \cdot h_{\mathrm{E}}$.

Goal: Find methods (of high order) with $\mathcal{C}_{\mathrm{eff}} = \mathcal{C}/\text{work}$ as large as possible.



Previous work

Shu/Osher 1988... Kraaijvanger 1991 ... Horváth 1998... Higueras 2004 ... Spijker 2007... Constantinescu/Sandu 2009 ... Ketcheson/Gottlieb/Macdonald 2011... and many more

Buckley-Leverett Equation, Hundsdorfer/Verwer, 2003

Consider the hyperbolic equation

$$u_t + f(u)_x = 0, \quad f(u) = u^2/(u^2 + \frac{1}{3}(1-u)^2)$$

with periodic boundary conditions $x \in \Omega = [0,1]$. Because

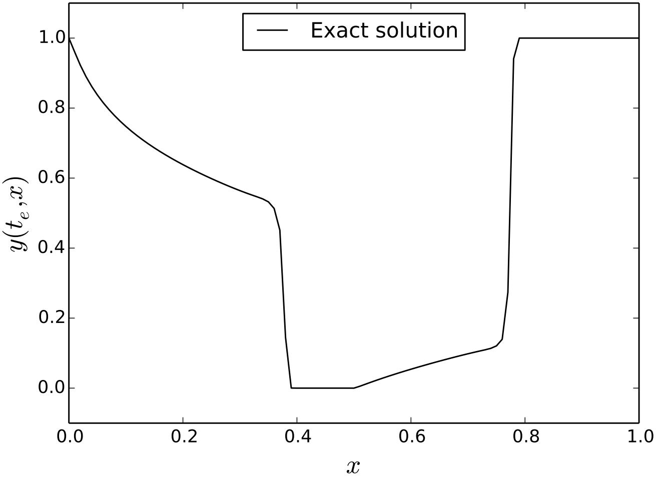
$$\int_\Omega u_x(t+h)\,dx \le \int_\Omega u_x(t)\,dx$$

we want no spurios oscillations in the numerical solution

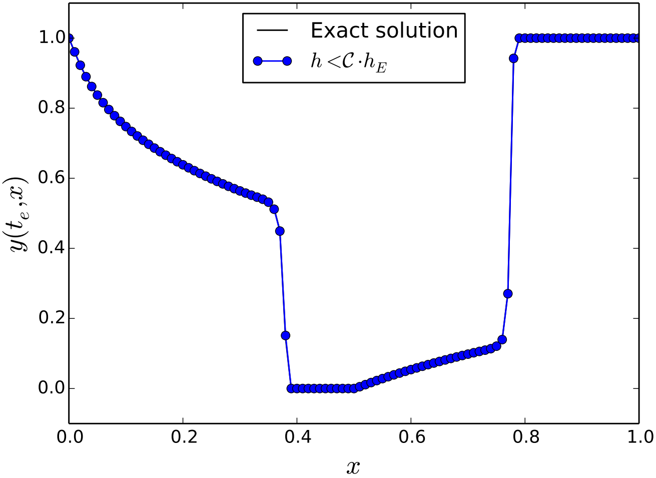
$$\|y_{m+1}\|_{\mathrm{TV}} \le \|y_m\|_{\mathrm{TV}}.$$

In other words, $S = \{y : \|y\|_{\mathrm{TV}} = c\}$ shall be preserved.
The scheme is total variation diminishing or TVD.

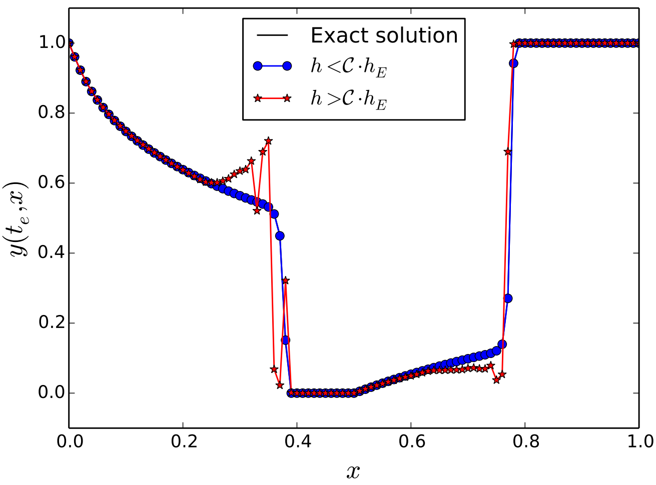
Buckley-Leverett, numerical results



Buckley-Leverett, numerical results



Buckley-Leverett, numerical results



Explicit Runge–Kutta methods and SSP

Let $Y_m \in \mathbb{R}^{n\times(s+1)}$ be stages and solution of a method $\begin{array}{c|c} c & A \\ \hline & b^T \end{array}$.

Transforming the scheme

$$Y_m = \mathbb{1} y_m + hRF_m, \quad \text{with} \quad R = \begin{pmatrix} A & 0 \\ b^T & 0 \end{pmatrix}$$

into Shu-Osher form (= convex combination of Euler steps)

$$\begin{aligned} (I + rR)Y_m &= \mathbb{1} y_m + rR(Y_m + \frac{h}{r}F_m) \\ Y_m &= (I + rR)^{-1}\mathbb{1} y_m + r(I + rR)^{-1}R(Y_m + \frac{h}{r}F_m). \end{aligned}$$

The method is SSP, i.e. $\max_i \|Y_{m,i}\| \le \|y_m\|$, iff $h \le \mathcal{C} \cdot h_E$ with

$$\mathcal{C} = \max\{r : (I + rR)^{-1}(\mathbb{1}, rR) \ge 0\}.$$

("⇒" is straightforward, "⇐" involves non-reducibility)

Fair comparison of different methods

Stability. The method is SSP if $h \leq \mathcal{C} \cdot h_E$. For fairness, we must take the number of stages, s, into account: $\mathcal{C}_{\text{eff}} = \mathcal{C}/s$.

Accuracy. Assume we have two method A and B with

$$R_A(z) = \exp(z) - \eta^A_{p+1} z^{p+1} + \mathcal{O}(z^{p+2}),$$
$$R_B(z) = \exp(z) - \eta^B_{p+1} z^{p+1} + \mathcal{O}(z^{p+2}).$$

If B is s times more expensive than A and the amount of work is fixed, we must take larger steps with B:

$$\begin{aligned}(R_B(sz))^{1/s} &= \left(\exp(sz) - \eta^B_{p+1}(sz)^{p+1}\right)^{1/s} + \mathcal{O}(z^{p+2}) \\ &= \exp(z) - \eta^B_{p+1} s^p z^{p+1} + \mathcal{O}(z^{p+2})\end{aligned}$$

Therefore

$$\eta_{p+1,\text{eff}} = (\text{work})^p \times \eta_{p+1}$$

Explicit Runge–Kutta methods and SSP, Results

p	s	$\mathcal{C}_{\text{eff}}$	$\eta_{p+1,\text{eff}}$	Reference
2	2	0.5	0.67	Heun 1900
3	3	0.33	1.93	Shu/Osher 1988
3	5	0.53	6.39	Gottlieb/Ketcheson/Shu 2011
4	4	0	2.13	Kutta 1901
4	5	0.30	2.4	Kraaijevanger 1991
4	10	0.67	4.62	Ketcheson 2008

$$\eta_{p+1,\text{eff}} = (\text{number of stages})^p \times (\text{error constant for } y' = y)$$

- No high order RK method ($p \geq 5$) can be positive.
- Larger $\mathcal{C}_{\text{eff}}$ implies larger truncation errors $\eta_{p+1,\text{eff}}$.

Linear Multistep methods

Again, we write the method as convex combination of Euler steps.

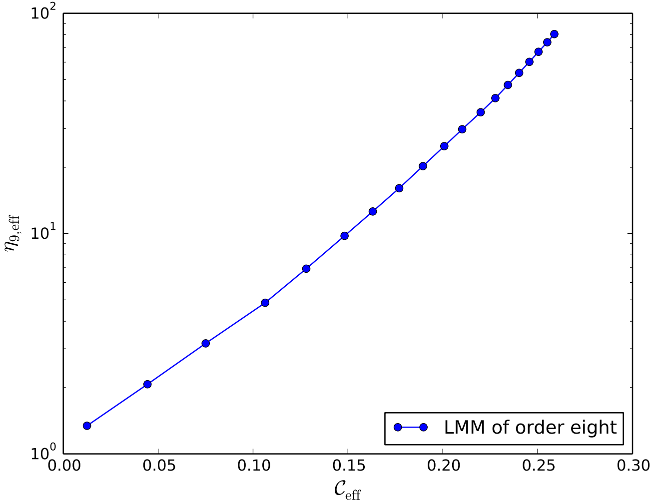
$$\begin{aligned} y_m &= \sum_{i=1}^{k} \alpha_i y_{m-i} + h \sum_{i=1}^{k} \beta_i f(y_{m-i}) \\ &= \sum_{i=1}^{k} \alpha_i \left(y_{m-i} + h \frac{\beta_i}{\alpha_i} f(y_{m-i}) \right) \end{aligned}$$

Therefore

$$\mathcal{C} = \mathcal{C}_{\text{eff}} = \min \frac{\beta_i}{\alpha_i}$$

Linear Multistep methods (cont.)

With take order $p = 8$ as an example.



Explicit peer methods

Stage values $Y_{m,i} \approx y(t_m + c_i h)$, $i = 1, \dots, s$ are computed by

$$Y_m = BY_{m-1} + hAf(Y_{m-1}) + hRf(Y_m) \qquad \text{(Peer)}$$

with $B, A, R \in \mathbb{R}^{s \times s}$ and R strictly lower triangular.

We require uniform order p for all components, i.e.,

$$e^{cz} = Be^{(c-1)z} + zAe^{(c-1)z} + zRe^{cz} + \mathcal{O}(z^{p+1}) \qquad \text{(Order } p\text{)}$$

We want to find (c, B, A, R) such that r is maximal with

$$(I + rR)^{-1}(R, A, B - rA) \geq 0 \qquad \text{(SSP)}$$

Tasks

Solve a constraint optimization problem, detect and use sparsity, deal with rounding errors, verify and sell the result.

Note (for selling)

Optimal positive methods are positive as well as stable and civilised. Moreover, they can exhibit an interesting structure.

Two weakly coupled Euler methods

The following two-stage parallel method with $c = (-\eta, 1)$

$$Y_m = \begin{pmatrix} \frac{\eta^2+2\eta}{(\eta+1)^2} & \frac{1}{(\eta+1)^2} \\ \frac{1}{(\eta+1)^2} & \frac{\eta^2+2\eta}{(\eta+1)^2} \end{pmatrix} Y_{m-1} + \begin{pmatrix} \frac{\eta}{\eta+1} & 0 \\ 0 & \frac{\eta+2}{\eta+1} \end{pmatrix} hf(Y_{m-1})$$

is of second order and SSP with $\mathcal{C} = \eta/(\eta+1)$.

For example, take $\eta = 9$ to obtain the method

$$\begin{pmatrix} Y_{1,t-9h} \\ Y_{2,t+h} \end{pmatrix} = \begin{pmatrix} \frac{99}{100} & \frac{1}{100} \\ \frac{1}{100} & \frac{99}{100} \end{pmatrix} \begin{pmatrix} Y_{1,t-10h} \\ Y_{2,t} \end{pmatrix} + \begin{pmatrix} \frac{9}{10} & 0 \\ 0 & \frac{11}{10} \end{pmatrix} \begin{pmatrix} hf(Y_{1,t-10h}) \\ hf(Y_{2,t}) \end{pmatrix}$$

with $\mathcal{C} = \frac{9}{10}$.

The method looks like a joke. Two Euler methods living at different times profit from a small conversation about their local dynamics. Maybe this scheme is even useful. Note that it is parallel.

Two weakly coupled Euler methods

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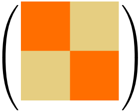
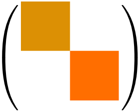
For example, take $\eta = 9$ to obtain the method

$$\begin{pmatrix} Y_{1,t-9h} \\ Y_{2,t+h} \end{pmatrix} =$$



$$\begin{pmatrix} Y_{1,t-10h} \\ Y_{2,t} \end{pmatrix} +$$



$$\begin{pmatrix} hf(Y_{1,t-10h}) \\ hf(Y_{2,t}) \end{pmatrix}$$

with $\mathcal{C} = \frac{9}{10}$.

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Constraint optimization

$$\max_{r,c,B,A,R} r$$

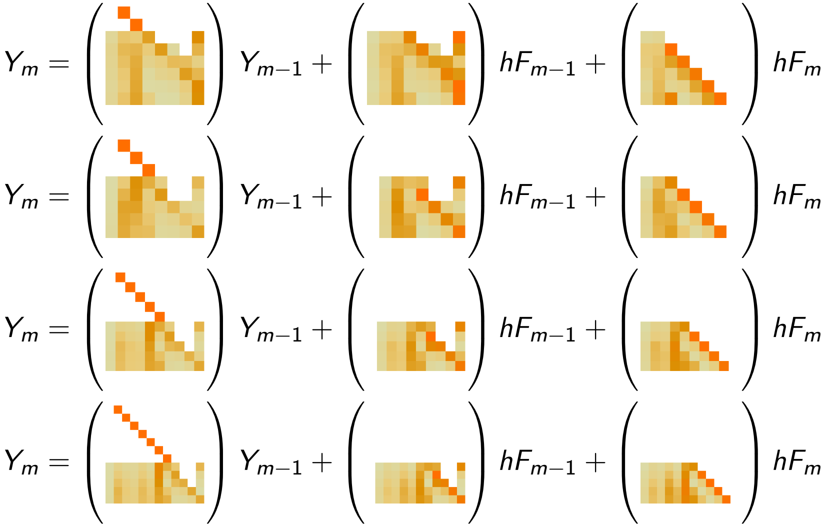
subject to

$$(I + rR)^{-1}(R, A, B - rA) \geq 0 \qquad \text{(SSP)}$$

$$e^{cz} = Be^{(c-1)z} + zAe^{(c-1)z} + zRe^{cz} + \mathcal{O}(z^{p+1}) \qquad \text{(Order } p\text{)}$$

- Matlab: `FMINCON`
- Mathematica: `NMaximize` and `FindMaximum`
- We have found positive peer methods up to order 13.
- We need extended precision for higher orders (condition number of (Order p) is about 10^8 for $p = 13$)
- Main result: optimized methods are sparse

Optimized methods are sparse, Orders 7,8,10 and 12



Methods with effectively five stages plus some copying.

Technical details

1. Run numerical optimization
2. Chop off tiny elements
3. Use the non-tiny elements to project onto the order conditions (the conditions are linear after freezing the nodes c)
4. Re-calculate r with $(I + rR)^{-1}(R, A, B - rA) \geq 0$

Steps 2 to 4 can be carried out with rational numbers rather than floating point numbers.

Further work/discussion

- Continue to test/evaluate the methods
- Construct methods of order greater than 13 (needs good tools)
- Variable step sizes
- Implicit methods