Arbitrary high-order, conservative and positive preserving Patankar-type deferred correction schemes

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Outline

1. Production–Destruction system
2. Deferred Correction
3. Modified Patankar DeC (mPDeC)
4. Numerics

Outline

Production–Destruction system

Consider production-destruction systems (PDS)

$$\begin{cases} d_t c_i = P_i(\mathbf{c}) - D_i(\mathbf{c}), \quad i = 1, \dots, I, & P_i(\mathbf{c}) = \sum_{j=1}^{I} p_{i,j}(\mathbf{c}), \\ \mathbf{c}(t=0) = \mathbf{c}_0, & D_i(\mathbf{c}) = \sum_{j=1}^{I} d_{i,j}(\mathbf{c}), \end{cases} \tag{1}$$

where

$$p_{i,j}(\mathbf{c}), d_{i,j}(\mathbf{c}) \geq 0, \qquad \forall i,j \in I, \quad \forall \mathbf{c} \in \mathbb{R}^{+,I}.$$

Applications: Chemical reactions, biological systems, population evolutions and PDEs.
Example: SIRD

$$\begin{cases} d_t S = -\beta \frac{SI}{N} \\ d_t I = \beta \frac{SI}{N} - \gamma I - \delta I \\ d_t R = \gamma I \\ d_t D = \delta I \end{cases}$$

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Property 1: Conservation

$$\sum_{i=1}^{I} c_i(0) = \sum_{i=1}^{I} c_i(t), \quad \forall t \geq 0$$

$$\iff \quad p_{i,j}(\mathbf{c}) = d_{j,i}(\mathbf{c}), \qquad \forall i,j \in I, \quad \forall \mathbf{c} \in \mathbb{R}^{+,I}.$$

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Property 2: Positivity

If P_i, D_i Lipschitz, and if when $c_i \to 0 \Rightarrow D_i(\mathbf{c}) \to 0 \Longrightarrow$
$c_i(0) > 0\, \forall i \in I \Longrightarrow c_i(t) > 0\, \forall i \in I\; \forall t > 0.$

Production–Destruction system

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$$p_{i,j}(\mathbf{c}), d_{i,j}(\mathbf{c}) \geq 0, \qquad \forall i, j \in I, \quad \forall \mathbf{c} \in \mathbb{R}^{+,I}.$$

Goal:

- One step method
- Unconditionally positive
- Unconditionally conservative
- High order accurate

Solvers

Explicit Euler

- $\mathbf{c}^{n+1} = \mathbf{c}^n + \Delta t \left(\mathbf{P}(\mathbf{c}^n) - \mathbf{D}(\mathbf{c}^n) \right)$
- Conservative
- First order
- Not unconditionally positive, if Δt is too big... CFL conditions

Implicit Euler

- $\mathbf{c}^{n+1} = \mathbf{c}^n + \Delta t \left(\mathbf{P}(\mathbf{c}^{n+1}) - \mathbf{D}(\mathbf{c}^{n+1}) \right)$
- Conservative & positive
- First order
- Expensive to be solved/not unique solution: Nonlinear solvers!!!

Patankar trick

$$c_i^{n+1} = c_i^n + \Delta t \left(P_i(\mathbf{c}^n) - D_i(\mathbf{c}^n) \frac{c_i^{n+1}}{c_i^n} \right)$$

$$\left(1 + \Delta t \frac{D_i(\mathbf{c}^n)}{c_i^n} \right) c_i^{n+1} = c_i^n + \Delta t P_i(\mathbf{c}^n)$$

- Not conservative
- First order
- Positive
- Implicit, but easy

Solvers

Modified Patankar (mP)
Burchard, Deleersnijder & Meister

$$c_i^{n+1} = c_i^n + \Delta t \left(\sum_j p_{i,j}(\mathbf{c}^n) \frac{c_j^{n+1}}{c_j^n} - \sum_j d_{i,j}(\mathbf{c}^n) \frac{c_i^{n+1}}{c_i^n} \right) \tag{2}$$

$\mathrm{M}(\mathbf{c}^n)\mathbf{c}^{n+1} = \mathbf{c}^n$ where M is

$$\begin{cases} m_{i,i}(\mathbf{c}^n) = 1 + \Delta t \sum_{k=1}^{I} \frac{d_{i,k}(\mathbf{c}^n)}{c_i^n}, & i = 1, \dots, I, \\ m_{i,j}(\mathbf{c}^n) = -\Delta t \frac{p_{i,j}(\mathbf{c}^n)}{c_j^n}, & i,j = 1, \dots, I,\ i \neq j. \end{cases} \tag{3}$$

- Conservative
- First order
- Positive
- Linear system at each timestep

- Extension to RK2 and RK3 (Burchard, Deleersnijder, Meister, Kopecz)
- Extension to PDEs (Huang, Zhao, Shu)

Outline

Deferred Correction discretization

We should discretize our variable on $[t^n, t^{n+1}]$ in M substeps $(\mathbf{c}^{n,m})$.

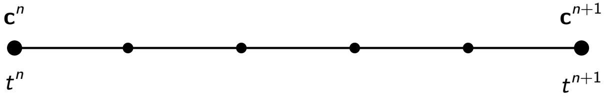

Figure: Subtimeintervals

Then, we can rewrite $\mathbf{c}^m = \mathbf{c}^0 + \int_{t^0}^{t^m} \mathbf{P}(\mathbf{c}(s)) - \mathbf{D}(\mathbf{c}(s))\, ds$.
Equispaced points $\Rightarrow$ order $= M + 1$.

$$\underline{\mathbf{c}} := (\mathbf{c}^0, \dots, \mathbf{c}^M) \in \mathbb{R}^{M \times I} \tag{4}$$

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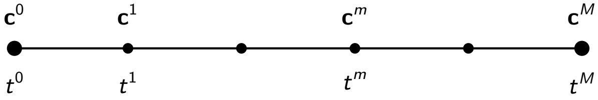

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DeC operators

$\mathcal{L}^2$ operator

$$\mathbf{E} := \mathbf{P} - \mathbf{D}$$

$$\mathcal{L}^2(\mathbf{c}^0, \dots, \mathbf{c}^M) = \mathcal{L}^2(\underline{\mathbf{c}}) :=$$

$$\begin{cases} \mathbf{c}^M - \mathbf{c}^0 - \int_{t^0}^{t^M} \mathbf{E}(\mathbf{c}(s))ds \\ \vdots \\ \mathbf{c}^1 - \mathbf{c}^0 - \int_{t^0}^{t^1} \mathbf{E}(\mathbf{c}(s))ds \end{cases}$$

- Implicit RK
- Order of accuracy $\geq M+1$
- Difficult to solve directly

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$$\begin{cases}\mathbf{c}^M-\mathbf{c}^0-\Delta t\sum_{r=0}^M\theta_r^M\mathbf{E}(\mathbf{c}^r)\\ \dots\\ \mathbf{c}^1-\mathbf{c}^0-\Delta t\sum_{r=0}^M\theta_r^1\mathbf{E}(\mathbf{c}^r)\end{cases}$$

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- Implicit RK
- Order of accuracy $\geq M+1$
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$\mathcal{L}^1$ operator

$$\mathcal{L}^1(\mathbf{c}^0,\dots,\mathbf{c}^M) = \mathcal{L}^1(\underline{\mathbf{c}}) :=$$
$$\begin{cases} \mathbf{c}^M - \mathbf{c}^0 - \Delta t \beta^M \mathbf{E}(\mathbf{c}^0) \\ \dots \\ \mathbf{c}^1 - \mathbf{c}^0 - \Delta t \beta^1 \mathbf{E}(\mathbf{c}^0) \end{cases}$$

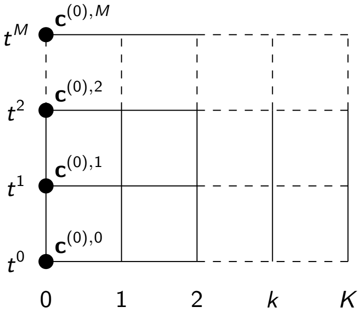
- First order accurate
- Explicit or easy to solve

Deferred Correction

How to combine two methods keeping the accuracy of the second and the stability and simplicity of the first one?

- $\mathcal{L}^1(\underline{\mathbf{c}}) = 0$, first order accuracy, easily invertible.
- $\mathcal{L}^2(\underline{\mathbf{c}}) = 0$, high order $M+1$.

$$\mathbf{c}^{0,(k)} := \mathbf{c}(t^n), \quad k = 0, \dots, K,$$
$$\mathbf{c}^{m,(0)} := \mathbf{c}(t^n), \quad m = 1, \dots, M$$
$$\mathcal{L}^1(\underline{\mathbf{c}}^{(k)}) = \mathcal{L}^1(\underline{\mathbf{c}}^{(k-1)}) - \mathcal{L}^2(\underline{\mathbf{c}}^{(k-1)}) \text{ with } k = 1, \dots, K.$$



DeC Theorem

- $\mathcal{L}^1$ coercive
- $\mathcal{L}^1 - \mathcal{L}^2$ Lipschitz

DeC converges and $\min(K, M+1)$ is the order of accuracy.

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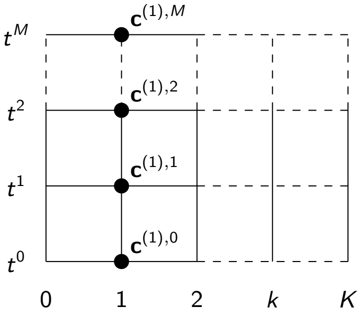

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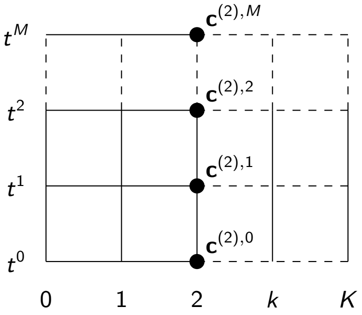

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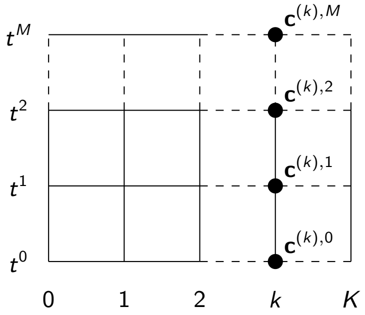

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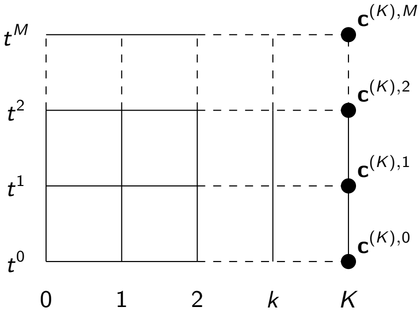

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Explicit DeC

If we write explicitly the DeC step we see that

$$
\begin{aligned}
\mathcal{L}_i^{1,m}(\underline{\mathbf{c}}^{(k)}) = \mathcal{L}_i^{1,m}(\underline{\mathbf{c}}^{(k-1)}) - \mathcal{L}_i^{2,m}(\underline{\mathbf{c}}^{(k-1)}) \iff \\
c_i^{(k),m} - c_i^0 - \Delta t \beta^m E_i(\mathbf{c}^0) = c_i^{(k-1),m} - c_i^0 - \Delta t \beta^m E_i(\mathbf{c}^0) \\
- c_i^{(k-1),m} + c_i^0 + \Delta t \sum_{r=0}^{M} \theta_r^m E_i(\mathbf{c}^{(k-1),r}) \iff \\
c_i^{(k),m} = c_i^0 + \Delta t \sum_{r=0}^{M} \theta_r^m E_i(\mathbf{c}^{(k-1),r}) \iff \\
c_i^{(k),m} = c_i(t^n) + \Delta t \sum_{r=0}^{M} \theta_r^m E_i(\mathbf{c}^{(k-1),r})
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c_i^{(k),m} - c_i^0 - \Delta t \beta^m E_i(\mathbf{c}^0) = c_i^{(k-1),m} - c_i^0 - \Delta t \beta^m E_i(\mathbf{c}^0) \\
- c_i^{(k-1),m} + c_i^0 + \boxed{\Delta t \sum_{r=0}^{M} \theta_r^m E_i(\mathbf{c}^{(k-1),r})} \Longleftrightarrow \\
c_i^{(k),m} = c_i^0 + \Delta t \sum_{r=0}^{M} \theta_r^m E_i(\mathbf{c}^{(k-1),r}) \Longleftrightarrow \\
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\end{aligned}
\tag{5}
$$

Ingredients

- We want to use the DeC for high order accuracy
- We want to recast positivity and conservation
- We will use the Patankar trick
- We want an implicit method (to get positivity), but only linearly implicit (no nonlinear solvers)
- We have to modify $\mathcal{L}^2$ using the trick

Outline

Modified Patankar $\mathcal{L}^2$

Modify the operator $\mathcal{L}^2$ according to the Patankar trick!

$$\mathcal{L}_i^2(\mathbf{c}^{0,(k-1)},\dots,\mathbf{c}^{M,(k-1)} \qquad\qquad\qquad) = \mathcal{L}_i^2(\underline{\mathbf{c}}^{(k-1)} \qquad) :=$$

$$\begin{cases} c_i^{M,(k-1)} - c_i^{0,(k-1)} - \Delta t \sum_{r=0}^{M} \color{red}{\theta_r^M} \sum_{j=1}^{I} \left(p_{i,j}(\mathbf{c}^{r,(k-1)}) \qquad\qquad - d_{i,j}(\mathbf{c}^{r,(k-1)}) \qquad\qquad \right), \\ \vdots \\ c_i^{1,(k-1)} - c_i^{0,(k-1)} - \Delta t \sum_{r=0}^{M} \color{red}{\theta_r^1} \sum_{j=1}^{I} \left(p_{i,j}(\mathbf{c}^{r,(k-1)}) \qquad\qquad - d_{i,j}(\mathbf{c}^{r,(k-1)}) \qquad\qquad \right), \end{cases}$$

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$$\mathcal{L}^2_i(\mathbf{c}^{0,(k-1)},\dots,\mathbf{c}^{M,(k-1)},\mathbf{c}^{0,(k)},\dots,\mathbf{c}^{M,(k)}) = \mathcal{L}^2_i(\underline{\mathbf{c}}^{(k-1)},\underline{\mathbf{c}}^{(k)}) :=$$

$$\begin{cases} c_i^{M,(k-1)} - c_i^{0,(k-1)} - \Delta t \sum_{r=0}^M \theta_r^M \sum_{j=1}^I \left(p_{i,j}(\mathbf{c}^{r,(k-1)}) \frac{c_j^{M,(k)}}{c_j^{M,(k-1)}} - d_{i,j}(\mathbf{c}^{r,(k-1)}) \frac{c_i^{M,(k)}}{c_i^{M,(k-1)}} \right), \\ \vdots \\ c_i^{1,(k-1)} - c_i^{0,(k-1)} - \Delta t \sum_{r=0}^M \theta_r^1 \sum_{j=1}^I \left(p_{i,j}(\mathbf{c}^{r,(k-1)}) \frac{c_j^{1,(k)}}{c_j^{1,(k-1)}} - d_{i,j}(\mathbf{c}^{r,(k-1)}) \frac{c_i^{1,(k)}}{c_i^{1,(k-1)}} \right), \end{cases}$$

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where $\gamma(a,b,\theta) = a$ if $\theta > 0$ and $\gamma(a,b,\theta) = b$ if $\theta < 0$.

Modified Patankar DeC (mPDeC)

Reminder: initial states $c_i^{0,(k)}$ are identical for any correction (k)
DeC Patankar can be rewritten for $k = 1, \dots, K$, $m = 1, \dots, M$ and $\forall i \in I$ into

$$\mathcal{L}_i^{1,m}(\underline{\mathbf{c}}^{(k)}) - \mathcal{L}_i^{1,m}(\underline{\mathbf{c}}^{(k-1)}) + \mathcal{L}_i^{2,m}(\underline{\mathbf{c}}^{(k)}, \underline{\mathbf{c}}^{(k-1)}) = 0$$
$$c_i^{m,(k)} - c_i^0 - \Delta t \sum_{r=0}^{M} \theta_r^m \sum_{j=1}^{I} \left(p_{i,j}(\mathbf{c}^{r,(k-1)}) \frac{c^{m,(k)}_{\gamma(j,i,\theta_r^m)}}{c^{m,(k-1)}_{\gamma(j,i,\theta_r^m)}} - d_{i,j}(\mathbf{c}^{r,(k-1)}) \frac{c^{m,(k)}_{\gamma(i,j,\theta_r^m)}}{c^{m,(k-1)}_{\gamma(i,j,\theta_r^m)}} \right) = 0. \tag{6}$$

- Conservation
- Positivity
- High order accuracy

Conservation

The mPDeC scheme is unconditionally conservative for all substages, i.e.,

$$\sum_{i=1}^{I} c_i^{m,(k)} = \sum_{i=1}^{I} c_i^0,$$

for all $k = 1, \dots, K$ and $m = 0, \dots, M$.
Using formulation (6), we can easily see that $\forall k, m$

$$\sum_{i\in I} c_i^{m,(k)} - \sum_{i \in I} c_i^0 =$$

$$=\Delta t \sum_{i,j=1}^{I} \sum_{r=0}^{M} \theta_r^m \left(p_{i,j}(\mathbf{c}^{r,(k-1)}) \frac{c^{m,(k)}_{\gamma(j,i,\theta_r^m)}}{c^{m,(k-1)}_{\gamma(j,i,\theta_r^m)}} - d_{i,j}(\mathbf{c}^{r,(k-1)}) \frac{c^{m,(k)}_{\gamma(i,j,\theta_r^m)}}{c^{m,(k-1)}_{\gamma(i,j,\theta_r^m)}} \right) =$$

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Using formulation (6), we can easily see that $\forall k, m$

$$\sum_{i\in I} c_i^{m,(k)} - \sum_{i \in I} c_i^0 =$$

$$= \Delta t \sum_{i,j=1}^{I} \sum_{r=0}^{M} \theta_r^m \left(d_{i,j}(\mathbf{c}^{r,(k-1)}) \frac{c^{m,(k)}_{\gamma(i,j,\theta_r^m)}}{c^{m,(k-1)}_{\gamma(i,j,\theta_r^m)}} - d_{i,j}(\mathbf{c}^{r,(k-1)}) \frac{c^{m,(k)}_{\gamma(i,j,\theta_r^m)}}{c^{m,(k-1)}_{\gamma(i,j,\theta_r^m)}} \right) = 0.$$

Positivity

At each step (m,k) implicit linear system with mass matrix

$$\mathrm{M}(\mathbf{c}^{m,(k-1)})_{ij} =$$
$$\begin{cases} 1+\Delta t \sum_{r=0}^{M} \sum_{l=1}^{I} \frac{\theta_r^m}{c_i^{m,(k-1)}} \left(d_{i,l}(\mathbf{c}^{r,(k-1)}) \chi_{\{\theta_r^m>0\}} - p_{i,l}(\mathbf{c}^{r,(k-1)}) \chi_{\{\theta_r^m<0\}} \right) & \text{for } i=j \\ -\Delta t \sum_{r=0}^{M} \frac{\theta_r^m}{c_j^{m,(k-1)}} \left(p_{i,j}(\mathbf{c}^{r,(k-1)}) \chi_{\{\theta_r^m>0\}} - d_{i,j}(\mathbf{c}^{r,(k-1)}) \chi_{\{\theta_r^m<0\}} \right) & \text{for } i \neq j \end{cases}$$

- Diagonally dominant by columns
- Invertible
- $\mathrm{M}^{-1} > 0$

High order accuracy

Let $\underline{\mathbf{c}}^*$ be the solution of the $\mathcal{L}^2$ operator, i.e., $\mathcal{L}^2(\underline{\mathbf{c}}^*,\underline{\mathbf{c}}^*)=0$.

- Coercivity operator $\mathcal{L}^1$: $||\mathcal{L}^1(\underline{\mathbf{c}})-\mathcal{L}^1(\underline{\mathbf{c}}^*)|| \geq C_1||\underline{\mathbf{c}}-\underline{\mathbf{c}}^*||$
- Lipschitz continuity operator $\mathcal{L}^1-\mathcal{L}^2$:
  $||\mathcal{L}^1(\underline{\mathbf{c}}^{(k-1)})-\mathcal{L}^2(\underline{\mathbf{c}}^{(k-1)},\underline{\mathbf{c}}^{(k)})-\mathcal{L}^1(\underline{\mathbf{c}}^*)+\mathcal{L}^2(\underline{\mathbf{c}}^*,\underline{\mathbf{c}}^*)|| \leq C_L\Delta t||\underline{\mathbf{c}}^{(k-1)}-\underline{\mathbf{c}}^*||.$

  Intermediate steps for Lipschitz continuity
  - $\mathbf{c}^{m,(k)}=\mathbf{c}^0+\Delta t G(\mathbf{c}^{m,(k-1)})\mathbf{c}^0$
  - $\frac{c_i^{(k)}}{c_i^{(k-1)}}=1+\Delta t^{k-1}g_i+\mathcal{O}(\Delta t^k)$

Proof of DeC

$$
\begin{aligned}
||\underline{\mathbf{c}}^{(k)} - \underline{\mathbf{c}}^*|| \leq & C_0 ||\mathcal{L}^1(\underline{\mathbf{c}}^{(k)}) - \mathcal{L}^1(\underline{\mathbf{c}}^*)|| = & (7)\\
= & C_0 ||\mathcal{L}^1(\underline{\mathbf{c}}^{(k-1)}) - \mathcal{L}^2(\underline{\mathbf{c}}^{(k-1)}, \underline{\mathbf{c}}^{(k)}) - \mathcal{L}^1(\underline{\mathbf{c}}^*) + \mathcal{L}^2(\underline{\mathbf{c}}^*, \underline{\mathbf{c}}^*)|| \leq & (8)\\
\leq & C\Delta t ||\underline{\mathbf{c}}^{(k-1)} - \underline{\mathbf{c}}^*|| & (9)
\end{aligned}
$$

After K iterations

$$
||\underline{\mathbf{c}}^{(K)} - \underline{\mathbf{c}}^*|| \leq C^K \Delta t^K ||\underline{\mathbf{c}}^0 - \underline{\mathbf{c}}^*||. \qquad (10)
$$

Outline

Linear test

$$\begin{aligned} c_1'(t) &= c_2(t) - 5c_1(t), \qquad & c_2'(t) &= 5c_1(t) - c_2(t), \\ c_1(0) &= c_1^0 = 0.9, & c_2(0) &= c_2^0 = 0.1\,. \end{aligned} \tag{11}$$

with

$$p_{1,2}(\mathbf{c}) = d_{2,1}(\mathbf{c}) = c_2, \quad p_{2,1}(\mathbf{c}) = d_{1,2}(\mathbf{c}) = 5c_1$$

and $p_{i,i}(\mathbf{c}) = d_{i,i}(\mathbf{c}) = 0$ for $i = 1, 2$.
Analytical solution is

$$c_1(t) = \frac{1}{6}\left(1 + \frac{22}{5}\exp(-6t)\right) \text{ and } c_2(t) = 1 - c_1(t). \tag{12}$$

Linear test

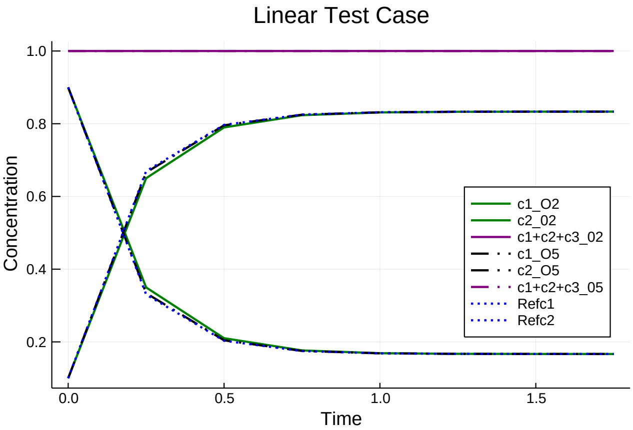


Figure: Second and fifth order methods together with the reference solution (12)

Linear test: Convergence

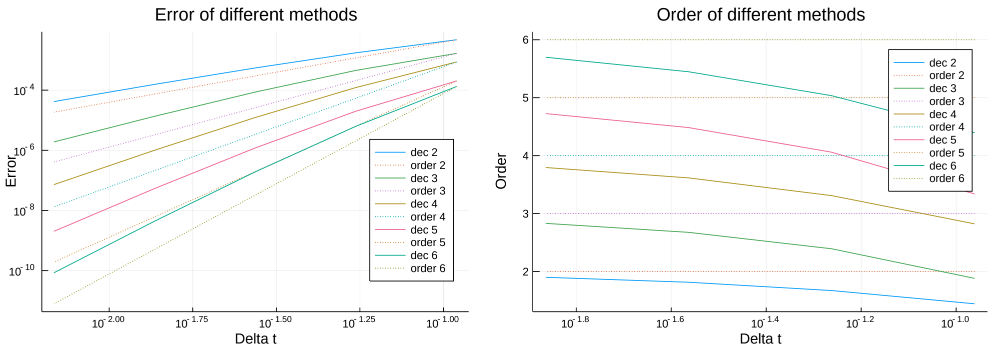


Figure: Second to sixth order error decay and slope of the errors

Nonlinear test

$$\begin{cases} c_1'(t) &= -\frac{c_1(t)c_2(t)}{c_1(t)+1}, \\ c_2'(t) &= \frac{c_1(t)c_2(t)}{c_1(t)+1} - 0.3c_2(t), \\ c_3'(t) &= 0.3c_2(t) \end{cases} \tag{13}$$

with initial condition $\mathbf{c}^0 = (9.98, 0.01, 0.01)^T$.
The PDS system in the matrix formulation can be expressed by

$$p_{2,1}(\mathbf{c}) = d_{1,2}(\mathbf{c}) = \frac{c_1(t)c_2(t)}{c_1(t)+1}, \quad p_{3,2}(\mathbf{c}) = d_{2,3}(\mathbf{c}) = 0.3c_2(t)$$

and $p_{i,j}(\mathbf{c}) = d_{i,j}(\mathbf{c}) = 0$ for all other combinations of i and j.

Nonlinear test

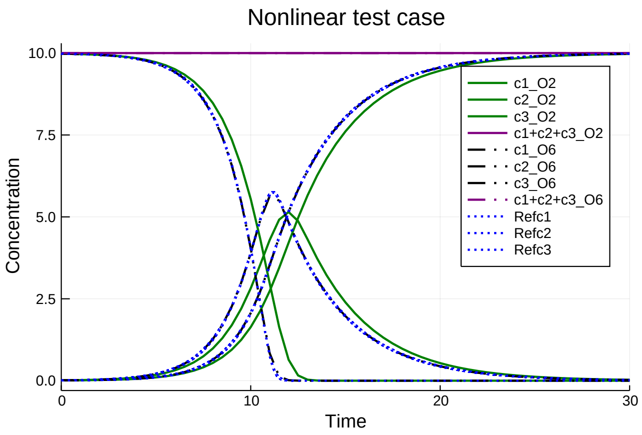


Figure: Second order and sixth order methods together with the reference solution (SSPRK104)

Nonlinear test: Convergence

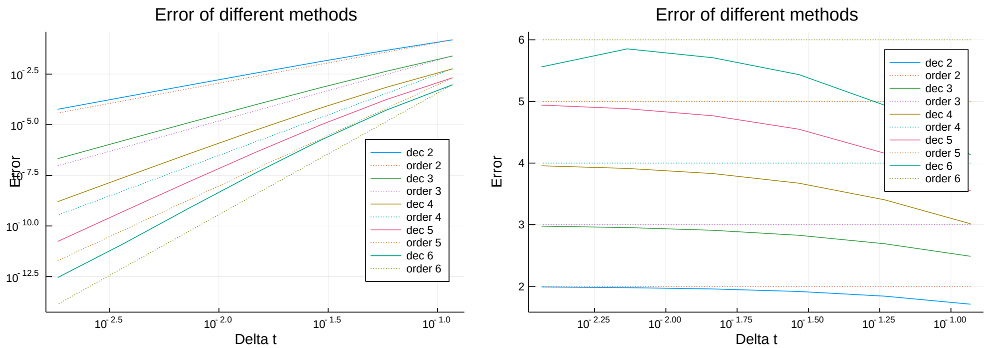
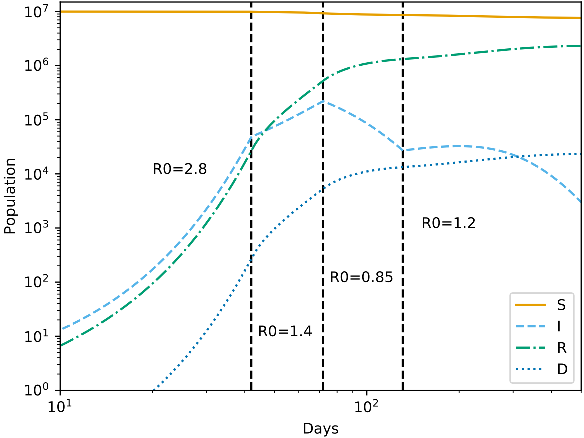


Figure: Second to sixth order error behaviors and slopes of the errors

SIRD

$$\begin{cases} d_t S = -\beta \frac{SI}{N} \\ d_t I = \beta \frac{SI}{N} - \gamma I - \delta I \\ d_t R = \gamma I \\ d_t D = \delta I \end{cases}$$

Solved with mPDeC5



Robertson test

$$
\begin{aligned}
c_1'(t) &= 10^4 c_2(t)c_3(t) - 0.04c_1(t)\\
c_2'(t) &= 0.04c_1(t) - 10^4 c_2(t)c_3(t) - 3\cdot 10^7 c_2(t)^2\\
c_3'(t) &= 3\cdot 10^7 c_2(t)^2
\end{aligned}
\tag{14}
$$

with initial conditions $\mathbf{c}^0 = (1, 0, 0)$.
The time interval of interest is $[10^{-6}, 10^{10}]$. The PDS for (14) reads

$$
\begin{aligned}
&p_{1,2}(\mathbf{c}) = d_{2,1}(\mathbf{c}) = 10^4 c_2(t)c_3(t), \quad p_{2,1}(\mathbf{c}) = d_{1,2}(\mathbf{c}) = 0.04c_1(t),\\
&p_{3,2}(\mathbf{c}) = d_{2,3}(\mathbf{c}) = 3\cdot 10^7 c_2(t)
\end{aligned}
$$

and zero for the other combinations.
We use exponential timesteps to better catch the behaviour of the solution $\Delta t^n = 2\cdot\Delta t^{n-1}$.

Robertson test

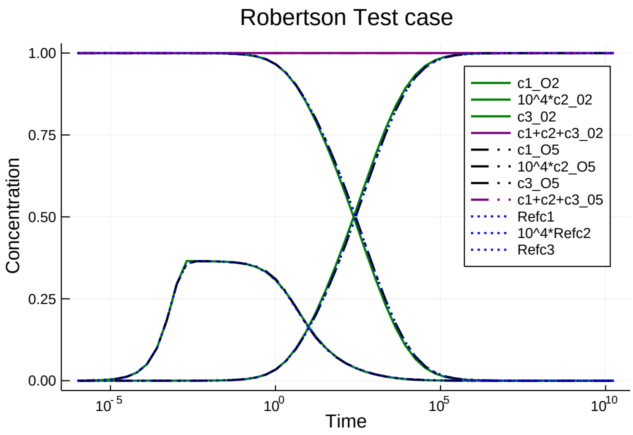


Figure: Second and fifth order solutions and references

Application to Shallow Water equations

$$\begin{cases} \partial_t h + \nabla \cdot (h\mathbf{u}) = 0 \\ \partial_t \mathbf{u} + \nabla \cdot (h\mathbf{u} \otimes \mathbf{u} + g\frac{h^2}{2}\mathrm{I}) = -gh\nabla b(\mathbf{x}) \end{cases}$$

- Slides
- Article post

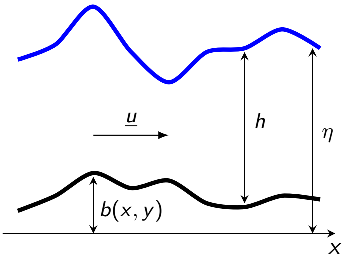


Figure: Shallow Water Equations: definition of the variables.

- MPDeC Code: If you want to check out the code, it's really easy ($\sim$ 150 lines), in Julia, on git. `https://git.math.uzh.ch/abgrall_group/deferred-correction-patankar-scheme`
- MPDeC Shallow Water code (Fortran) `https://github.com/accdavlo/sw-mpdec`