On Unconditionally Positivity Preserving and Conservative Methods for Systems of Advection-Diffusion-Reaction Equations

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An unconditionally positivity preserving finite difference scheme (UPFD) for systems of advection-diffusion-reaction equations with non-linear reaction terms is proposed. A modified Patankar approach is employed with respect to the reaction part in order to ensure both conservativity and positivity without any additional constraints on the time step size.

1 Introduction

Introducing an additional reaction term into advection-diffusion equations may yield a dramatic increase in stiffness and thus usually requires a significant adaptation of the time step size such that the numerical scheme becomes inefficient. Recently, Chen-Charpentier and Kojouharov proposed an unconditionally positivity preserving finite difference scheme (UPFD) for linear advection-diffusion-reaction equations [1]. The key idea is an implicit approach to discretize the sink terms as well as the local terms within both the advection and diffusion part, while the remaining terms are evaluated explicitly.

Some applications like geobiochemical marine systems model a closed cycle and lead to systems including non-linear and even conservative source terms, such that the sum of the production and destruction terms over all constituents always cancels out. The system

$$\partial_t c_k + v_k\,\partial_x c_k - D_k\,\partial^2_{xx} c_k = \sum_{j=1, j\neq k}^{N} \big(p_{kj}\left(\widetilde{\mathbf{c}}\right) - d_{kj}\left(\widetilde{\mathbf{c}}\right)\big) \quad \text{for } k = 1,\ldots,N \text{ in } [a,b]\times\mathbb{R}^+ \tag{1}$$

presents an example of such a system, since $p_{kj}\left(\widetilde{\mathbf{c}}\right) = d_{jk}\left(\widetilde{\mathbf{c}}\right)$ describes the production as well as destruction terms. Here, v_k denotes the velocity of the advection, $D_k \geq 0$ the diffusivity, and $\widetilde{\mathbf{c}} = (c_1,\ldots,c_N)$ represents the vector of the N unknown constituents. The system requires suitable boundary and initial conditions, where $\widetilde{\mathbf{c}}(x,0) > \mathbf{0}$ for all $x \in [a,b]$.

Burchard et al. [2] presented an unconditionally positivity preserving and conservative method. This paper combines the strategies to obtain an efficient semi-implicit unconditionally positivity preserving and conservative finite difference method for systems of advection-diffusion-reaction equations with linear advection and diffusion as well as non-linear reaction terms. Semi-implicit means here that even for non-linear reaction terms only one linear equation system has to be solved per timestep.

2 Numerical Method and Results

Using constant step sizes Δx and Δt, the UPFD method [1] applied to the advection-diffusion part reads

$$\underbrace{\left(\frac{1}{\Delta t} + \frac{v_k}{\Delta x} + \frac{D_k}{\Delta x^2}\right)}_{UPFD^k_{impl}>0} c^{n+1}_{k,i} = \underbrace{\frac{D_k}{\Delta x^2} c^n_{k,i+1} + \frac{c^n_{k,i}}{\Delta t} + \left(\frac{v_k}{\Delta x} + \frac{D_k}{\Delta x^2}\right) c^n_{k,i-1}}_{UPFD^k_{expl,i}(\mathbf{c}^n_k)>0},$$

where $c^n_{k,i} \approx c_k(x_i,t^n)$ using $x_i = a + (i-1)\Delta x$, $t^n = n\,\Delta t$, $i = 1,\ldots,M$, and $\mathbf{c}^n_k = (c^n_{k,1},\ldots,c^n_{k,M})$.

Employing a slight modification of Burchard et al. [2] the reaction terms are incorporated due to

$$UPFD^k_{impl} c^{n+1}_{k,i} = UPFD^k_{expl,i}(\mathbf{c}^n_k) + \sum_{j=1,j\neq k}^{N} p_{kj}(\widetilde{\mathbf{c}}^n_i)\frac{c^{n+1}_{j,i}}{c^n_{j,i}}\frac{UPFD^k_{impl}}{UPFD^j_{impl}} - \sum_{j=1,j\neq k}^{N} d_{kj}(\widetilde{\mathbf{c}}^n_i)\frac{c^{n+1}_{k,i}}{c^n_{k,i}}$$

using $\widetilde{\mathbf{c}}^n_i \approx \widetilde{\mathbf{c}}(x_i,t^n) \in \mathbb{R}^N$ or equivalently

$$c^{n+1}_{k,i} = \frac{UPFD^k_{expl,i}(\mathbf{c}^n_k)}{UPFD^k_{impl}} + \sum_{j=1,j\neq k}^{N} \frac{p_{kj}(\widetilde{\mathbf{c}}^n_i)}{UPFD^j_{impl}}\frac{c^{n+1}_{j,i}}{c^n_{j,i}} - \sum_{j=1,j\neq k}^{N} \frac{d_{kj}(\widetilde{\mathbf{c}}^n_i)}{UPFD^k_{impl}}\frac{c^{n+1}_{k,i}}{c^n_{k,i}} \tag{2}$$

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for $k = 1, \dots, N$ and $i = 1, \dots, M$. Note that the modified Patankar approach [2] has to be weighted with $1/UPFD^j_{impl}$ to ensure conservativity for the system, even if $UPFD^i_{impl} \neq UPFD^j_{impl}$ for some $i \neq j$.

Theorem 2.1 *The method* (2) *is unconditionally positivity preserving and conservative.*

Proof. Positivity can be shown by writing the method as $\mathbf{A}\mathbf{c}^{n+1} = \mathbf{UPFD_{expl}}$, where $\mathbf{c}^{n+1} = (\widetilde{\mathbf{c}}_1^{n+1}, \dots, \widetilde{\mathbf{c}}_M^{n+1})^T \in \mathbb{R}^{M \cdot N}$, $\mathbf{UPFD_{expl}} \in \mathbb{R}^{M \cdot N}$ with $(\mathbf{UPFD_{expl}})_{(i-1)N+k} = UPFD^k_{expl,i}(\mathbf{c}^n_k)$ and $\mathbf{A} \in \mathbb{R}^{(M\cdot N)\times(M\cdot N)}$ is a block diagonal matrix of blocks $\mathbf{A}^\ell \in \mathbb{R}^{N\times N}$, $\ell = 1, ..., M$ with

$$a^\ell_{ij} = \begin{cases} -\frac{p_{ij}(\widetilde{\mathbf{c}}^n_\ell)}{c^n_{j,\ell}} \frac{UPFD^i_{impl}}{UPFD^j_{impl}} = -\frac{d_{ji}(\widetilde{\mathbf{c}}^n_\ell)}{c^n_{j,\ell}} \frac{UPFD^i_{impl}}{UPFD^j_{impl}}, & \text{if } i \neq j, \\ UPFD^i_{impl} + \sum_{k=1,k\neq i}^N \frac{d_{ik}(\widetilde{\mathbf{c}}^n_\ell)}{c^n_{i,\ell}}, & \text{if } i = j. \end{cases}$$

Using the diagonal matrix $\mathbf{D} := \mathrm{diag}\{\mathbf{D_B}, \dots, \mathbf{D_B}\} \in \mathbb{R}^{(M\cdot N)\times(M\cdot N)}$ with $\mathbf{D_B} := \mathrm{diag}\{UPFD^1_{impl}, \dots, UPFD^N_{impl}\} \in \mathbb{R}^{N\times N}$ we obtain $\mathbf{B} := \mathbf{D^{-1}AD}$ with

$$b^\ell_{ij} = \begin{cases} d^{-1}_{ii} a^\ell_{ij} d_{jj} = \frac{1}{UPFD^i_{impl}} \frac{-d_{ji}(\widetilde{\mathbf{c}}^n_\ell)}{c^n_{j,\ell}} \frac{UPFD^i_{impl}}{UPFD^j_{impl}} UPFD^j_{impl} = -\frac{d_{ji}(\widetilde{\mathbf{c}}^n_\ell)}{c^n_{j,\ell}}, & \text{if } j \neq i, \\ d^{-1}_{ii} a^\ell_{ii} d_{ii} = a^\ell_{ii}, & \text{if } j = i. \end{cases}$$

Thus $|b^\ell_{ii}| = UPFD^i_{impl} + \sum_{k=1,k\neq i}^N \frac{d_{ik}(\widetilde{\mathbf{c}}^n_\ell)}{c^n_{i,\ell}} > \sum_{k=1,k\neq i}^N \frac{d_{ik}(\widetilde{\mathbf{c}}^n_\ell)}{c^n_{i,\ell}} = \sum_{k=1,k\neq i}^N |b^\ell_{ki}|$ for $i \in \{1, \dots, N\}$, $\ell \in \{1, \dots, M\}$, which implies that $\mathbf{B}^T$ is strictly diagonal dominant. Using a result of [3] yields that $\mathbf{A}$ is a M-matrix and therefore $\mathbf{A}^{-1} \geq \mathbf{0}$ [4]. Considering $\mathbf{c}^{n+1} = \mathbf{A}^{-1}\mathbf{UPFD_{expl}} > 0$ proves the positivity. Conservativity follows directly from

$$\sum_{k=1}^N \sum_{i=1}^M c^{n+1}_{k,i} = \sum_{k=1}^N \sum_{i=1}^M \sum_{j=1,j\neq k}^N \left(\frac{p_{kj}(\widetilde{\mathbf{c}}^n_i)}{UPFD^j_{impl}} \frac{c^{n+1}_{j,i}}{c^n_{j,i}} - \frac{\overbrace{d_{kj}(\widetilde{\mathbf{c}}^n_i)}^{=p_{jk}(\widetilde{\mathbf{c}}^n_i)}}{UPFD^k_{impl}} \frac{c^{n+1}_{k,i}}{c^n_{k,i}} \right) + \sum_{k=1}^N \sum_{i=1}^M \frac{UPFD^k_{expl,i}(\mathbf{c}^n_k)}{UPFD^k_{impl}}$$

$$= \sum_{k=1}^N \sum_{i=1}^M \frac{UPFD^k_{expl,i}(\mathbf{c}^n_k)}{UPFD^k_{impl}} = \sum_{k=1}^N \sum_{i=1}^M c^n_{k,i} + \sum_{k=1}^N \underbrace{\frac{\frac{D_k}{\Delta x^2}(c^n_{k,M+1} - c^n_{k,1}) + (\frac{v_k}{\Delta x} + \frac{D_k}{\Delta x^2})(c^n_{k,0} - c^n_{k,M})}{UPFD^k_{impl}}}_{\text{inflow and outflow}},$$

which shows that the total value of all quantities does not change between the time levels n and $n+1$, except for fluxes over the boundaries of the domain. □

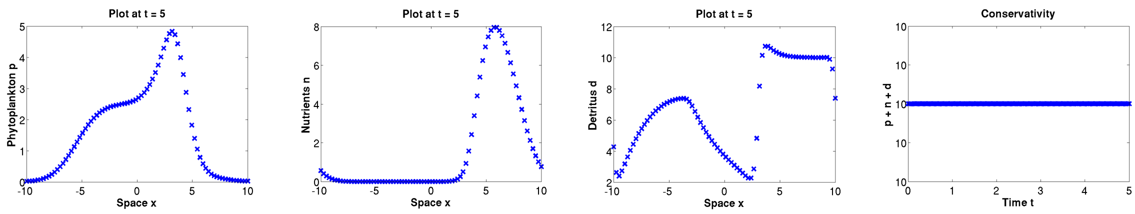
To confirm the properties of the numerical method developed, we consider the model problem

$$\left.\begin{array}{lllcrcl} \partial_t p & +\partial_x p & -0.2 \;\; \partial^2_{xx} p & = & & \frac{pn}{n+1} & - \;\; 0.3\, p \\ \partial_t n & +\partial_x n & -0.15 \;\; \partial^2_{xx} n & = & - & \frac{pn}{n+1} & \\ \partial_t d & & -0.01 \;\; \partial^2_{xx} d & = & & & 0.3\, p \end{array}\right\} \quad \text{in} \quad [-10, 10] \times (0, 30],$$

where p, n, d denote phytoplankton, nutrients, and detritus, respectively. With periodic boundary conditions as well as

$$p(x,0) = \begin{cases} 9.98, & x < -3, \\ 0.01, & \text{else}, \end{cases} \quad d(x,0) = \begin{cases} 9.98, & x > 3, \\ 0.01, & \text{else}, \end{cases} \quad n(x,0) = \begin{cases} 9.98, & -3 \leq x \leq 3, \\ 0.01 & \text{else}, \end{cases}$$

the results at time $t = 5$ computed using $\Delta x = 0.25$ and $\Delta t = 0.31$ are depicted in the plots. The constituents are obviously always positive, and additionally the right plot shows the conservativity of the scheme.



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