PATANKAR–TYPE LINEAR MULTISTEP SCHEMES

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INTRODUCTION

We present a novel class of high order, unconditionally positive and conservative linear multistep methods for **Production-Destruction Systems** (PDSs).

PRODUCTION-DESTRUCTION SYSTEMS

A general differential PDS has the form

$$y_i'(t) = \sum_{j=1}^{N} p_{ij}(y(t)) - \sum_{j=1}^{N} d_{ij}(y(t)), \qquad i = 1, \ldots, N,$$

where $t \geq 0$, the initial values $y_i^0 = y_i(0)$ are given and

- $y(t) = (y_1(t), \ldots, y_N(t))^{\mathsf{T}} \in \mathbb{R}^N$;
- $p_{ij}(\boldsymbol{y}) \geq 0$ is the rate of production of the i-th component consuming the j-th constituent;
- $d_{ij}(\boldsymbol{y}) \geq 0$ is the rate of destruction of the i-th component tranformed into the j-th constituent.

PDSs find relevant applications to

Chemistry, Biogeochemistry, Hydrodynamics, Finance, Epidemiology, Astrophysics

POSITIVE AND CONSERVATIVE PDS

A PDS is referred to as **positive** if for all $1 \leq i \leq N$,

$$y_i^0 > 0 \implies y_i(t) > 0, \quad \forall t \geq 0.$$

Theoretical positivity criteria are established in [1, 2].

A PDS is **fully conservative** if for all $1 \leq i, j \leq N$,

$$p_{ij}(y) = d_{ji}(y) \quad \text{and} \quad p_{ii}(y) = 0, \quad \forall y \in \mathbb{R}^N.$$

The solution to a positive and fully conservative PDS satisfies the following **conservation law**

$$\sum_{i=1}^{N} y_i(t) = \sum_{i=1}^{N} y_i^0, \qquad \forall t \geq 0.$$

EMBEDDING TECHNIQUE

The implementation of order p MPLM-k schemes requires

- accurate, positive and conservative starting values,
- PWDs that are order $p-1$ approximations of the continuous solution.

We address both tasks with an embedding technique based on the recursive integration by MPLM methods

- for $p = 1$ we just consider the one-step **Modified Patankar Euler** (MPE) scheme in [4];
- for $p > 1$ we employ a **k^*-steps order $p-1$** MPLM method, with $k^* \leq k$.

Theorem 5.

Let α_r^*, β_r^* and σ_i^{*n} be the coefficients and the PWDs of a MPLM-$k^*(p-1)$ integrator. A MPLM-$k(p)$ scheme is then **consistent and convergent of order p** if the PWDs are given, for $1 = 1, \ldots, N$ and $n \geq k$, by

$$\sigma_i^n = \sum_{r=1}^{k^*} \alpha_r^* y_i^{n-r} + h \sum_{r=1}^{k^*} \beta_r^* \sum_{j=1}^{N} \left(p_{ij}(y^{n-r}) \frac{\sigma_j^n}{\sigma_j^{*n}} - h \sum_{r=1}^{k^*} \beta_r^* \sum_{j=1}^{N} \left(d_{ij}(y^{n-r}) \frac{\sigma_i^n}{\sigma_i^{*n}} \right) \right).$$

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MODIFIED PATANKAR LINEAR MULTISTEP METHODS

Let $k > 1$ be an integer number. Let $\alpha_r \geq 0$ and $\beta_r \geq 0$, $r = 1, \ldots, k$, be the coefficients of an explicit k-steps **Linear Multistep** (LM) method. A **Modified Patankar Linear Multistep** k-steps scheme (MPLM-k) reads

$$y_i^n = \sum_{r=1}^{k} \alpha_r y_i^{n-r} + h \sum_{r=1}^{k} \beta_r \sum_{j=1}^{N} \left(p_{ij}(y^{n-r}) \frac{y_j^n}{\sigma_j^n} - d_{ij}(y^{n-r}) \frac{y_i^n}{\sigma_i^n} \right), \qquad i = 1, \ldots, N, \qquad n \geq k,$$

where $h > 0$, $t_n = nh$ and $y^n = (y_1^n, \ldots, y_N^n)^{\mathsf{T}} \approx y(t_n)$, for $n \geq 0$. The starting values $y^0, \ldots, y^{k-1} \in \mathbb{R}^N$ are given and the **Patankar Weight Denominators** (PWDs) satisfy

- σ_i^n unconditionally positive, $i = 1, \ldots, N$ and $n \geq k$;
- σ_i^n independent of y_i^n, $i = 1, \ldots, N$ and $n \geq k$.

Theorem 1.

Assume that $y_i^m > 0$, for each $1 \leq i \leq N$ and $0 \leq m < k$. Then, **independently of the stepsize h**,

$$y_i^n > 0, \quad \text{for all } i = 1, \ldots, N \text{ and } n \geq k.$$

Theorem 2.

Let $\sum_{i=1}^{N} y_i^m = \sum_{i=1}^{N} y_i^0$, for each $0 < m < k$. Then, $\forall h > 0$ the following **discrete conservation law** holds

$$\sum_{i=1}^{N} y_i^n = \sum_{i=1}^{N} y_i^0, \qquad \forall n \geq 0.$$

The MPLM methods are **linearly implicit**, **unconditionally positive** and **conservative** numerical integrators.

HIGH ORDER CONSISTENCY AND CONVERGENCE

Consider $\Omega = \left[0, \sum_{i=1}^{N} y_i^0\right]^N \subset \mathbb{R}^N$ and assume that

- $p \geq 1$ is a positive integer,
- the functions $p_{ij}(y)$ and $d_{ij}(y)$ belong to $C^p(\Omega)$,
- the underlying LM scheme is convergent of order p, so

$$\sum_{r=1}^{k} \alpha_r = 1, \quad \sum_{r=1}^{k} \left(r^q \alpha_r - q r^{q-1} \beta_r \right) = 0, \quad 1 \leq q \leq p.$$

Theorem 3.

A MPLM-k scheme is **consistent of order p** with the continuous-time PDS **if and only if**

$$\sigma_i(y(t_{n-1}), \ldots, y(t_{n-k})) = y_i(t_n) + \mathcal{O}(h^p),$$

for $i = 1, \ldots, N$ and $n \geq k$.

Theorem 4.

An order p consistent MPLM-k scheme is **convergent of order p** if the PWDs are continuously differentiable functions on $\Omega^k = \Omega \times \ldots \times \Omega$ and $\|y(t_m) - y^m\| = \mathcal{O}(h^p)$ for $m = 0, \ldots, k-1$.

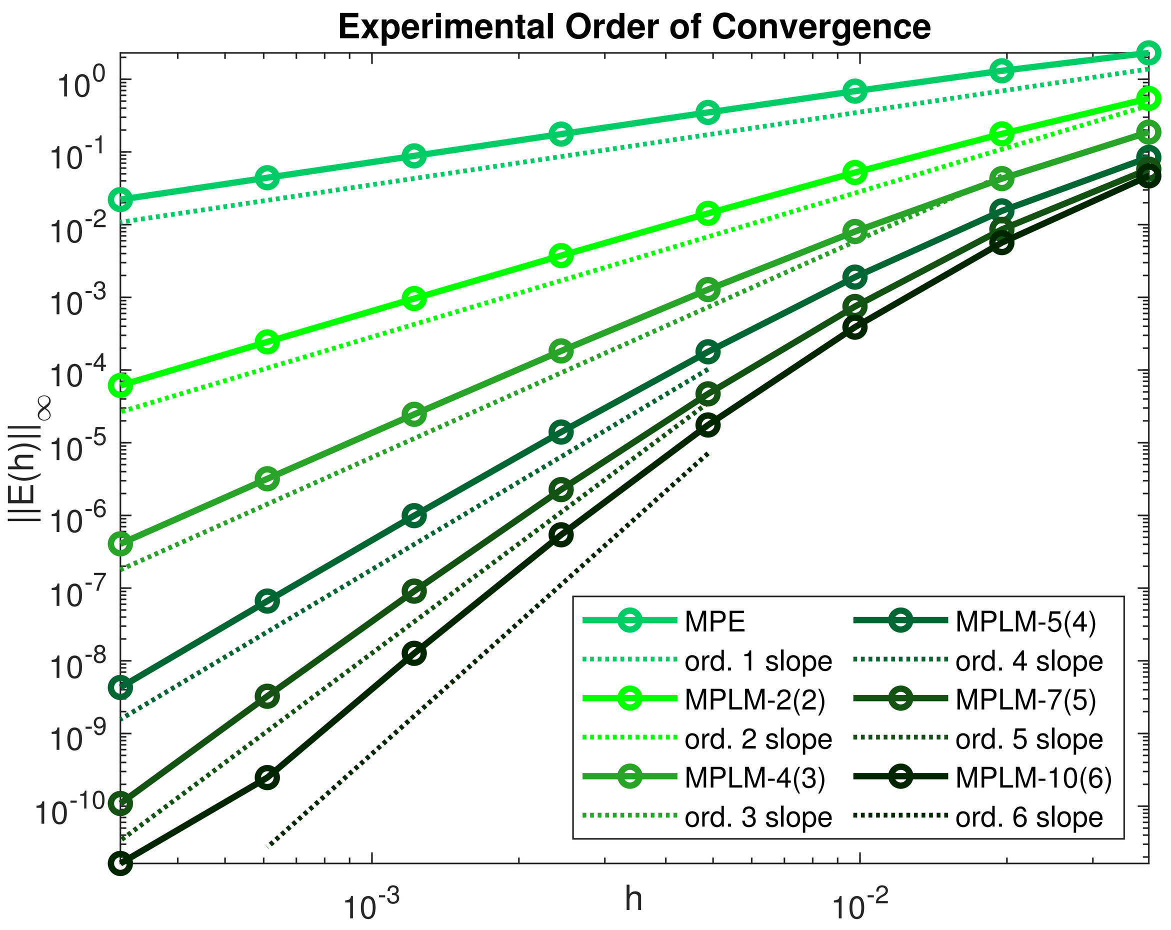


Figure 1: Brusselator test problem [3], maximum absolute error as a function of the stepsize. Here, MPLM-$k(p)$ denotes a k-steps, order p convergent method.

NUMERICAL EXPERIMENTS: EPIDEMIC MODEL

I test: the modified SIRD epidemic model in [5]
with $y(t) = (S(t), A(t), C(t), E(t), I(t), R(t), Q(t), D(t))^{\mathsf{T}}$,

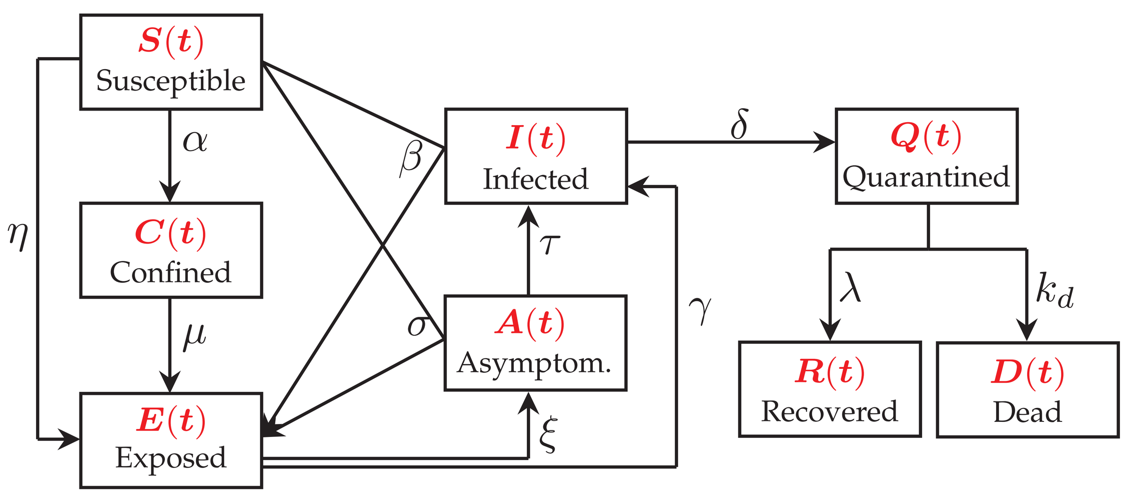
$$S'(t) = -\left(\alpha + \frac{\beta I(t) + \sigma A(t)}{N_P} + \eta \right) S(t),$$

$$A'(t) = -\tau A(t) + \xi E(t), \qquad C'(t) = \alpha S(t) - \mu C(t),$$

$$E'(t) = \left(\frac{\beta I(t) + \sigma A(t)}{N_P} + \eta \right) S(t) + \mu C(t) - (\gamma + \xi) E(t),$$

$$I'(t) = \tau A(t) + \gamma E(t) - \delta I(t), \qquad R'(t) = \lambda Q(t),$$

$$Q'(t) = \delta I(t) - \lambda Q(t) - k_d Q(t), \qquad D'(t) = k_d Q(t).$$



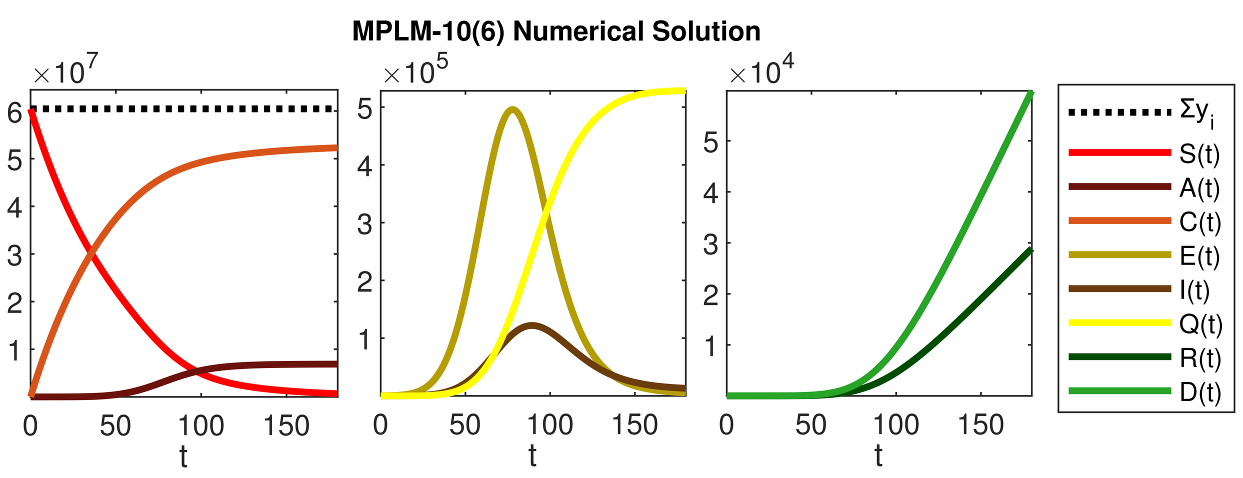


Figure 2: Modified SIRD model simulation with $h = 5.5 \cdot 10^{-3}$. The parameters, set accordingly to early-stage Covid-19 data [5], are $N_P = 6.046 \cdot 10^7$, $\alpha = 0.0194$, $\beta = 7.567$, $\mu = 2.278 \cdot 10^{-6}$, $\eta = 9.180 \cdot 10^{-7}$, $\sigma = 1.4633 \cdot 10^{-3}$, $\tau = 1.109 \cdot 10^{-4}$, $\xi = 0.263$, $\gamma = 0.021$, $\delta = 0.077$, $\lambda = 6.28 \cdot 10^{-4}$, $k_d = 0.0013$, $y^0 = (60459997, 0, 0, 1, 1, 0, 1, 0)^{\mathsf{T}}$.

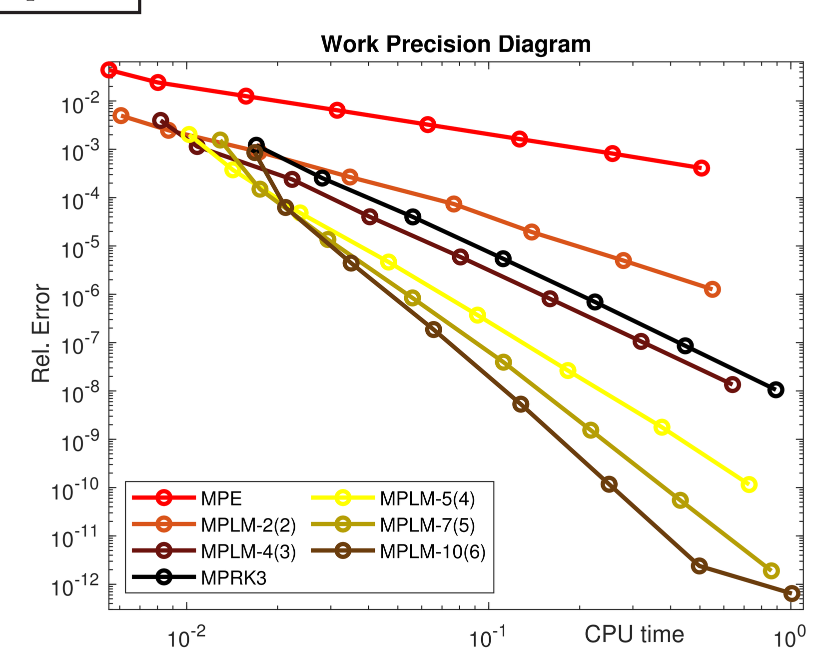


Figure 3: Work precision diagram and comparison of MPLM methods with the 3^{rd} order **Modified Patankar Runge-Kutta** (MPRK3) scheme in [3, Lemma 6, Case II, $\gamma = 0.5$].

NUMERICAL EXPERIMENTS: ALGAL BLOOM MODEL

II test: the non-linear model in [3],

$$y_1'(t) = -\frac{y_1(t) y_2(t)}{y_1(t) + 1}, \qquad y_1^0 = 9.98,$$

$$y_2'(t) = \frac{y_1(t) y_2(t)}{y_1(t) + 1} - 0.3 y_2(t), \qquad y_2^0 = 0.01,$$

$$y_3'(t) = 0.3 y_2(t), \qquad y_3^0 = 0.01.$$

MPLM schemes are compared to **Modified Patankar Deferred Correction** (MPDeC) methods [2], by computing the mean error and the residual

$$R(h) = \max_{0 \leq n \leq \frac{30}{h}} \left| \sum_{i=1}^{N} y_i^n - \sum_{i=1}^{N} y_i^0 \right|.$$

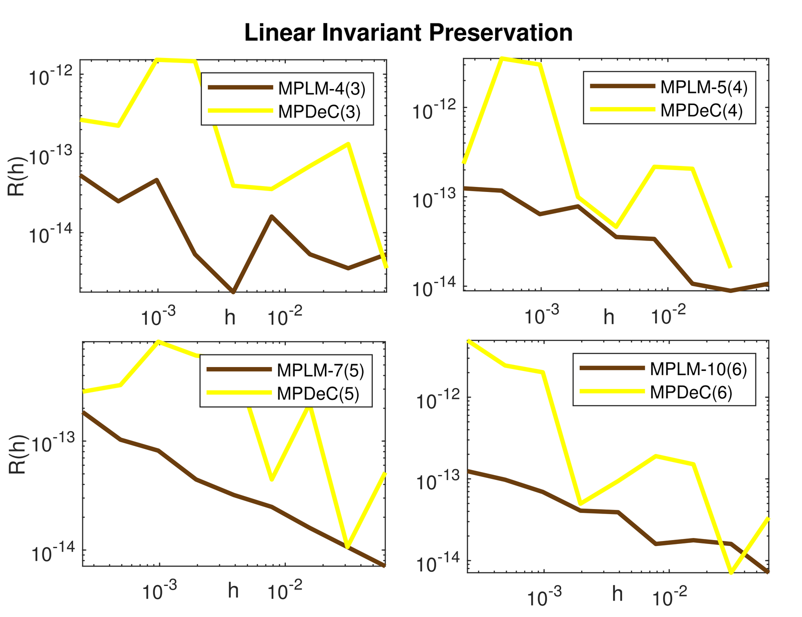


Figure 4: Linear invariant residual as a function of the stepsize. Here, MPDeC(p) denotes an order p MPDeC method.

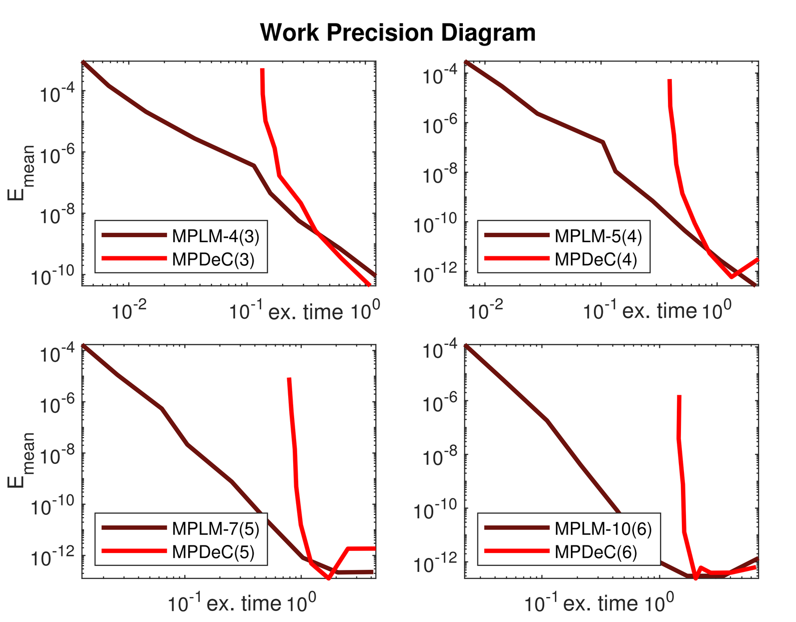


Figure 5: Mean error as a function of the execution time. Here, Julia codes from the repository in [2, Pag. 22] are used for MPDeC schemes.