Positivity-Preserving Patankar Approaches for Production-Destruction Systems: Simulation and Optimal Control

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Abstract

The mathematical modeling of various real life phenomena involving the interplay of formation and consumption processes leads to non-linear *Production–Destruction Systems* (PDS) of the form

$$\boldsymbol{y}'(t) = \big(P(\boldsymbol{y}(t)) - D(\boldsymbol{y}(t))\big)\boldsymbol{e}, \qquad \text{where} \qquad P, D : \mathbb{R}^N \to \mathbb{R}^{N\times N}, \qquad \boldsymbol{e} = [1,\dots,1]^\mathsf{T} \in \mathbb{R}^N.$$

In many practical applications, the underlying physics naturally yields PDS that are both positive and fully conservative for which $\Omega = \{[x_1,\dots,x_N]^\mathsf{T} : 0 \le x_i \le \boldsymbol{e}^\mathsf{T}\boldsymbol{y}(t_0),\ i = 1,\dots,N\}$ is a positively-invariant set and the conservation law $\boldsymbol{e}^\mathsf{T}(\boldsymbol{y}(t) - \boldsymbol{y}(t_0)) = 0,\ \forall t \ge t_0$ holds true. As a result, there is an increasing demand for numerical integrators that retain both the positivity of the solution and the system's linear invariant with no limitations on the discretization steplength. In this context, *Modified Patankar* (MP) methods have proven particularly beneficial (see [1, 5, 6, 8] and references therein).

The purpose of this contribution is twofold. First, we present the results of [7], where a novel class of k-step, unconditionally positive and conservative *Modified Patankar Linear Multistep* (MPLM) methods is introduced. A thorough theoretical analysis is conducted, with emphasis placed upon the conditions on the *Patankar Weight Denominators* (PWDs) required to achieve arbitrarily high orders of convergence. Additionally, the σ-embedding technique is proposed as a practical tool for the effective computation of PWDs. A comparison with other well-established MP discretizations reveals the competitiveness of the proposed methods for the simulation of PDS.

The second part of the present work explores the findings of [2], where the framework of a *Controlled PDS* (CPDS)

$$\boldsymbol{y}'(t) = \big(P(\boldsymbol{y}(t)) \odot \mathcal{P}(\boldsymbol{\alpha}(t)) - D(\boldsymbol{y}(t)) \odot \mathcal{D}(\boldsymbol{\alpha}(t))\big)\boldsymbol{e}, \quad \boldsymbol{\alpha} : \mathbb{R}^+ \to A \subset \mathbb{R}^M, \qquad \mathcal{P}, \mathcal{D} : A \to \mathbb{R}^{N\times N},$$

is outlined with the aim of influencing the dynamics of a PDS without altering its inherent properties. A general finite horizon *Optimal Control Problem* (OCP) is formulated and addressed via the dynamic programming approach. Specifically, the OCP is restated in terms of a backward-in-time Hamilton-Jacobi-Bellman (HJB) equation, whose unique viscosity solution corresponds to the value function [3]. We then propose a parallel-in-space *Modified Patankar Semi-Lagrangian* (MPSL) approximation scheme for the HJB equation [4] and design an uncondionally positive and conservative reconstruction procedure for the optimal control in feedback and open-loop forms. The application to two case studies, specifically enzyme catalyzed biochemical reactions and infectious diseases, highlights the advantages of the proposed methodology over classical semi-Lagrangian discretizations.

References

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