Positive and mass-conservative integrators for biochemical systems

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The state variables involved in a biochemical process are non-negative, since they model the concentration of chemical elements and compounds. In addition, biochemical systems are mass-conservative, in the sense that the total amount of any chemical element involved in the process does not change over time. The numerical schemes for the integration of this type of equations must be unconditionally positive and mass-conservative, if they are to produce meaningful results.

In this talk I will give an overview of the existing numerical schemes for biochemical systems in the recent literature [1, 4]. Then, I will propose a novel explicit scheme based on the composition of the (non-Newtonian) geometric Euler scheme in [2] with a non-standard positive integrator [3]. This work has been supported by GNCS-INDAM.

References

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