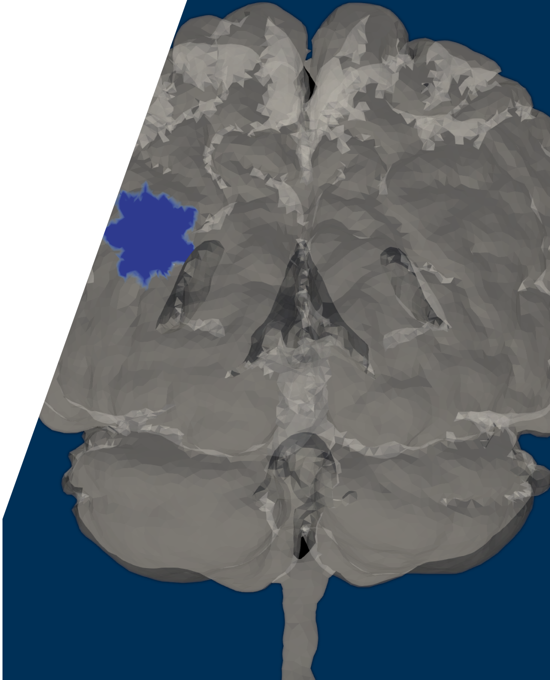
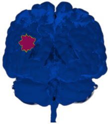
Fully-Discrete Lyapunov Consistent Discretizations for Parabolic Reaction-Diffusion Equations with r Species

R. Al Jahdali[1] D.C. Del Rey Fernández[2] L. Dalcin[1] **M. Sayyari**[1,4]
P. Markowich[3] M. Parsani[1,3]

[1]CEMSE, ECRC, KAUST, Thuwal, Saudi Arabia
[2]Dep. of Appl. Math., UWaterloo, Waterloo, Canada
[3]PSE, KAUST, Thuwal, Saudi Arabia
[4]Dep. of Math. & Stat., ODU, Norfolk, VA

November 2, 2024





Lyapunov consistency: A form of nonlinear stability

A more well known form of nonlinear stability is entropy stability:

- Mostly used in CFD applications.
- Practically allows for the derivation of a bound on solutions [1, 2].

$$\int_{\Omega} \frac{\partial \mathcal{S}}{\partial t} \leq \mathcal{C}_{\text{DATA}} \tag{1}$$

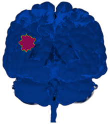
$$\implies \left\| u(x, t_f) \right\|_{L^2(\Omega)} \leq \frac{\mathcal{C}_{\text{DATA}}}{\lambda_{\min}\left(\frac{\partial^2 S}{\partial u^2}(\theta)\right)} + \| u(x, 0) \|_{L^2(\Omega)} \tag{2}$$

Entropy stability in practice

	Degree	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
ES-C	3^3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
	6^3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
	12^3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
	24^3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
	48^3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
SF-KG	3^3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
	6^3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
	12^3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
	24^3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
	48^3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
DC	3^3	✓	✓	×	×	×	×	×	×	×	×	×	×	×	×	×
	6^3	✓	✓	×	×	×	×	×	×	×	×	×	×	×	×	×
	12^3	✓	✓	×	×	×	×	×	×	×	×	×	×	×	×	×
	24^3	✓	✓	✓	×	×	×	×	×	×	✓	×	✓	✓	✓	✓
	48^3	✓	✓	✓	✓	×	×	✓	✓	✓	✓	✓	✓	✓	✓	✓
	96^3	✓	✓	✓	✓	✓	✓	✓	–	–	–	–	–	–	–	–

	Degree	1	2	3	4
ES-C	4^3	✓	✓	✓	✓
	8^3	✓	✓	✓	✓
	16^3	✓	✓	✓	✓
	32^3	✓	✓	✓	✓
	64^3	✓	✓	✓	✓
SF-KG	4^3	×	✓	✓	✓
	8^3	×	✓	✓	✓
	16^3	×	✓	✓	✓
	32^3	×	✓	✓	✓
	64^3	✓	✓	✓	✓
DC	4^3	×	×	×	×
	8^3	×	×	×	×
	16^3	×	×	×	✓
	32^3	×	×	✓	✓
	64^3	✓	✓	✓	✓

Figure: Numerical stability for the Taylor–Green vortex (TGV), left, and homogeneous-isotropic turbulence (HIT), right. $\surd$ = success, $\times$ = failures. The entropy stable discretization is noted ES-C. The discretization that uses the Kennedy and Gruber (2008) flux is noted SF-KG. The standard discontinuous collocation is noted DC. Adapted from [3].



ODE to PDE: reaction equation

We are interested in equations the form

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{F}\left(\mathbf{U}\right), \quad t \in \left[t_0, T_f\right). \tag{3}$$

With globally asymptotically stable equilibrium points U_{eq}, and a Lyapunov function V s.t.

$$V > 0, \qquad \frac{dV}{dt} \leq 0 \tag{4}$$

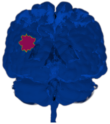
ODE to PDE: reaction-diffusion equation

We extend the reaction equation to a PDE via a diffusion term

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{F}\left(\mathbf{U}\right) + \sum_{l,m=1}^{d} \frac{\partial}{\partial x_l}\left(\mathsf{C}_{l,m}\frac{\partial \mathbf{U}}{\partial x_m}\right), \quad \mathbf{x} \in \Omega, \quad t \in [t_0, T_f). \tag{5}$$

This system inherits the ODE equilibrium points because they are constant in space. Define the Lyapunov functional

$$\tilde{V} = \int_\Omega V d\Omega, \qquad \text{we would like} \qquad \tilde{V} > 0, \text{ and } \frac{d\tilde{V}}{dt} \leq 0 \tag{6}$$



Lyapunov consistency

Define $W = dV/dU$. We consider systems where

1. $W^\top F \leq 0$
2. V is convex and locally positive definite
3. $\hat{\mathsf{M}} + \hat{\mathsf{M}}^\top \geq 0$, where $\hat{\mathsf{M}}_{l,m} = \hat{\mathsf{C}}_{l,m}$
4. appropriate boundary conditions can be found such that

$$\oint_\Gamma \sum_{l,m}^{dim} W^\top \hat{\mathsf{C}}_{l,m} \frac{\partial W}{\partial x_m} n_{x_l} d\Gamma \leq 0 \qquad (7)$$

Theorem

Given the previous assumptions, if $\tilde{V}$ is locally positive definite, $d\tilde{V}/dt \leq 0$, and $\|U\| \to +\infty \implies \tilde{V}(U) \to +\infty$, then, $U_{eq} = 0$ is globally asymptotically stable.

Lyapunov consistency

We multiply the PDE from the left by the Lyapunov variables $W = dV/dU$ and integrate over the domain

$$\int_{\Omega} W^{\top} \frac{\partial \mathbf{U}}{\partial t} dx = \int_{\Omega} W^{\top} \mathbf{F}(\mathbf{U}) + W^{\top} \sum_{l,m=1}^{d} \frac{\partial}{\partial x_l} \left(\mathsf{C}_{l,m} \frac{\partial \mathbf{U}}{\partial x_m} \right) dx. \tag{8}$$

Using integration by parts and applying the previous assumptions

$$\frac{\partial \tilde{V}}{\partial t} \leq - \int_{\Omega} Z^{\top} \hat{\mathsf{M}} Z \, dx \leq 0, \tag{9}$$

where $Z = \left[\frac{\partial W}{\partial x_1}, \cdots, \frac{\partial W}{\partial x_m} \right]^{\top}$.

Semi-discrete Lyapunonv consistency: SBP operators

SBP operators define a discrete integration (quadrature) and high-order operators

$$\|x\|_{L^2}^2 = x^\top \mathcal{P} x, \quad \mathcal{D} = \mathcal{P}^{-1}\mathcal{Q}, \quad \mathcal{Q} + \mathcal{Q}^\top = \begin{bmatrix} -1 & & \\ & 0 & \\ & & 1 \end{bmatrix}, \quad \mathcal{D}x^j = jx^{j-1}, \forall j \leq p. \quad (10)$$

SBP operators are capable of inheriting the bounds into the semi-discrete representation by mimicing the integration by parts property discretely [4].

Semi-dicrete Lyapunov consistency: scheme

General form (curvilinear coordinates shown in the paper)

$$\frac{du_k}{dt} = f_k + \sum_{l,m=1}^{dim} \mathcal{D}_l [\mathsf{C}_{l,m}]_k \Theta_m^k + \mathbf{SAT}_V + \mathbf{SAT}_{IP} + \mathbf{SAT}_{BC}, \tag{11}$$

where

$$\Theta_m^k = \mathcal{D}_m w_k + \mathbf{SAT}_W. \tag{12}$$

SAT are penalty terms that apply at the interfaces between elements.

Semi-discrete Lyapunov consistency

Utilizing the discrete counterparts to the continuous operators,

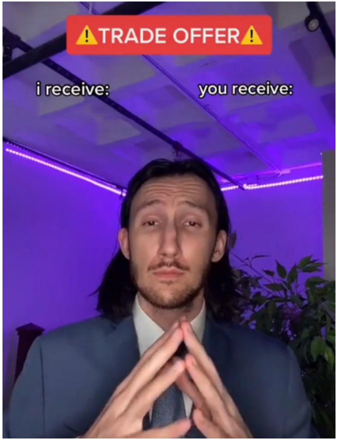
$$\sum_{k=1}^{K} \bar{\mathbf{1}}^{\top} \bar{\mathcal{P}}_k \frac{d\boldsymbol{v}_k}{dt} = \sum_{k=1}^{K} \boldsymbol{w}_k^{\top} \mathcal{P}_k \boldsymbol{f}_k - \sum_{k=1}^{K} \sum_{l,m=1}^{dim} \left(\Theta_l^k\right)^{\top} \hat{\mathsf{C}}_{l,m} \mathcal{P}_k \Theta_m^k + ST, \tag{13}$$

where ST are surface terms.

Semi-discrete Lyapunov consistency: interpretation

RD system with:

1. $W^\top F \leq 0$
2. $V > 0$ is convex
3. $\hat{\mathrm{M}} + \hat{\mathrm{M}}^\top \geq 0$
4. $ST \leq 0$



By bradeazy [5].

Theorem

Given the previous assumptions, if $\tilde{V}$ is locally positive definite, $d\tilde{V}/dt \leq 0$, and $\|u\| \to +\infty \implies \tilde{V}(u) \to +\infty$, then, $u_{eq} = 0$ is globally asymptotically stable.

Relaxation Runge–Kutta: fully discrete Lyapunov stability

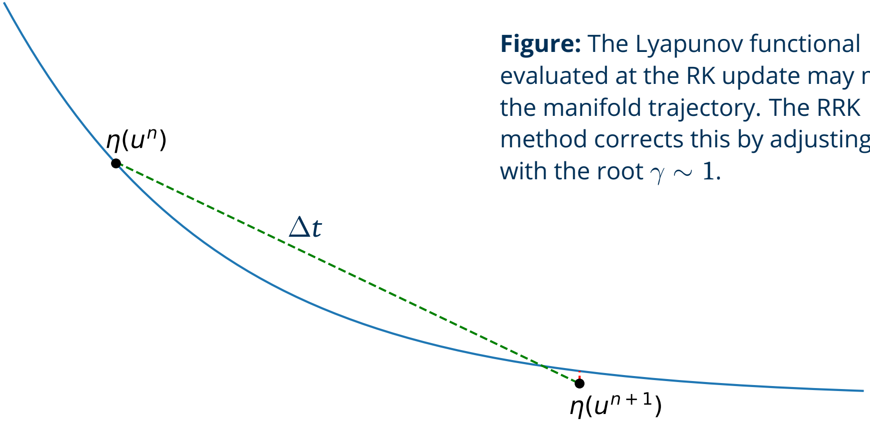


Figure: The Lyapunov functional evaluated at the RK update may miss the manifold trajectory. The RRK method corrects this by adjusting Δt with the root $\gamma \sim 1$.

Relaxation Runge–Kutta: fully discrete Lyapunov stability

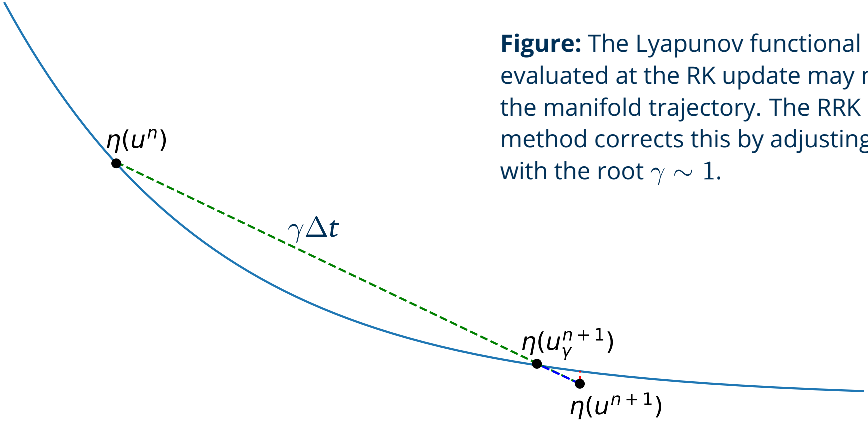


Figure: The Lyapunov functional evaluated at the RK update may miss the manifold trajectory. The RRK method corrects this by adjusting Δt with the root $\gamma \sim 1$.

Relaxation Runge–Kutta: fully discrete Lyapunov stability

We compute a γ_n at every timestep to adjust the update stepsize Δt

$$U_\gamma^{n+1} = U^n + \gamma_n \Delta t \sum_{i=1}^{s} b_i F_i, \tag{14}$$

Where γ_n is the positive root of

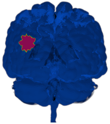
$$r(\gamma) = \eta\left(U^n + \gamma \Delta t \sum_{i=1}^{s} b_i F_i\right) - \eta(U^n) - \gamma \Delta t \sum_{i=1}^{s} b_i \left\langle \eta'(Y_i), F_i \right\rangle, \tag{15}$$

More on RRK methods for general functionals in [6].

RRK: important results

The RRK scheme:

- inherits the Lyapunov functional, and is dissipation preserving
- the local error is $\mathcal{O}(\Delta t^{p+1})$
- has a positive root γ
- fixed points retain the stability properties of the ODE equilibriums
- does not have spurious solutions



Numerical results: SI epidemiology

From [7, 8]

$$U = [S, I]^\top, \tag{16a}$$

$$F = \left[\nu R_d (S+I)\,(1-(S+I)) - R_0 \frac{SI}{S+I} - \nu S,\; R_0 \frac{SI}{S+I} - I\right]^\top, \tag{16b}$$

$$\mathsf{C} = \begin{bmatrix} D_S & 0 \\ 0 & D_I \end{bmatrix}, \tag{16c}$$

Where R_d, R_0 and ν depend on the parameters:

- r, the susceptible growth rate
- β, the transmission rate
- μ, the death rate

Numerical results: SI epidemiology

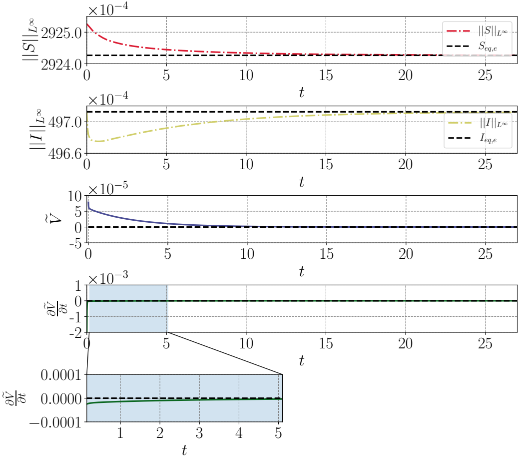


Figure: Temporal evolution of the maximum norm of the solution, (S, I), Lyapunov functional, $\widetilde{V}$, and time derivative of the Lyapunov functional, $\frac{d\widetilde{V}}{dt}$, for the SI PDE model.

Numerical results: SI epidemiology

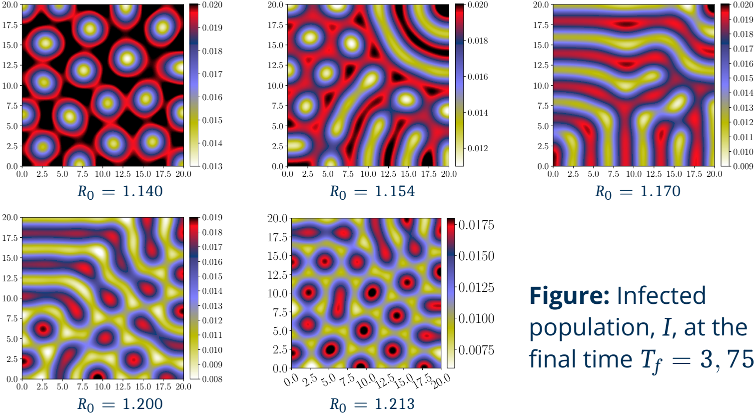
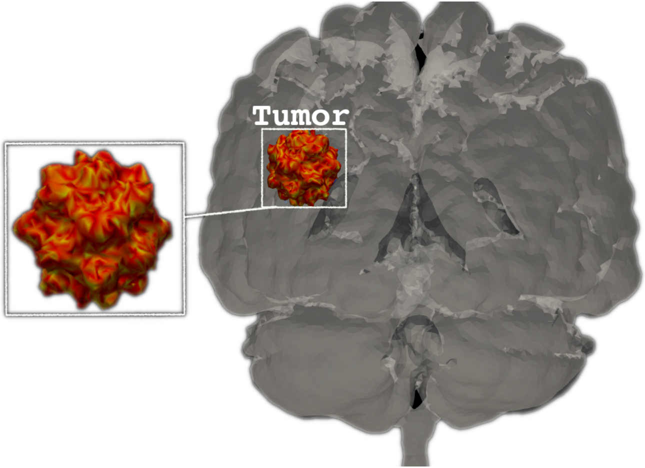


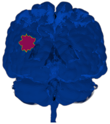
Figure: Infected population, I, at the final time $T_f = 3,750$.

Numerical results: tumor M1 virology

The model consists of [9]

- S nutrients consentration
- N normal cells
- T tumor cells
- $M1$ virus
- Z cytotoxic T lymphocytes (CTS)





Numerical results: tumor M1 virology

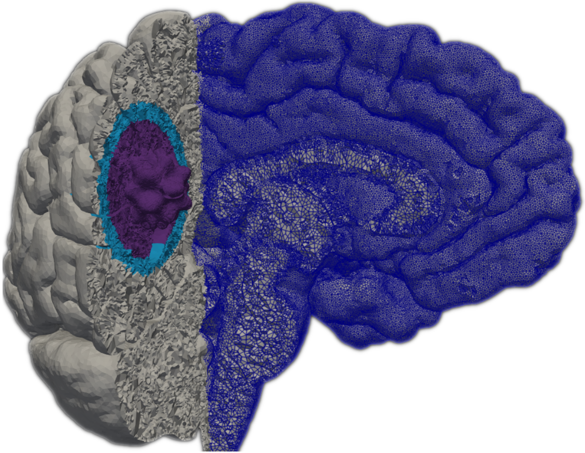
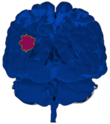


Figure: Brain mesh constructed from MRI images using SimNIBS [10]. The total number of hexahedral elements is $\simeq 3.2899 \times 10^6$, and the number of DOFs is $\simeq 18.9496 \times 10^6$.



Numerical results: tumor M1 virology

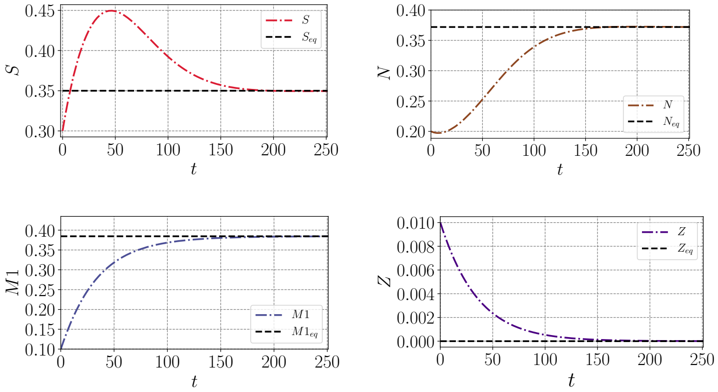


Figure: Temporal evolution of the nutrients, S, normal cells, N, tumor cells, T, free M1 virus, $M1$, immune response, Z.

Numerical results: tumor M1 virology

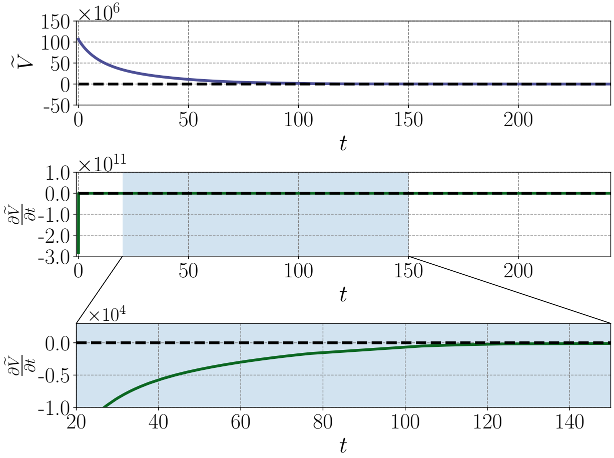


Figure: Temporal evolution of the Lyapunov functional, $\widetilde{V}$, and its time derivative, $\partial \widetilde{V} / \partial t$.

Numerical results: tumor M1 virology

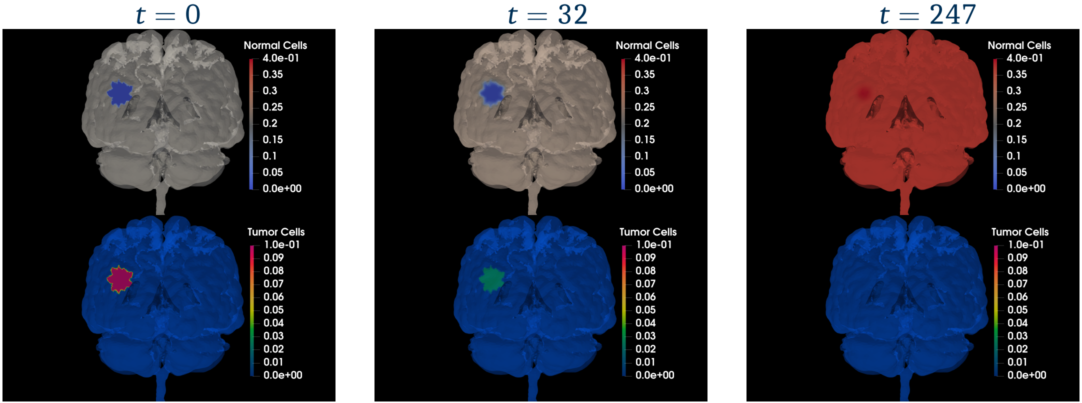
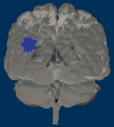


Figure: Response of the tumor to the oncolytic M1 virotherapy at $t = 0$ (initial condition), $t = 32.67$, and $t = 247.96$.



Open access available

Link to paper

Communications on Applied Mathematics and Computation
https://doi.org/10.1007/s42967-024-00425-7

ORIGINAL PAPER

Fully-Discrete Lyapunov Consistent Discretizations for Parabolic Reaction-Diffusion Equations with *r* Species

Rasha Al Jahdali[1] · David C. Del Rey Fernández[2] · Lisandro Dalcin[1] · Mohammed Sayyari[1] · Peter Markowich[1] · Matteo Parsani[1,3]

Received: 26 November 2023 / Revised: 1 April 2024 / Accepted: 3 May 2024

Abstract
Reaction-diffusion equations model various biological, physical, sociological, and environmental phenomena. Often, numerical simulations are used to understand and discover the dynamics of such systems. Following the extension of the nonlinear Lyapunov theory applied to some class of reaction-diffusion partial differential equations (PDEs), we develop the first fully discrete Lyapunov discretizations that are consistent with the stability properties of the continuous parabolic reaction-diffusion models. The proposed framework provides a systematic procedure to develop fully discrete schemes of arbitrary order in space and time for solving a broad class of equations equipped with a Lyapunov functional. The new schemes are applied to solve systems of PDEs, which arise in epidemiology and oncolytic M1 virotherapy. The new computational framework provides physically consistent and accurate results without exhibiting scheme-dependent instabilities and converging to unphysical solutions. The proposed approach represents a capstone for developing efficient, robust, and predictive technologies for simulating complex phenomena.

Rasha Al Jahdali
rasha.aljahdali@kaust.edu.sa

Matteo Parsani
matteo.parsani@kaust.edu.sa

David C. Del Rey Fernández
dcdelrey@gmail.com

Lisandro Dalcin
dalcinl@gmail.com

Mohammed Sayyari
mohammed.alsayyari@kaust.edu.sa

Peter Markowich
peter.markowich@kaust.edu.sa

1 Computer Electrical and Mathematical Science and Engineering Division (CEMSE), Extreme Computing Research Center (ECRC), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

2 Department of Applied Mathematics, University of Waterloo, Waterloo, Canada

3 Physical Science and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

Published online: 23 September 2024

Springer

References:

- M. Svärd, “Weak solutions and convergent numerical schemes of modified compressible navier–stokes equations,” *Journal of Computational Physics*, vol. 288, pp. 19–51, 2015.
- M. Sayyari, *The capabilities of summation-by-parts and structure-preserving operators for compressible computational fluid dynamics and reaction-diffusion models*. PhD thesis, 2022.
- D. B. Rojas, *Application of Robust Entropy Stable Numerical Methods for Modeling Shock Waves, Turbulence, and Pollutant Dispersion in the Planetary Boundary Layer*. PhD thesis, 2021.
- D. C. D. R. Fernández, J. E. Hicken, and D. W. Zingg, “Review of summation-by-parts operators with simultaneous approximation terms for the numerical solution of partial differential equations,” *Computers & Fluids*, vol. 95, pp. 171–196, 2014.
- @bradeazy *TikTok*.
- H. Ranocha, M. Sayyari, L. Dalcin, M. Parsani, and D. I. Ketcheson, “Relaxation runge–kutta methods: Fully discrete explicit entropy-stable schemes for the compressible euler and navier–stokes equations,” *SIAM Journal on Scientific Computing*, vol. 42, no. 2, pp. A612–A638, 2020.
- W. Wang and X.-Q. Zhao, “Basic reproduction numbers for reaction-diffusion epidemic models,” *SIAM Journal on Applied Dynamical Systems*, vol. 11, no. 4, pp. 1652–1673, 2012.
- Y. Cai, D. Chi, W. Liu, and W. Wang, “Stationary patterns of a cross-diffusion epidemic model,” *Abstract and Applied Analysis*, vol. 2013, 2013.
- A. M. Elaiw, A. D. Hobiny, and A. D. Al Agha, “Global dynamics of reaction-diffusion oncolytic M1 virotherapy with immune response,” *Applied Mathematics and Computation*, vol. 367, p. 124758, 2020.
- A. Thielscher, A. Antunes, and G. B. Saturnino, “Field modeling for transcranial magnetic stimulation: A useful tool to understand the physiological effects of tms?,” in *2015 37th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC)*, pp. 222–225, 2015.

Thanks for your attention

For further questions: malsayya@odu.edu

ResearchGate

Suggested References:

M. Sayyari. "The capabilities of summation-by-parts and structure-preserving operators for compressible computational fluid dynamics and reaction-diffusion models." (2022).

R. Al Jahdali, et.al. "Fully-Discrete Lyapunov Consistent Discretizations for Parabolic Reaction-Diffusion Equations with r Species." Commun. Appl. Math. Comput. (2024).