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Energy stable numerical schemes for a chemo-repulsion model with linear production term - Nº 9

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Chemotaxis model

Chemotaxis is understood as the biological process of the movement of living organisms in response to a chemical stimulus which can be given towards a higher (attractive) or lower (repulsive) concentration of a chemical substance. Specifically, we focus on the following chemorepulsion model:

$$\begin{cases} \partial_t u - \Delta u = \nabla\cdot(u\nabla v) \ \text{ in } \Omega,\ t>0,\\ \partial_t v - \Delta v + v = u \text{ in } \ \Omega,\ t>0,\\ \frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0 \ \text{ on } \partial\Omega,\ t>0,\\ u(x,0)=u_0(x)>0,\ v(x,0)=v_0(x)>0 \ \text{ in } \Omega, \end{cases} \tag{1}$$

where $\Omega\subseteq\mathbb{R}^d$ $(d=2,3)$, and $u>0$ denotes the cell density and $v>0$ the chemical concentration.

Some properties

Problem (1) is well-posed ([1]), and is conservative in u, that is,

$$\int_\Omega u(t) = \int_\Omega u_0, \quad \forall t>0.$$

Moreover, formally testing $(1)_1$ by $ln\ u$ and $(1)_2$ by $-\Delta v$, we obtain

$$\frac{d}{dt}\int_\Omega \left(u(ln\ u-1)+\frac{1}{2}|\nabla v|^2\right)dx + \int_\Omega \left(4|\nabla\sqrt{u}|^2+|\Delta v|^2+|\nabla v|^2\right)dx = 0.$$

Truncated functions and operators

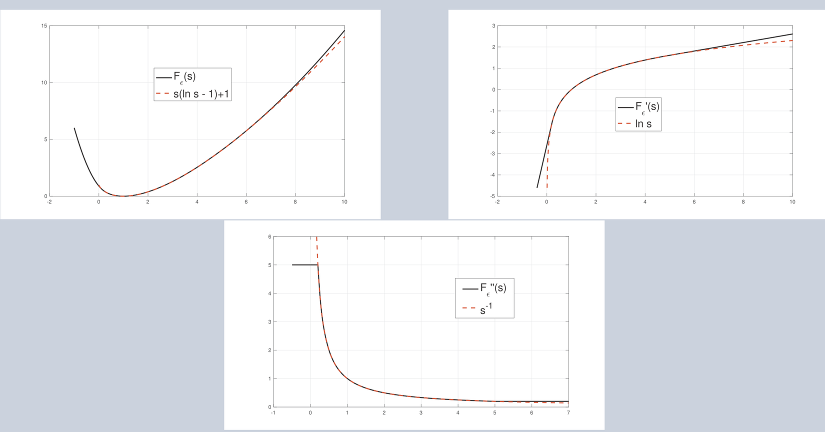

Figure: The function F_ε and its derivatives.

- F_ε: Truncation of $s(ln\ s-1)+1$.
- F'_ε: Truncation of $ln\ s$.
- F''_ε: Truncation of s^{-1}.
- λ_ε: Truncation of s.
- Λ_ε: Constant by elements matrix (key for the energy-stability of scheme **UV**).
- π^h: Lagrange interpolator.
- $(\cdot,\cdot)^h$: Mass lumping.

Main assumptions on the space discretization

- For the scheme **UV** are required right angled simplices.
- For the schemes **UV** and **US**, U_h is approximated by $\mathbb{P}_1$-continuous FE.
- For all schemes, V_h, Σ_h, Z_h, W_h are approximated by $\mathbb{P}_k$-continuous FE, $k\geq 1$.

Scheme UV

Time step n: Given $(u_\varepsilon^{n-1}, v_\varepsilon^{n-1})\in U_h\times V_h$, compute $(u_\varepsilon^n, v_\varepsilon^n)\in U_h\times V_h$ s.t.

$$\begin{cases} (\delta_t u_\varepsilon^n,\bar u)^h + (\nabla u_\varepsilon^n,\nabla\bar u) + (\Lambda_\varepsilon(u_\varepsilon^n)\nabla v_\varepsilon^n,\nabla\bar u) = 0, \quad \forall \bar u\in U_h,\\ (\delta_t v_\varepsilon^n,\bar v) + (A_h v_\varepsilon^n,\bar v) - (u_\varepsilon^n,\bar v) = 0, \quad \forall\bar v\in V_h. \end{cases}$$

Scheme US

Time step n: Given $(u_\varepsilon^{n-1}, \sigma_\varepsilon^{n-1})\in U_h\times \Sigma_h$, compute $(u_\varepsilon^n, \sigma_\varepsilon^n)\in U_h\times \Sigma_h$ s.t.

$$\begin{cases} (\delta_t u_\varepsilon^n,\bar u)^h + (\lambda_\varepsilon(u_\varepsilon^n)\nabla\pi^h(F'_\varepsilon(u_\varepsilon^n)),\nabla\bar u) = -(\lambda_\varepsilon(u_\varepsilon^n)\sigma_\varepsilon^n,\nabla\bar u), \ \forall\bar u\in U_h,\\ (\delta_t\sigma_\varepsilon^n,\bar\sigma) + (B_h\sigma_\varepsilon^n,\bar\sigma) = (\lambda_\varepsilon(u_\varepsilon^n)\nabla\pi^h(F'_\varepsilon(u_\varepsilon^n)),\bar\sigma), \quad \forall\bar\sigma\in\Sigma_h. \end{cases}$$

Here, the auxiliary variable σ_ε^n try to approximate ∇v_ε^n.

Scheme UZSW

Time step n: Given $(u_\varepsilon^{n-1}, \sigma_\varepsilon^{n-1}, w_\varepsilon^{n-1})\in U_h\times\Sigma_h\times W_h$, compute $(u_\varepsilon^n, z_\varepsilon^n, \sigma_\varepsilon^n, w_\varepsilon^n)\in U_h\times Z_h\times\Sigma_h\times W_h$ s.t.

$$\begin{cases} (\delta_t u_\varepsilon^n,\bar z) + (\lambda_\varepsilon(u_\varepsilon^{n-1})\nabla z_\varepsilon^n,\nabla\bar z) = -(u_\varepsilon^{n-1}\sigma_\varepsilon^n,\nabla\bar z), \quad \forall\bar z\in Z_h,\\ (\delta_t\sigma_\varepsilon^n,\bar\sigma) + (B_h\sigma_\varepsilon^n,\bar\sigma) = (u_\varepsilon^{n-1}\nabla z_\varepsilon^n,\bar\sigma), \quad \forall\bar\sigma\in\Sigma_h,\\ (\delta_t w_\varepsilon^n,\bar w) = (H'_\varepsilon(u_\varepsilon^{n-1})\delta_t u_\varepsilon^n,\bar w), \quad \forall\bar w\in W_h,\\ (z_\varepsilon^n,\bar u) = 2(w_\varepsilon^n H'_\varepsilon(u_\varepsilon^{n-1}),\bar u), \quad \forall\bar u\in U_h. \end{cases}$$

Here, the auxiliary variables σ_ε^n, z_ε^n and w_ε^n try to approximate ∇v_ε^n, $F'_\varepsilon(u_\varepsilon^n)$ and $\sqrt{F_\varepsilon(u_\varepsilon^n)}$

Main Theoretical results

- Well-posedness of these numerical schemes.
- Unconditional energy-stability (for modified energies) and mass-conservation of the schemes. In fact, the following discrete energy laws hold:

$$\delta_t\left((F_\varepsilon(u_\varepsilon^n),1)^h+\frac{1}{2}\|\nabla v_\varepsilon^n\|_0^2\right)+\varepsilon\|\nabla u_\varepsilon^n\|_0^2+\|\Delta_h v_\varepsilon^n\|_0^2+\|\nabla v_\varepsilon^n\|_0^2\leq 0, \ (\mathbf{UV})$$

$$\delta_t\left((F_\varepsilon(u_\varepsilon^n),1)^h+\frac{1}{2}\|\sigma_\varepsilon^n\|_0^2\right)+\varepsilon\|\nabla\pi^h(F'_\varepsilon(u_\varepsilon^n))\|_0^2 d+\|\sigma_\varepsilon^n\|_1^2\leq 0, \ (\mathbf{US})$$

$$\delta_t\left(\|w_\varepsilon^n\|_0^2+\frac{1}{2}\|\sigma_\varepsilon^n\|_0^2\right)+\varepsilon\|\nabla z_\varepsilon^n\|_0^2+\|\sigma_\varepsilon^n\|_1^2\leq 0, \ (\mathbf{UZSW}).$$

- Uniform in time energy estimates.
- Approximated positivity of u_ε^n and v_ε^n for schemes **UV** and **US**, when $\varepsilon\to 0$.

Main Numerical results

- There are initial conditions for which **UZSW** is not energy stable with respect to the energy

$$\mathcal{E}_e(u,v) := \int_\Omega u_+(ln\ u_+ -1)\ dx + \frac{1}{2}\|\nabla v\|_0^2,$$

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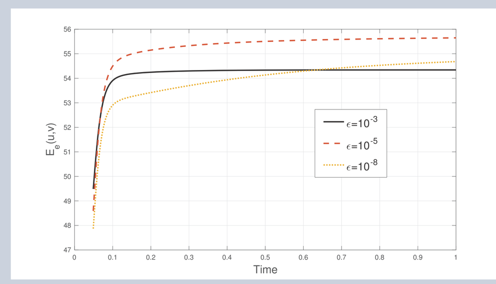

Figure: $E_e(u_\varepsilon^n, v_\varepsilon^n)$ of **UZSW**.

- The scheme **US** has convergence problems with the linear iterative method, which are overcome considering thinner meshes.
- **UV** and **US** have decreasing energy $\mathcal{E}_e(u,v)$. In fact, it holds

$$RE_e(u_\varepsilon^n,v_\varepsilon^n) := \delta_t\mathcal{E}_e(u^n,v^n)+4\int_\Omega|\nabla\sqrt{[u^n]_+}|^2\ dx+\|\Delta_h v^n\|_0^2+\|\nabla v^n\|_0^2\leq 0.$$

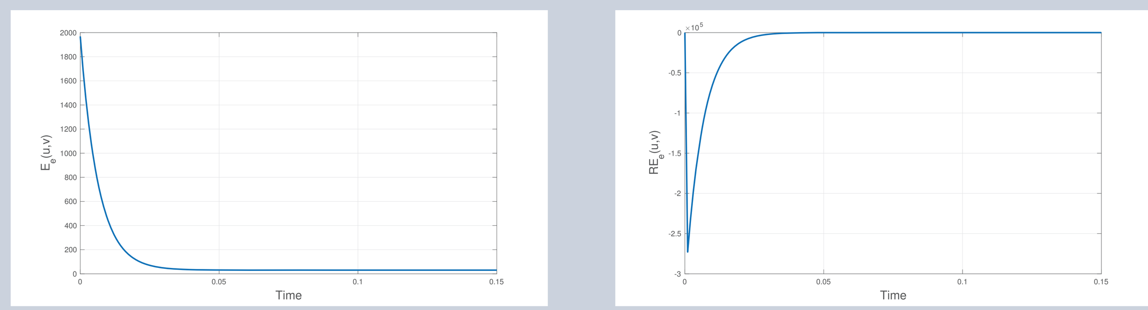

Figure: Energy $\mathcal{E}_e(u^n,v^n)$ and $RE_e(u^n,v^n)$ of **UV** and **US**.

- The scheme **BEUV** (the classical backward Euler for model (1)) has decreasing in time energy $\mathcal{E}_e(u,v)$. However, for some cases, the discrete energy inequality $RE_e(u^n,v^n)\leq 0$ is not satisfied.

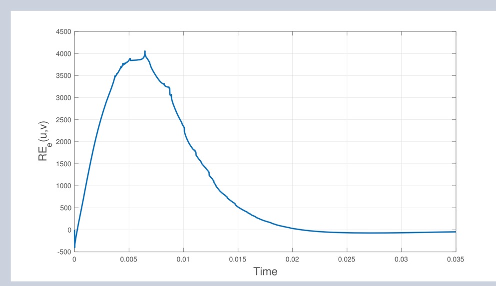

Figure: $RE_e(u_\varepsilon^n, v_\varepsilon^n)$ of **BEUV**.

- For **UV** and **US**, $[u_\varepsilon^n]_-\to 0$ when $\varepsilon\to 0$, while for **UZSW** this behavior is not observed. Finally, for **BEUV** negative values (greater than the obtained in **UV** and **US**) for the minimum of u^n in some times $t_n>0$ are observed.

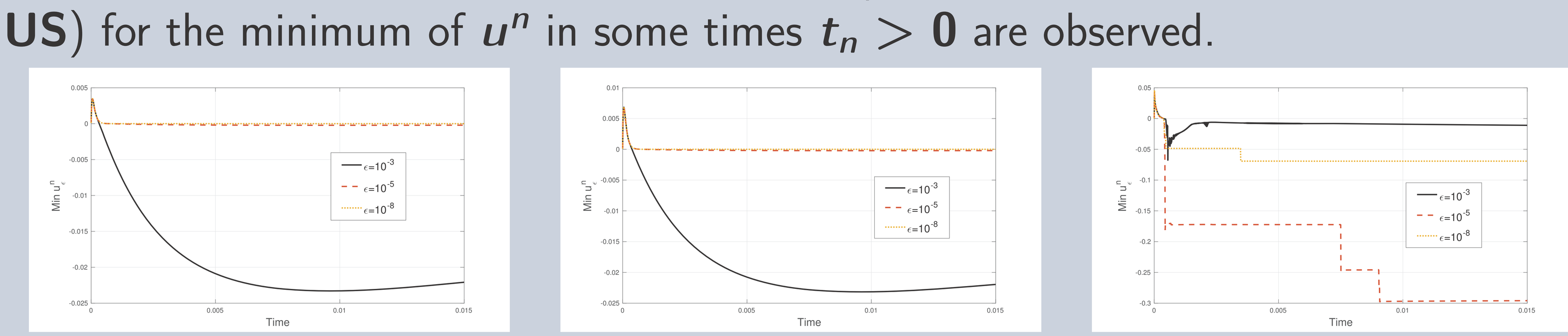

Figure: Minimum values of u_ε^n computed with **UV**, **US** and **UZSW** respectively.

- In all schemes, for the variable v_ε^n is observed that if $v_\varepsilon^0>0$ then $v_\varepsilon^n>0$ for all n.

References

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[2] F. Guillén-González, M.A. Rodríguez-Bellido, D.A. Rueda-Gómez. *Unconditionally energy stable fully discrete schemes for a chemo-repulsion model.* (Preprint).

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