On the stabilization method for chemotaxis system

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Contents

$$\mathscr{L}u := -\varepsilon\Delta u + \mathbf{b}.\nabla u + cu = f \qquad \text{in} \qquad \Omega, \tag{1}$$
$$u = u_b \qquad \text{on} \qquad \partial\Omega,$$

- $\Omega \subset \mathbb{R}^d$, $d = 2, 3, ...,$
- $\varepsilon > 0$, constant,
- $\mathbf{b} \in W^{1,\infty}(\Omega)^d$,
- $c \in L^\infty(\Omega)$,
- $f \in L^2(\Omega)$,
- $u_b \in H^{1/2}(\partial\Omega)$,
- $c - \frac{1}{2} div\mathbf{b} \geqslant 0$

Convection-dominate

If $\varepsilon \ll |\mathbf{b}|$ convection dominates the diffusion and causes narrow layer or spurious oscillation

There are two ways:

- Mesh adaptation on layers
- Coarse mesh+modifications of a standard discretization
  - * special discretization of the convective term (Upwinding method)
  - * introduction of additional terms (stabilization)[1]

Weak formulation: Find $u \in H^1(\Omega)$ such that $u = u_b$ on $\partial\Omega$:

$$\begin{aligned} a(u,v) &= (f,v) \qquad \forall\, v \in H_0^1(\Omega), \\ a(u,v) &= \varepsilon(\nabla u, \nabla v) + (\mathbf{b}\cdot\nabla u, v) + (c\,u, v), \end{aligned} \tag{2}$$

Galekin FEM: Find $u_h \in W_h \subset H^1(\Omega)$ such that $u_h = u_{bh} \in W_h$ on $\partial\Omega$ and

$$a(u_h, v_h) = (f, v_h) \qquad \forall\, v_h \in V_h = W_h \cap H_0^1(\Omega).$$

Stabilized FEM: Find $u_h \in W_h$ such that $u_h = u_{bh}$ on $\partial\Omega$ and

$$a(u_h, v_h) + \sum_{K \in \mathcal{T}_h} \tau_K\, s_K(u_h, v_h) = (f, v_h) \qquad \forall\, v_h \in V_h,$$

[1] Brooks, Hughes (1982); Hughes, Franca, Hulbert (1989); Franca, Frey, Hughes (1992); Franca, do Carmo (1989); Becker, Braack(2004); Burman, Hansbo (2004); Burman, Ern, CMAME (2002); Burman, Ern (2005); Volker, Knobloch, CMAME (2007).

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* manipulations at algebraic level (AFC schemes)[2]
  Aim: manipulate the algebraic system in such a way that the solution satisfies DMP and layers are not smeared.

[2] Kuzmin et al. (2001–now); Barrenechea, Volker, Knobloch, IMAJNA (2015); Barrenechea, Volker, Knobloch, SINUM (2016); Barrenechea, Volker, Knobloch, M3AS (2017).

Cross-diffusion cancer invasion model: [1,2,3]

$$\frac{\partial u}{\partial t} = \mu u(1-u) - \chi \nabla \cdot (u \nabla c), \quad x \in \Omega \times [0,l],$$
$$\frac{\partial c}{\partial t} = -pc, \quad x \in \Omega \times [0,l],$$
$$\frac{\partial p}{\partial t} = \varepsilon^{-1}(uc - p), \quad x \in \Omega \times [0,l],$$
$$\frac{\partial u}{\partial n} = 0, \quad x \in \partial\Omega \times [0,l],$$

$u = u(x,t)$: the concentration of invasive cells
$c = c(x,t)$: the concentration of healthy tissue
$p = p(x,t)$: protease

[1] Fuest, H, Knobloch, Lankeit, and Wick: Global existence of classical solutions and numerical simulations of a cancer invasion model. Preprint, arXiv:2205.08168, 2022.

[2] H, Knobloch, and Wick: On the AFC stabilization of an evolutionary cross-diffusion cancer invasion model(In Progress, 2022.)

[3] Fuest, H: A cross-diffusion system modelling rivaling gangs: global existence of bounded solutions and numerical evidence for total separation (In progress, 2022.)

$$\left(M+\theta\Delta t A^{n+1,c}\right)\mathbf{c}_k^{n+1} = (M-(1-\theta)\Delta t A^{n,c})\,\mathbf{c}^n, \tag{3}$$

$$\begin{aligned}\left((1+\varepsilon^{-1}\theta\Delta t)M\right)\mathbf{p}_k^{n+1} &= \left((1-\varepsilon^{-1}(1-\theta)\Delta t)M\right)\mathbf{p}^n \\ &\quad +\varepsilon^{-1}\Delta t\left(\theta F^{n+1,p}+(1-\theta)F^{n,p}\right),\end{aligned} \tag{4}$$

$$\left(M+\theta\Delta t A^{n+1,u}\right)\mathbf{u}_k^{n+1} = (M-(1-\theta)\Delta t A^{n,u})\,\mathbf{u}^n \tag{5}$$

$\mathbf{c}_k^{n+1} = \left(c_{j,k}^{n+1}\right)^T_{j=1,\dots,M}$, $\mathbf{p}_k^{n+1} = \left(p_{j,k}^{n+1}\right)^T_{j=1,\dots,M}$ and $\mathbf{u}_k^{n+1} = \left(u_{j,k}^{n+1}\right)^T_{j=1,\dots,M}$ denote the vector of unknowns at time t^{n+1} and iteration $k, k = 1, 2, \dots,$

$$M_{ij} = \int_{\mathcal{T}_h} \phi_i(x)\phi_j(x)dx,$$

$$A^{n+1,c} = \int_{\mathcal{T}_h} \phi_i(x)\phi_j(x)p_{h,k-1}^{n+1}dx,$$

$$A^{n,c} = \int_{\mathcal{T}_h} \phi_i(x)\phi_j(x)p_h^n dx,$$

$$F^{n+1,p} = \int_{\mathcal{T}_h} \phi_i(x)u_{h,k-1}^{n+1}c_{h,k}^{n+1}dx,$$

$$F^{n,p} = \int_{\mathcal{T}_h} \phi_i(x)u_h^n c_h^n dx,$$

$$A^{n+1,u} = -\mu \int_{\mathcal{T}_h} \phi_i(x)\phi_j(x)(1-u_{h,k-1}^{n+1})dx - \chi \int_{\mathcal{T}_h} \phi_i(x)\nabla c_{h,k}^{n+1}\cdot\nabla\phi_j(x)dx,$$

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$M_L = (m_{ij}^L)_{j=1,\dots,M}^{i=1,\dots,M}$ with entries $m_{ij}^L = 0, \quad \forall\, i \neq j$ and $m_{ii}^L = \sum_{i=1}^{M} m_{ij}^c$,

$D^{n+1,u} = (d_{ij}^{n+1,u})_{j=1,\dots,M}^{i=1,\dots,M}$ possesing the entries

$$d_{ij}^{n+1,u} = -\max\{a_{ij}^{n+1,u}, 0, a_{ji}^{n+1,u}\}\ \forall\, i \neq j,$$

$$d_{ii}^{n+1,u} = -\sum_{i \neq j} d_{ij}^{n+1,u}.$$

Then the equation for u can be rewritten as follow:

$$\left[M_L + \theta \Delta t \tilde{A}^{n+1,u}\right] \mathbf{u}_k^{n+1} = \left[M_L - (1-\theta)\Delta t \tilde{A}^{n,u}\right] \mathbf{u}^n. \qquad (6)$$

$\tilde{A}^{n+1,u} = A^{n+1,u} + D^{n+1,u}$ and $\tilde{A}^{n,u} = A^{n,u} + D^{n,u}$.

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$D^{n+1,u} = (d^{n+1,u}_{ij})^{i=1,\dots,M}_{j=1,\dots,M}$ possesing the entries

$$d^{n+1,u}_{ij} = -\max\{a^{n+1,u}_{ij}, 0, a^{n+1,u}_{ji}\} \;\forall\, i \neq j,$$
$$d^{n+1,u}_{ii} = -\sum_{i \neq j} d^{n+1,u}_{ij}.$$

Then the equation for u can be rewritten as follow:

$$\left[M_L + \theta \Delta t \tilde{A}^{n+1,u}\right] \mathbf{u}^{n+1}_k = \left[M_L - (1-\theta)\Delta t \tilde{A}^{n,u}\right] \mathbf{u}^n. \qquad (6)$$

$\tilde{A}^{n+1,u} = A^{n+1,u} + D^{n+1,u}$ and $\tilde{A}^{n,u} = A^{n,u} + D^{n,u}$.

Positivity-preservation of low-order scheme (6)[3]:
Let us set $\theta = 1$ and choose Δt such that

$$M_L \mathbb{I}_M + \Delta t \tilde{A}^{n+1,u} \mathbb{I}_M \geqslant 0, \qquad m_i - \Delta t \tilde{A}^{n,u} \geqslant 0, \quad i = 1, ..., M.$$

Since $\tilde{A}^{n+1,u}$ and $\tilde{A}^{n,u}$ are of non-negative type, then the matrix $B = M_L + \Delta t \tilde{A}^{n+1,u}$ is strictly diagonally dominant and hence it is non-singular, which implies that B is an M-matrix. Thus $B^{-1} \geqslant 0$. On the other hand $K = M_L - \Delta t \tilde{A}^{n,u} \geqslant 0$. This immediately implies that the method is positivity-preserving, i.e,

$$\mathbf{u}^n \geqslant 0 \Rightarrow \mathbf{u}^{n+1} \geqslant 0.$$

[3] Barrenechea, Volker , Knobloch :Finite element methods respecting the discrete maximum principle for convection-diffusion equations, arXiv preprint arXiv:2204.07480, 2022.

by subtracting (6) and (5):

$$f_{ij}^{u} = m_{ij}(u_i^{n+1} - u_j^{n+1}) - m_{ij}(u_i^{n} - u_j^{n})$$

$$- \theta \Delta t d_{ij}^{n+1,u}(u_i^{n+1} - u_j^{n+1}) - (1-\theta)\Delta t d_{ij,u}^{n}(u_i^{n} - u_j^{n}) = -f_{ji}^{u},$$

$$F^{u} = \sum_{i \neq j} \bar{f}_{ij}^{u}$$

where

$$\bar{f}_{ij}^{u} = \alpha_{ij}^{u} f_{ij}^{u}$$

Compute the $\tilde{u}$ from (6) and determine the flux limiter α_{ij}^u as [4]:

$$P_i^+ = \sum_{i \neq j} \max\{0, f_{ij}^u\}, \quad P_i^- = \sum_{i \neq j} \min\{0, f_{ij}^u\},$$

$$Q_i^+ = \max\{0, \max_{j \in S(i)} (\tilde{u}_j - \tilde{u}_i)\}, \quad Q_i^- = \min\{0, \min_{j \in S(i)} (\tilde{u}_j - \tilde{u}_i)\},$$

$$R_i^+ = \min\left\{1, \frac{m_i Q_i^+}{P_i^+}\right\}, \quad R_i^- = \min\left\{1, \frac{m_i Q_i^-}{P_i^-}\right\}$$

$$\alpha_{ij}^u = \begin{cases} \min\{R_i^+, R_j^-\}, & \text{if } f_{ij}^u > 0 \\ \min\{R_i^-, R_j^+\}, & \text{otherwise} \end{cases}, \quad \alpha_{ij}^u \in [0,1], \; \alpha_{ij}^u = \alpha_{ji}^u$$

$$\bar{f}_{ij}^u = \alpha_{ij}^u f_{ij}^u,$$

Then the high-order schme of (6) reads:

$$\left[M_L + \theta \Delta t \tilde{A}^{n+1,u}\right] \mathbf{u}_k^{n+1} = \left[M_L - (1-\theta)\Delta t \tilde{A}^{n,u}\right] \mathbf{u}^n + F^u. \qquad (7)$$

[4] S. T. Zalesak. Fully multidimensional flux-corrected transport algorithms for fluids. Journal of computational physics, 31(3):335â362, 1979.

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$$\alpha_{ij}^u = \begin{cases} \min\{R_i^+, R_j^-\}, & \text{if } f_{ij}^u > 0 \\ \min\{R_i^-, R_j^+\}, & \text{otherwise} \end{cases}, \;\; \alpha_{ij}^u \in [0,1], \; \alpha_{ij}^u = \alpha_{ji}^u$$
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$$M_L \bar{u}^{n+1} = M_L \tilde{u}^{n+1} + F^u, \tag{9}$$

$$\left[M_L + \theta \Delta t \tilde{A}^{n+1,u} \right] \mathbf{u}_k^{n+1} = M_L \bar{u}, \tag{10}$$

positivity-preservation of high-order scheme (7):

* let $u^n \geqslant 0$ and $\Delta t < \frac{m_i}{(1-\theta)l_{ii}}$, M_L is diagonal matrix with positive diagonal entries, then $\tilde{u} \geqslant 0$,
* the limiter are determined in such a way that $\bar{u} \geqslant 0$,
* $M_L \geqslant 0$ and $\tilde{A}^{n+1,u}$ is of nonnegative type, then the matrix $B = \left[M_L + \theta \Delta t \tilde{A}^{n+1,u} \right]$ is strictly diagonally dominant and non-singular, so it is a M-matix, therefore $u^{n+1} \geqslant 0$.

DMP:
If we simplify (6) as

$$Bu^{n+1} = Ku^n,$$

where $B, K \in \mathbb{R}^{M\times M}$ and $u^{n+1}, u^n \in \mathbb{R}^M$. Assuming that

$$B^{-1} \geqslant 0, \qquad K \geqslant 0 \qquad , B\mathbb{I}_M \geqslant K\mathbb{I}_M,$$

one obtains with $N_1 = (\max u^n)^+, N_2 = (\min u^n)^-$

$$u^{n+1} = B^{-1}Ku^n \leqslant N_1 B^{-1} K\mathbb{I}_M \leqslant N_1 B^{-1} B\mathbb{I}_M = N_1 \mathbb{I}_M,$$

$$u^{n+1} = B^{-1}Ku^n \geqslant N_2 B^{-1} K\mathbb{I}_M \geqslant N_2 B^{-1} B\mathbb{I}_M = N_2 \mathbb{I}_M,$$

i.e.,

$$(\min u^n)^- \leqslant u_i^{n+1} \leqslant (\max u^n)^+.$$

Algorithm

Step 1 : initialize at time $t = 0$ with $\mathbf{c}^0 = c(x,0), \mathbf{p}^0 = p(x,0)$ and $\mathbf{u}^0 = u(x,0)$,

Step 2 : for $n \geq 1$ (time step number index)
first set $\mathbf{c}_0^{n+1} = \mathbf{c}^n, \mathbf{p}_0^{n+1} = \mathbf{p}^n$ and $\mathbf{u}_0^{n+1} = \mathbf{u}^n$,
for $k \geq 1$ (fixed-point iteration index)

(a) determine $\mathbf{c}_k^{n+1}$ using (3),

(b) determine $\mathbf{p}_k^{n+1}$ using (4),

(c) (1.) compute $\tilde{\mathbf{u}}_k^{n+1}$

$$\left[M_L + \theta \Delta t \tilde{A}^{n+1,u}\right] \tilde{\mathbf{u}}_k^{n+1} = \left[M_L - (1-\theta)\Delta t \tilde{A}^{n,u}\right] \mathbf{u}^n.$$

(2.) compute α_{ij}^u using $\tilde{\mathbf{u}}_k^{n+1}$,

(3.) set $\mathbf{u}_k^{n+1} = \tilde{\mathbf{u}}_k^{n+1}$ or $\mathbf{u}_k^{n+1} = \mathbf{u}_{k-1}^{n+1}$ to compute F^u explicitly or implicitly, respectively.

(4.) determine $\mathbf{u}_k^{n+1}$ from

$$\left[M_L + \theta \Delta t \tilde{A}^{n+1,u}\right] \mathbf{u}_k^{n+1} = \left[M_L - (1-\theta)\Delta t \tilde{A}^{n,u}\right] \mathbf{u}^n + F^u.$$

Step3 : if $\left\{\|\mathbf{c}_k^{n+1}-\mathbf{c}_{k-1}^{n+1}\|_{l^2}, \|\mathbf{p}_k^{n+1}-\mathbf{p}_{k-1}^{n+1}\|_{l^2}, \|\mathbf{u}_k^{n+1}-\mathbf{u}_{k-1}^{n+1}\|_{l^2}\right\} < Tol = 10^{-8}$ stop and set

$$\mathbf{u}^{n+1}=\mathbf{u}_k^{n+1}, \mathbf{c}^{n+1}=\mathbf{c}_k^{n+1}, \mathbf{p}^{n+1}=\mathbf{p}_k^{n+1},$$

and go back to step 2 (proceed to next time point).

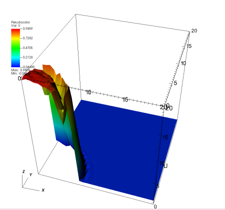
Step 4 : else set

$$\mathbf{c}_{h,k}^{n+1}=\beta\mathbf{c}_{h,k}^{n+1}+(1-\beta)\mathbf{c}_{h,k-1}^{n+1},$$

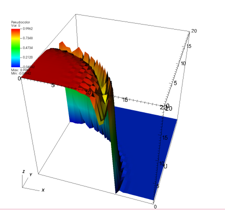
$$\mathbf{p}_{h,k}^{n+1}=\beta\mathbf{p}_{h,k}^{n+1}+(1-\beta)\mathbf{p}_{h,k-1}^{n+1},$$

$$\mathbf{u}_{h,k}^{n+1}=\beta\mathbf{u}_{h,k}^{n+1}+(1-\beta)\mathbf{u}_{h,k-1}^{n+1},$$

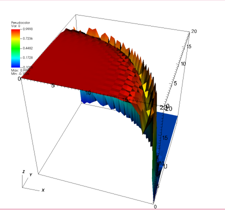
for some $\beta \in [0,1]$ and go to (a) and increment $k \mapsto k+1$ (next fixed-point iteration), here we set $\beta = 0.5$.



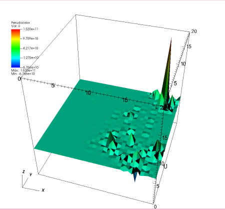
(a) t = 10



(b) t=20

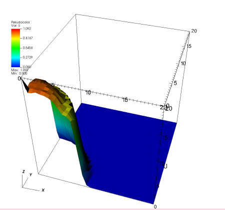


(c) t=30



(d) t=40

Figure: Cancer density, Galerkin method, $\mu = 1$ and $\chi = 1$ Crank-Nicolson method $\theta = 0.5$ with $\Delta t = 1$, 20×20 mesh, Q_1.



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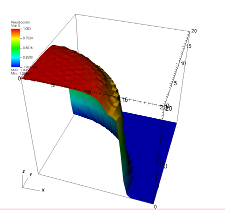
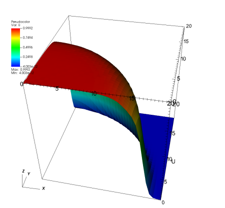
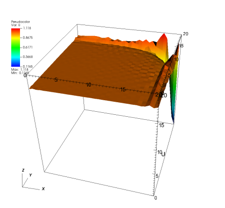


(b) t=20



(c) t=30



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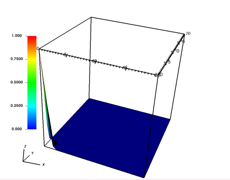
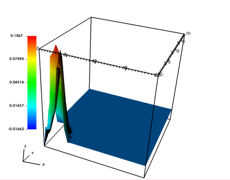
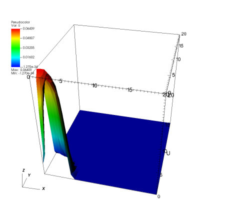


(a) t = 0

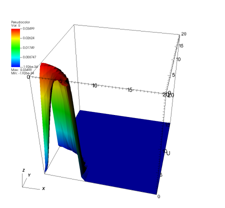


(b) t=5

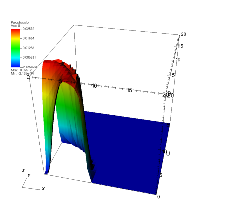
Figure: Cancer density, Galerkin method, $\mu = 0.001$ and $\chi = 1$ Crank-Nicolson method $\theta = 0.5$ with $\Delta t = 1$, 20×20 mesh, Q_1.



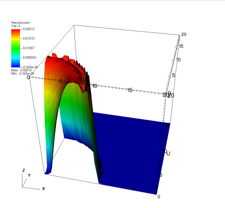
(a) t = 10



(b) t=20



(c) t=30

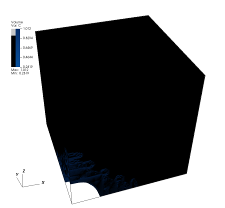


(d) t=40

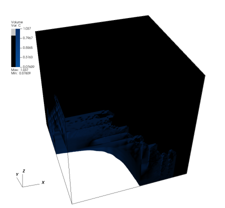
Figure: Cancer density, AFC method, $\mu = 0.001$ and $\chi = 1$ Crank-Nicolson method $\theta = 0.5$ with $\Delta t = 1$, 20×20 mesh, Q_1.

Table: The convergece of AFC scheme, $\mu = 1$ and $\chi = 1$
Crank-Nicolson method $\theta = 0.5$

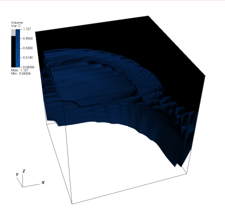
Δt	$\mathbf{u}_k^{n+1}$	$\mathbf{c}_k^{n+1}$	$\mathbf{p}_k^{n+1}$
0.5	0.9588	0.0998	0.0956
0.25	0.9636	0.0986	0.0957
0.125	0.9695	0.0984	0.0967
0.0625	0.9725	0.0976	0.0964
0.0313	0.9741	0.0967	0.0958



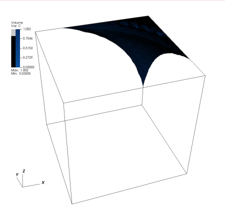
(a) t = 5



(b) t=15

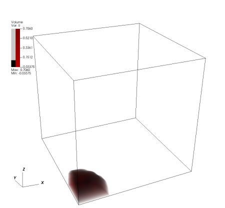


(c) t=25

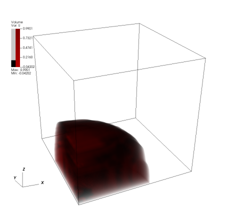


(d) t=35

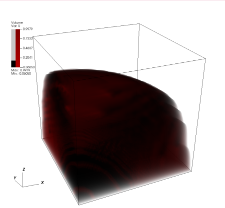
Figure: Healthy tissue density, AFC method, $\mu = 1$ and $\chi = 1$ Crank-Nicolson method $\theta = 0.5$ with $\Delta t = 1$, Q_1.



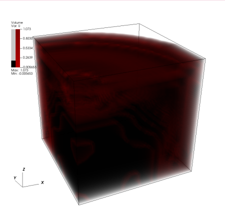
(a) t = 5



(b) t=15



(c) t=25



(d) t=35

Figure: Cancer cell density, AFC method, $\mu = 1$ and $\chi = 1$ Crank-Nicolson method $\theta = 0.5$ with $\Delta t = 1$, Q_1.

Outlook

- Existence of solutions of a FE-FCT scheme for chemotaxis system [5,6]
- Derive a posteriori error estimation
- Apply AFC method on fluid-structure interaction (FSI) problem
- Space-time method + AFC on FSI

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[e] Existence of solutions of a finite element flux-corrected-transport scheme, Volker ,Knobloch, 2021.

[f] On the solvability of the nonlinear problems in an algebraically stabilized finite element method for evolutionary transport-dominated equations, V. John, P. Knobloch, P. Korsmeier, 2020.


Thank You
For Your
Attention