WESTFÄLISCHE WILHELMS-UNIVERSITÄT MÜNSTER

Biological Transportation Networks PDE Modeling and Numerics

joint work with Martin Burger (WWU Münster), Jan Haskovec (KAUST), Peter Markowich (KAUST/Cambridge), Benoît Perthame (LLJL,UPMC)

Data-Rich Phenomena - Modelling, Analysing and Simulations using PDEs
Cambridge

living.knowledge
WWU Münster

Matthias Schlottbom

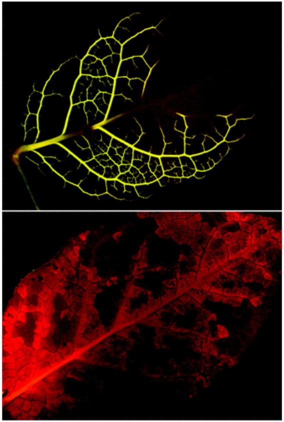
16th Dec 2016

Outline

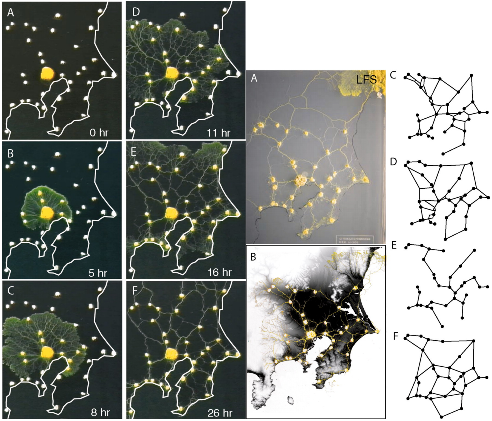
Modeling

Analysis

Numerics



Leaf venation



Slime mold growth and railway networks

E. Katifori et al: Damage and Fluctuations Induce Loops in Optimal Transport Networks, Phys Rev Letters 104: 048704 (2010). (left Fig.)

A. Tero et al: Rules for Biologically Inspired Adaptive Network Design, Science 327: 439–442 (2010). (right Fig.)

Modeling

Analysis

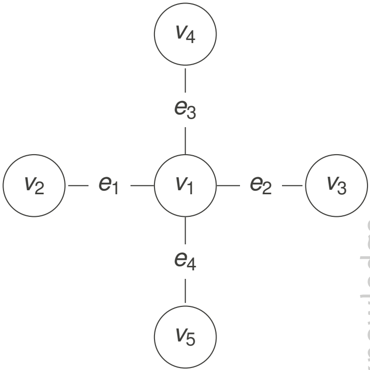
Numerics

Microscopic flow model

- Given network with nodes $v_j \in \mathbb{V}$ and edges $e_i \in \mathbb{E}$.
- $\mathbb{E}$ models vessels/veins.
- In edge $e_i = (j, k)$ between v_j and v_k, we have a flow

$$Q_i = C_i \Delta P_i = C_i \big(P_j - P_k\big)$$

- $C_i > 0$ vessel conductivity at edge e_i.
- P_j pressure at node v_j.
- ΔP_i pressure drop at edge e_i.



A. Tero et al: Rules for Biologically Inspired Adaptive Network Design, Science 327: 439–442 (2010).

D. Hu, D. Cai: Adaptation and Optimization of Biological Transport Networks, Phys Rev Letters 111: 138701 (2013).

Example: Hagen-Poiseuille flow (laminar flow)

- Small vessels (diameter $D_i < 0.6\text{mm}$)[1]

$$Q_i = \frac{\pi D_i^4}{128\eta} \frac{\Delta P_i}{L_i}$$

η is the blood viscosity, L_i length of vessel e_i.

- Leaf venation[2]: Leaf vein consists of a bundle of small tubes with similar diameter. Thus

$$C_i = nC_0 = \frac{\pi D_0^2 D_i^2}{128\eta L_i}.$$

n is the number of tubes C_0 and D_0 are the conductance and diameter of a single tube.

[1] A.R. Pries, T.W. Secomb, P. Gaehtgens: Structural adaptation and stability of microvascular networks: theory and simulations. Am J Physiol Heart Circ Physiol 275: H349–H360 (1998).

[2] D. Hu, D. Cai: Adaptation and Optimization of Biological Transport Networks, Phys Rev Letters 111: 138701 (2013).

Microscopic flow distribution

- Kirchhoff law:

Sum of incoming fluxes = Sum of outgoing fluxes.

- At node v_j we have

$$\sum_{v_k : e_i = (j,k) \in \mathbb{E}} Q_i = s_j .$$

- s_j allows modeling of sources and sinks for the flow.

Towards a macroscopic flow model

- C_i are scalars. What about the orientation of the vein?
- Main flow is in direction v_i of the vein e_i, $(|v_i| = 1)$

$$Q_i \cdot v_i = L_i C_i \frac{\Delta P_i}{L_i}.$$

- No flow perpendicular to v_i

$$Q_i \cdot v_i^{\perp} = 0.$$

- Setting $m = \sqrt{L_i C_i} v_i$, we obtain on the macroscopic level

$$Q(x) = \big(r(x)I + m(x) \otimes m(x)\big)\nabla p(x).$$

- $r(x)$ models background permeability.[3] [4]

[3] G. Albi, M. Artina, M. Fornasier, P. Markowich: Biological transportation networks: modeling and simulation (2015).

[4] S. Whitaker: Flow in Porous Media I: A Theoretical Derivation of Darcy's Law, Transport in Porous Media 1:3–25 (1986).

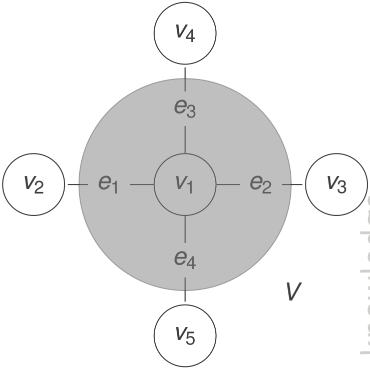
Towards a macroscopic pressure model

- Kirchhoff's law $\sum_{v_k : e_i = (j,k) \in \mathbb{E}} Q_i = s_j$.
- Continuous interpretation

$$\int_{\partial V} n \cdot Q d\partial V = - \int_V S dx .$$

- Using $Q = (rI + m \otimes m)\nabla p$, we obtain

$$-\mathrm{div}((rI + m \otimes m)\nabla p) = S \quad + \text{B.C.}$$



Network adaptation process

- The network will minimize its "costs"[5]:

$$E = \text{pumping power } + \text{maintaining costs.}$$

- Joule's law:

$$\text{power } = \text{potential } \cdot \text{ current} = \nabla p \cdot Q = r|\nabla p|^2 + |m \cdot \nabla p|^2.$$

- Maintaining costs $|m|^{2\gamma}$.
  - $\gamma = 1/2$ for blood vessel systems.
  - $1/2 \leq \gamma \leq 1$ for leaf venation.

[5] D. Hu, D. Cai: Adaptation and Optimization of Biological Transport Networks, Phys Rev Letters 111: 138701 (2013).

Continuous adaptation model

- Adaptation energy

$$\min_m E_a(m) = \frac{1}{2}\int_\Omega c^2\left(r|\nabla p(m)|^2 + |m\cdot\nabla p(m)|^2\right) + \frac{|m|^{2\gamma}}{\gamma}\,dx,$$

where $p = p(m)$ solves

$$-\mathrm{div}((rI + m\otimes m)\nabla p) = S \quad + \text{ B.C.}$$

- Adaptation and formation energy

$$E(m) = \frac{1}{2}\int_\Omega D^2|\nabla m|^2 + c^2 r|\nabla p(m)|^2 + c^2|m\cdot\nabla p(m)|^2 + \frac{|m|^{2\gamma}}{\gamma}\,dx.$$

Minimization via evolution

Consider the L^2-gradient flow

$$m_t = -\nabla E(m)$$

This leads to the system ($\gamma > 1/2$)

$$\begin{aligned} -\mathrm{div}((rI + m \otimes m)\nabla p) &= S \quad \text{in } \Omega \times (0,T) + \text{ B.C.}, \\ m_t - D^2 \Delta m &= c^2 \nabla p \otimes \nabla p m - |m|^{2(\gamma-1)} m, \quad \text{in } \Omega \times (0,T), \\ m &= 0 \quad \text{on } \partial\Omega \times (0,T), \\ m(t=0) &= m^0 \quad \text{in } \Omega. \end{aligned}$$

For $\gamma = 1/2$,

$$m_t - D^2 \Delta m - c^2 \nabla p \otimes \nabla p m \in \partial \mathcal{R}(m), \quad \text{in } \Omega \times (0,T),$$

where $\partial R(m)$ is the subdifferential of $\|m\|_{L^1(\Omega)}$.

Modeling

Analysis

Numerics

Analytical results

Let $\gamma \geq 1/2$, $S \in L^2(\Omega)$ and $m^0 \in H_0^1(\Omega)^d \cap L^{2\gamma}(\Omega)^d$. Then there exists a global weak solution $(m, p[m])$ with $E(m) \in L^\infty(0,\infty)$ and with

$$\begin{aligned} m &\in L^\infty(0,\infty; H_0^1(\Omega)) \cap L^\infty(0,\infty; L^{2\gamma}(\Omega)), \\ \partial_t m &\in L^2((0,\infty)\times\Omega), \\ \nabla p &\in L^\infty(0,\infty; L^2(\Omega)), \\ m\cdot\nabla p &\in L^\infty(0,\infty; L^2(\Omega)). \end{aligned}$$

Moreover,

$$E(m(t)) + \int_0^t \int_\Omega |\partial_t m(s,x)|^2 dxds \leq E(m^0) \qquad \text{for all } t \geq 0.$$

J. Haskovec, P. Markowich, B. Perthame: Math. Anal. of a PDE System for Biol. Netw. Formation, Comm. PDEs 40:5, 918–956 (2015).

J. Haskovec, P. Markowich, B. Perthame, M. Schlottbom: Notes on a PDE System for Biological Network Formation (2015).

Analytical results 2

- The energy is non-convex in general.[6]
- Many stationary states.
- For $\gamma < 1/2$ the solutions of the evolution equation will approach zero in finite time[7], i.e. finite-time breakdown.

[6] G. Albi, M. Artina, M. Fornasier, P. Markowich: Biological transportation networks: modeling and simulation (2015).

[7] J. Haskovec, P. Markowich, B. Perthame, M. Schlottbom: Notes on a PDE System for Biological Network Formation (2015).

Modeling

Analysis

Numerics

Mixed formulation

Setting $\sigma = \nabla m$, we consider

$$
\begin{aligned}
-\mathrm{div}((rI + m \otimes m)\nabla p) &= S \quad \text{in } \Omega \times (0,T),\\
p &= 0 \quad \text{on } \Gamma \times (0,T),\\
n \cdot (rI + m \otimes m)\nabla p &= 0 \quad \text{on } \partial\Omega \setminus \Gamma \times (0,T),\\
\partial_t m - D^2 \mathrm{div}\sigma &= c^2(\nabla p \otimes \nabla p)m - |m|^{2(\gamma-1)} m \quad \text{in } \Omega \times (0,T),\\
\sigma - \nabla m &= 0 \quad \text{in } \Omega \times (0,T),\\
m &= 0 \quad \text{on } \partial\Omega \times (0,T),
\end{aligned}
$$

with $m(t=0) = m^0$ in Ω.

Weak mixed formulation

Find

$(p, m, \sigma) \in L^\infty(0, T; H^1_{0,\Gamma}(\Omega)) \times L^2(0, T; L^2(\Omega)^2) \times L^2(0, T; H(\mathrm{div})^2)$

s.t.

$$\int_\Omega (rI + m \otimes m)\nabla p \cdot \nabla q \, dx = \int_\Omega Sq \, dx,$$

$$\int_\Omega \partial_t m \cdot v \, dx - \int_\Omega D^2 \mathrm{div}\sigma \cdot v \, dx = \int_\Omega f_{\gamma,c}(m, \nabla p) \cdot v \, dx,$$

$$\int_\Omega \sigma \cdot \mu \, dx + \int_\Omega m \cdot \mathrm{div}\mu \, dx = 0,$$

for all $(q, v, \mu) \in H^1_{0,\Gamma}(\Omega) \times L^2(\Omega)^2 \times H(\mathrm{div})^2$, $m(t = 0) = m^0$ in Ω,

$$f_{\gamma,c}(m, \nabla p) = c^2(\nabla p \otimes \nabla p)m - |m|_\rho^{2(\gamma-1)} m,$$

where $|m|_\rho = \sqrt{m_1^2 + m_2^2 + \rho}$.

Space discretization – approximation spaces

- Lagrangian finite elements, i.e. continuous, piecewise linear functions

$$p \approx p_h \in P_h = \{q_h \in C^0(\overline{\Omega}) : q_{h|T} \in \mathcal{P}_1(T)\ \forall T \in \mathcal{T}_h, v_{h|\Gamma} = 0\}.$$

- Piecewise constant functions

$$m \approx m_h \in M_h^2 = \{v_h \in L^2(\Omega) : v_{h|T} \in \mathcal{P}_0(T)\ \forall T \in \mathcal{T}_h\}^2.$$

- Raviart-Thomas elements

$$\sigma \approx \sigma_h \in V_h = \{\mu_h \in H(\mathrm{div}) : \mu_{h|T} \in \mathcal{P}_0(T)^2 + x\mathcal{P}_0(T)\ \forall T \in \mathcal{T}_h\}.$$

Galerkin semi-discretization

Find $(p_h, m_h, \sigma_h) \in L^\infty(0,T;P_h) \times L^2(0,T;M_h^2) \times L^2(0,T;V_h^2)$ s.t.

$$\int_\Omega (rI + m_h(t) \otimes m_h(t)) \nabla p_h(t) \cdot \nabla q_h dx = \int_\Omega S q_h dx,$$

$$\int_\Omega \partial_t m_h(t) \cdot v_h - D^2 \mathrm{div} \sigma_h(t) \cdot v_h dx = \int_\Omega f_{\gamma,c}(m_h(t), \nabla p_h(t)) \cdot v_h dx,$$

$$\int_\Omega \sigma_h(t) \cdot \mu_h dx + \int_\Omega m_h(t) \cdot \mathrm{div} \mu_h dx = 0,$$

for all $(q_h, v_h, \mu_h) \in P_h \times M_h^2 \times V_h^2$, and $m_h(t=0) = m_h^0$ in Ω.

Time discretization: IMEX Euler scheme

- Let $0 = t^0 < t^1 < \ldots < t^K = T$ be a partition of $[0, T]$.
- $m_h^k \approx m_h(t^k)$, $p_h^k \approx p_h(t^k)$ and $\sigma_h^k \approx \sigma_h(t^k)$, $0 \leq k \leq K$.
- time-stepping scheme

$$\int_\Omega (rI + m_h^k \otimes m_h^k)\nabla p_h^k \cdot \nabla q_h = \int_\Omega S q_h,$$

$$\int_\Omega (m_h^{k+1} - \delta^{k+1} D^2 \mathrm{div}\sigma_h^{k+1}) \cdot v_h = \int_\Omega \left(m_h^k + \delta^{k+1} f_{\gamma,c}(m_h^k, \nabla p_h^k)\right) \cdot v_h,$$

$$\int_\Omega \sigma_h^{k+1} \cdot \mu_h + \int_\Omega m_h^{k+1} \cdot \mathrm{div}\mu_h = 0,$$

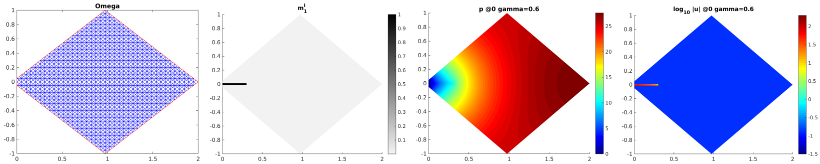
for all $(q_h, v_h, \mu_h) \in P_h \times M_h^2 \times V_h^2$, and $\delta^{k+1} = t^{k+1} - t^k$.

- $u_h^k = (rI + m_h^k \otimes m_h^k)\nabla p_h^k$ is the flow.

Issues for time-stepping schemes

- $-D^2 \Delta m$ is stiff $\rightsquigarrow$ implicit treatment.
- $c^2 \nabla p \otimes \nabla p$ has eigenvalues 0 and $c^2 |\nabla p|^2$.
  - $c^2 |\nabla p|^2 \gg 1 \rightsquigarrow$ implicit treatment ?
  - linearization errors $\rightsquigarrow \delta^k \ll 1$.
- $|m|^{2(\gamma-1)} m$ is non-differentiable for $\gamma < 1$, $\rightsquigarrow$ order of the method?
- Overall guideline: $E(m_h^{k+1}) \leq E(m_h^k)$.

Example

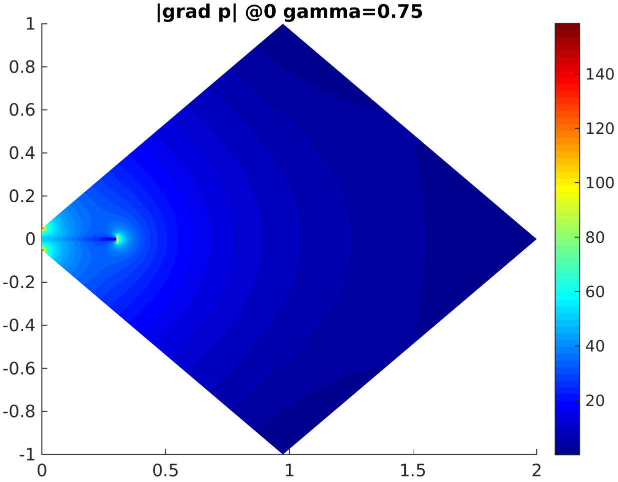


$\mathcal{T}_h$ contains 102, 905 vertices and 204, 544 triangles, i.e. $h \approx 0.0032$. Set

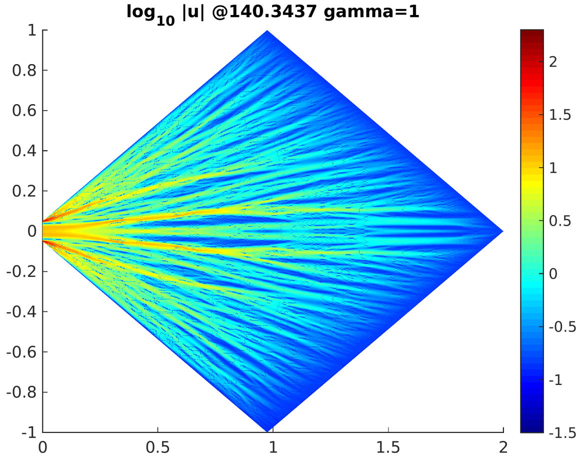
$$S = 1, \quad r = \frac{1}{10}, \quad c = 50, \quad D = \frac{1}{1000}, \quad \rho = 10^{-12},$$

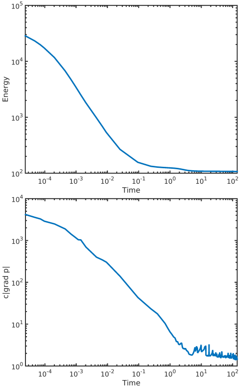
$$m_1^0(x) = \begin{cases} 1, & x \leq 0.3 \text{ and } |y| \leq 0.0125, \\ 0, & \text{else}, \end{cases} \qquad m_2^0 = 0.$$

Initial pressure: max $c|\nabla p| = 7926.36$

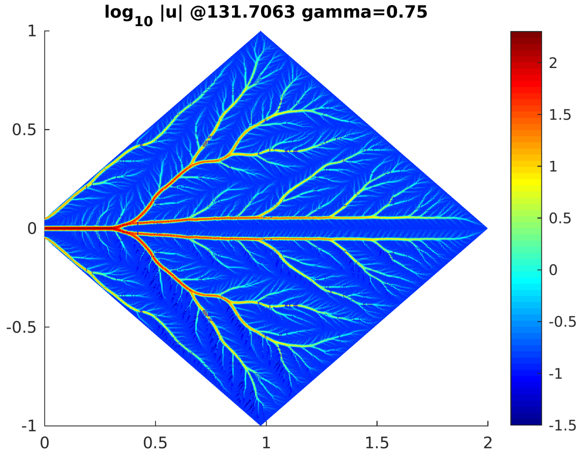


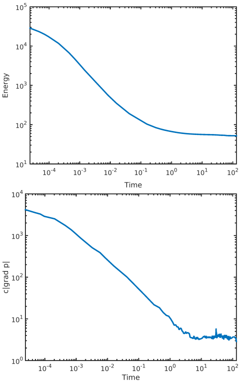
Near stationary state; $\gamma = 1$



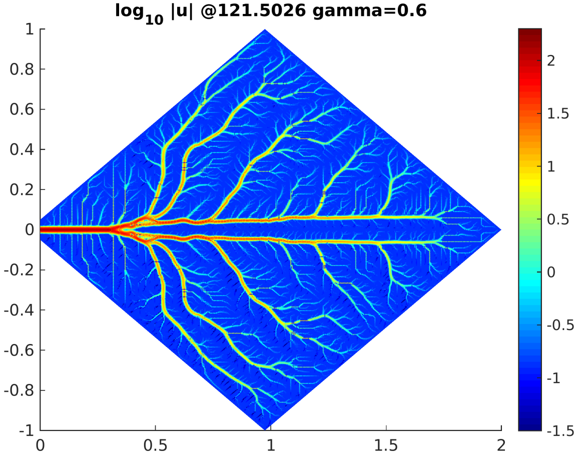


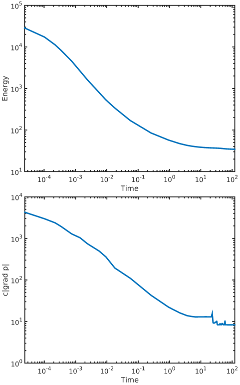
Near stationary state; $\gamma = 3/4$



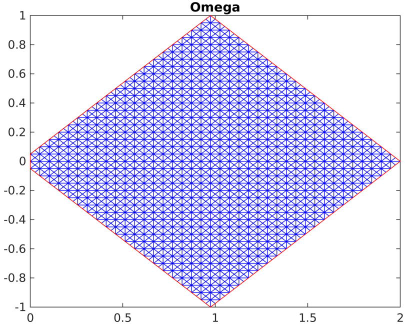


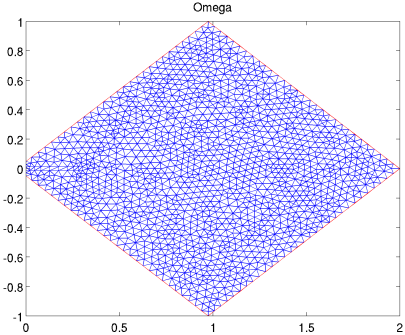
Near stationary state; $\gamma = 3/5$



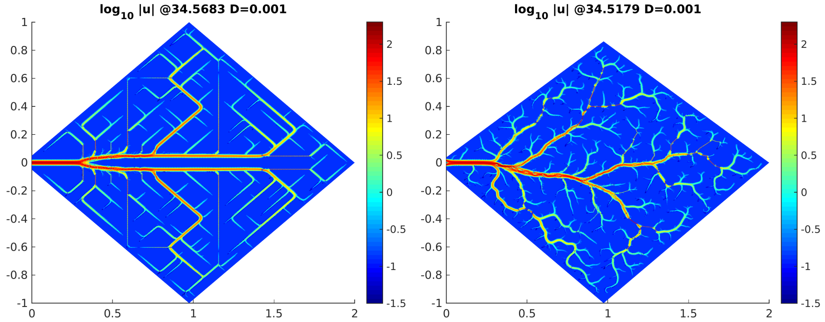


Comparison mesh dependency



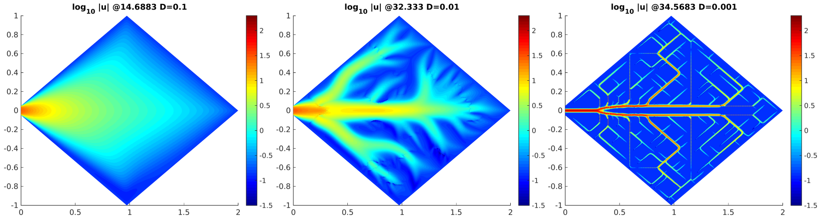


Comparison mesh dependency; $\gamma = 1/2$



$D \ll 1 \rightsquigarrow$ microscopic effects defined by the underlying triangulation.

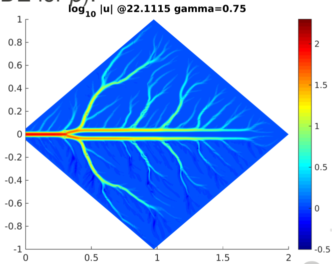
Comparison mesh dependency diffusion



$D = 1/10,$ $D = 1/100,$ $D = 1/1000.$

Other schemes

- higher-order IMEX schemes: [a] [b]
  - treat $f_{\gamma,c}(m, \nabla p)$ explicitly.
  - at each stage evaluate $f_{\gamma,c}(m, \nabla p)$ (solve PDE for p).
- Implicit integrating factor method (IIF): [c]
  - treats Δm exactly (matrix exponential).
  - treats $f_{\gamma,c}(m, \nabla p)$ implicitly.
  - updates require nonlinear solver.
  - fixed-points $\rightsquigarrow$ contraction property.
- Other splittings (future work). Split
  - Δm, $c\nabla p \otimes c\nabla p$: stiff, but differentiable.
  - $|m|^{2\gamma}$: convex optimization ($\gamma = 1/2$: shrinkage).



IIF, $D = 1/400$, $r = 3/4$.

[a] U.M. Ascher, S.J. Ruuth, R.J. Spiteri: Implicit-explicit Runge-Kutta methods for time-dependent PDEs, APNUM 25 (1997): 151–167

[b] T. Koto: IMEX Runge-Kutta schemes for reaction-diffusion equations, J. Comp & Appl Math 215 (2008):182–195

[c] Q. Nie, Y.-T. Zhang, R. Zhao: Efficient semi-implicit schemes for stiff systems, JCP 214 (2006): 521–537

Conclusions

- Derived a model for network adaptation and formation.
- Proposed a numerical method for simulation.
- First numerical results show the potential of the model.
- For small diffusion, it is likely that we solve a microscopic model.

Open/Future work

- More efficient numerical schemes.
- Regularity of the continuous solution.
- Source identification.

Acknowledgement

Financial support from the

European Research Council

Established by the European Commission

through grant

EU FP 7 - ERC Consolidator Grant 615216

Variational Methods for Dynamic Inverse Problems in the Life Sciences

is gratefully acknowledged