Accurate and robust finite element solvers for chemotaxis-dominated partial differential equations

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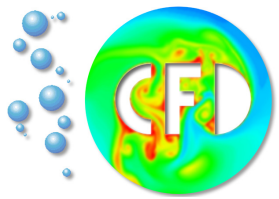
June 20, 2013



Outline

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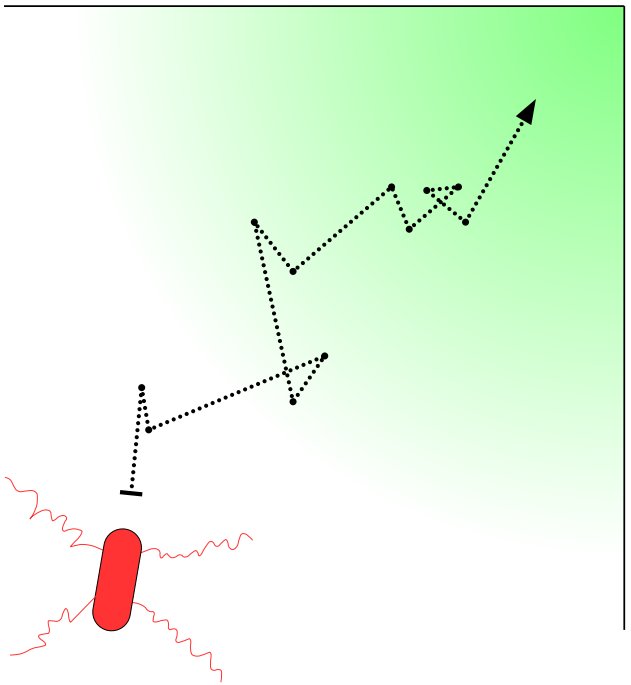
Concept

Chemotaxis describes an oriented movement towards or away from regions of higher concentrations of chemical agents and plays a vitally important role in the evolution of many living organisms.



(a) Slime mold, http://dictybase.org

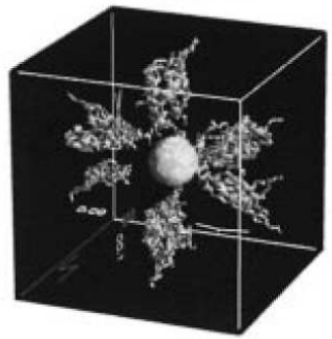
(b) Bacterial chemotaxis

Where to find chemotaxis?

Certainly, applied mathematicians look for practical benefits of their work. Since chemotaxis plays a key-role for many organisms, plenty applications come into mind.

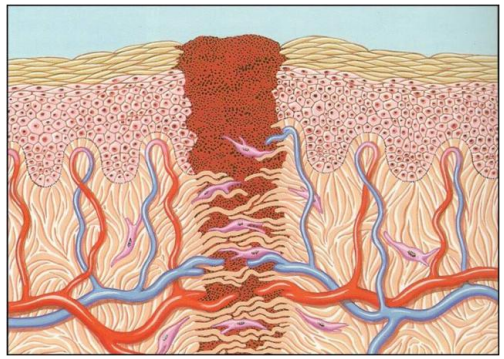
- proliferation of bacteria (not only in petri dishes)
- tumour growth/angiogenesis/haptotaxis
- breeding concerns (insemination of sea urchins)
- immunology/wound healing (production of chemokines at infection sites)

E. Ben-Jacob, http://star.tau.ac.il/∼eshel/image-flow.html



M.A.J. Chaplain, Journal of Neuro-Oncology

C. Pietschmann, MPI



www.surgical-blog.com/wound-healing-what-are-the-phases-of-wound-healing/

Basic model

It is common to use continuous models $\rightarrow$ system of partial differential equations (PDE)

A general Keller-Segel model for chemotaxis:

equation for motile species u:

$$\frac{\partial u}{\partial t} = \nabla \cdot \Big(\underbrace{D \nabla u}_{\text{diffusion}} - \underbrace{u \chi(v) \nabla v}_{\text{chemotaxis}} \Big) + \underbrace{u g(u)}_{\textit{kinetics}}$$

equation for the chemical agent v:

$$\frac{\partial v}{\partial t} = \underbrace{\Delta v}_{\text{diffusion}} - \underbrace{\beta v + u s(u)}_{\text{reaction}}$$

(nonlinear) coefficients modeling saturation effects: e.g. D, $\chi(v)$, $s(u) \overset{u \to \infty}{\to} 0$

introducing kinetics: e.g. $s(u) = \nu(1 - u)$ (logistic)

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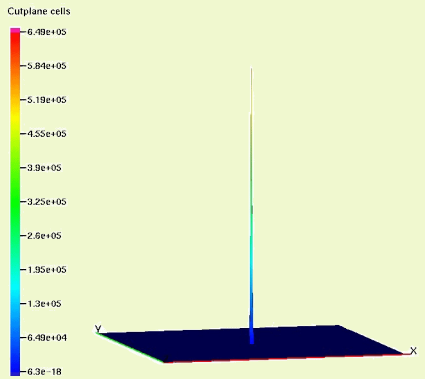
Blow-up

$$\begin{aligned} \partial_t u &= \Delta u - \nabla \cdot (u \chi \nabla v) \\ \partial_t v &= \Delta v - v + u \end{aligned}$$

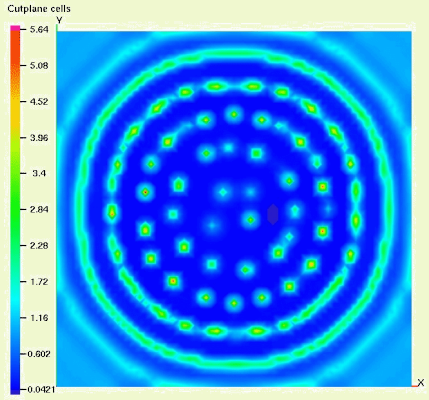


- solution might form singularities
- num. motivated by e.g. [Filbet '06, Chertock & Kurganov '08]
- theor. motivated by e.g. [Horstmann & Winkler '04, Tao & Winkler '11]
- theoretical results
  - $\mathbb{R}^1$: all solutions are bounded
  - $\mathbb{R}^2$: blow-up iff $||u_0||_1 > 8\pi/\chi$
  - $\mathbb{R}^{\geq 3}$: no explicit threshold is known

Features of chemotaxis models

Pattern formation

$$\begin{aligned} \partial_t u &= \Delta u - \nabla \cdot \left(u \chi \nabla v\right) + \nu u(1-u) \\ \partial_t v &= \Delta v - \alpha v + \beta u \end{aligned}$$



- well documented patterns arise (experimental and math.)
- existence of non-trivial steady states
- num. motivated by e.g.
  [Mimura et al. '93, Chertock & Kurganov '08]
- theor. motivated by e.g. [Myerscough et al. '98, Tyson et al. '99]
- theoretical results
  - $\mathbb{R}^{1,2}$: unique global weak solution (at least for $\nu \gg 1$)
  - $\mathbb{R}^{\geq 3}$: far less is known

Numerical challenges

Highly localized solutions with steep gradients reveal particular numerical challenges

- CPU costs
- Memory concerns
- Convenient user interfaces
- Accuracy of discretization
- Robustness with respect to reasonable parameters (e.g. preservation of physical properties)

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"*The purpose of computing is insight, not numbers*"
Hamming, 1971

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Numerical setting

Recapitulate the governing model

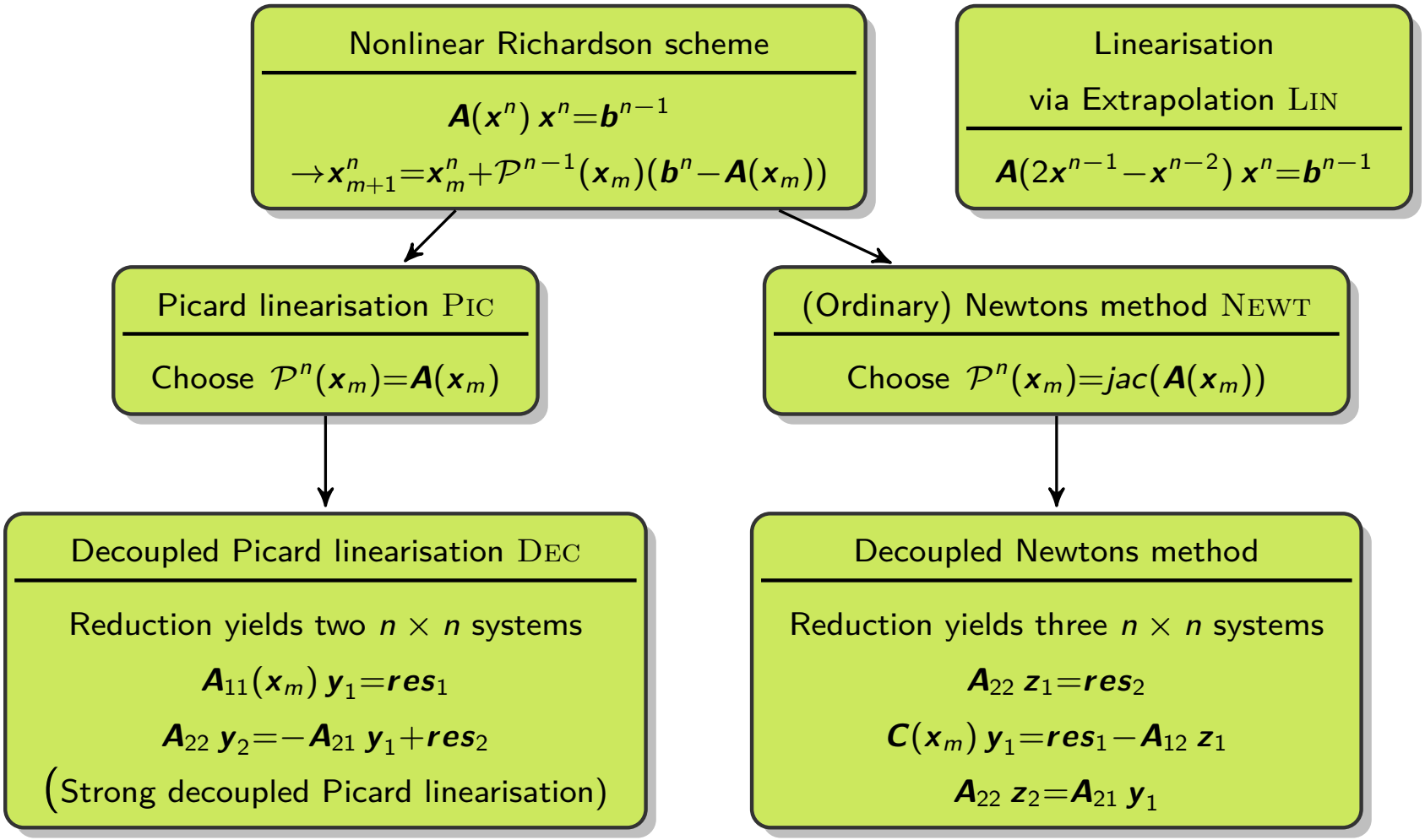
$$\begin{aligned} \partial_t u &= \nabla \cdot \left(D \nabla u - u \chi(v) \nabla v \right) + u\, g(u) \\ \partial_t v &= \Delta v - \beta v + u\, s(u) \end{aligned} \tag{1}$$

Discretisation techniques

We (currently) use

- a method of lines approach,
- a canonical, uniform refinement of the spatial grid,
- conform quadrilateral bilinear finite elements (Ritz-Galerkin),
- the standard $\theta-$scheme for temporal discretisation.

Survey of num. schemes



go on

Comparison of iteration schemes

Model under consideration: 2D Pattern model on a square
Plots show convergence to num. reference solution

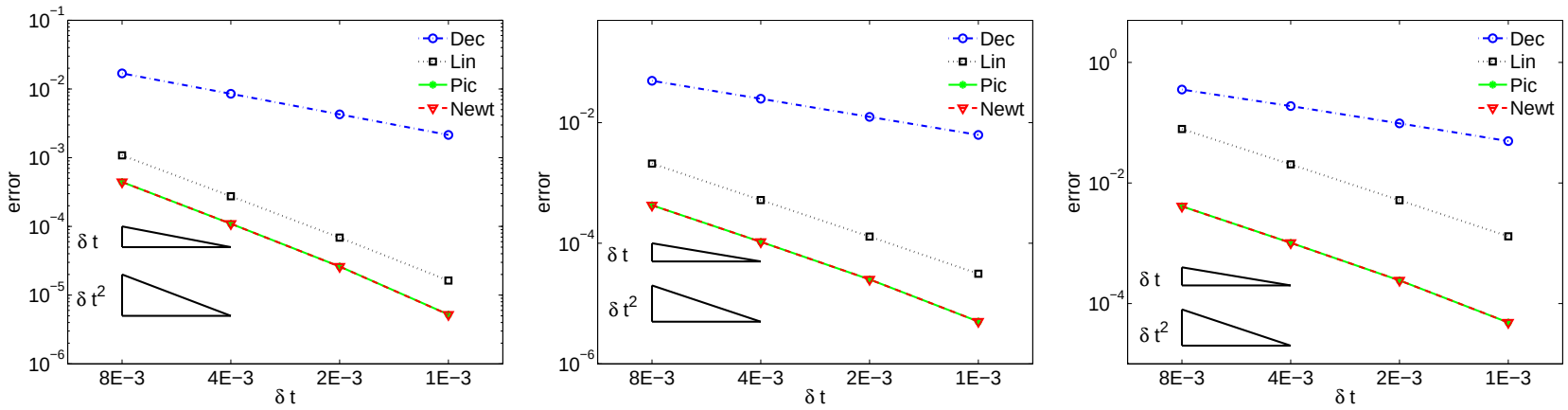


Figure : Convergence with varying chemosensitivities, $\chi = 10, 20, 50$.

- efficiency scales remarkably with χ
- Dec not comparable in terms of #IT
- Dec and Lin reveal inconsistencies
- Pic vs. Newt strongly emphasized for higher nonlinearity

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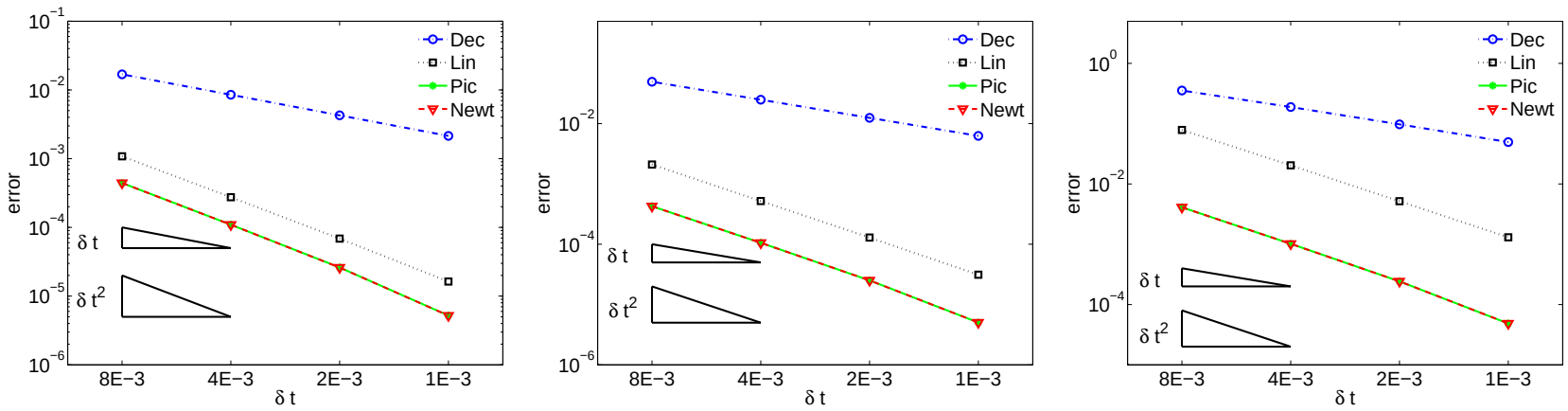

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Stabilisation via AFC

Motivation

- standard FEM fail for chemotaxis dominated PDEs
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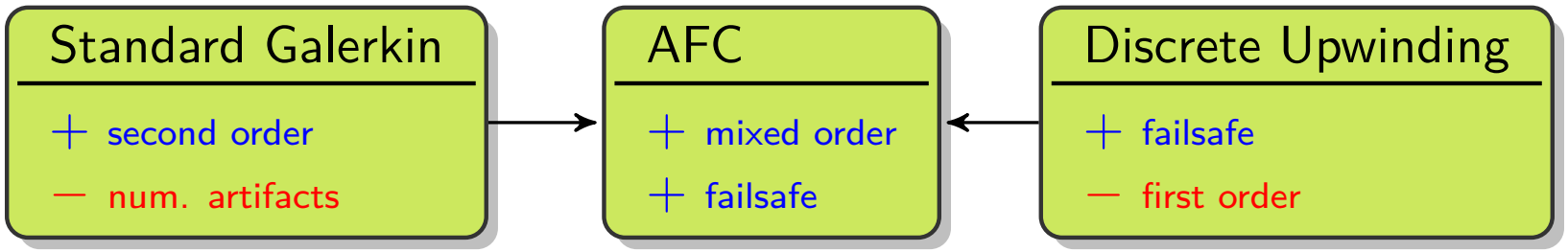
REMEDY: merging of the two approaches is the motivation of Algebraic Flux Correction (AFC), [Kuzmin '09]



AFC sketch

Standard Galerkin

+ second order
− num. artifacts

convenient semi-discretized formulation

$$\boldsymbol{M}\partial_t \boldsymbol{u} = \boldsymbol{B}(\boldsymbol{u})\boldsymbol{u}$$

Discrete Upwinding

+ failsafe
− first order

AFC

+ mixed order
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go on

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modification with discrete upwinding

$$\boldsymbol{M}^L\partial_t \boldsymbol{u} = (\boldsymbol{B}+\boldsymbol{D})(\boldsymbol{u})\boldsymbol{u} = \widetilde{\boldsymbol{B}}(\boldsymbol{u})\boldsymbol{u}$$

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correction of over-diffusive fluxes

$$\underbrace{\boldsymbol{M}^L\partial_t \boldsymbol{u} = \widetilde{\boldsymbol{B}}(\boldsymbol{u})\,\boldsymbol{u}}_{\text{low order scheme}} + \underbrace{\bar{\boldsymbol{f}}(\boldsymbol{u})}_{\substack{\text{antidiff.}\\ \text{flux}}}, \quad \bar{\boldsymbol{f}}_i = \sum_{j\neq i} \underbrace{\alpha_{ij}}_{\substack{\text{lim.}\\ \text{factors}}} \boldsymbol{f}_{ij}$$

go on

Discrete Upwinding

Consider the semi discretised system ($\boldsymbol{B}$ having zero row-sum)

$$\boldsymbol{M}\partial_t \boldsymbol{u} \quad = \quad \boldsymbol{B}(\boldsymbol{u})\boldsymbol{u} \tag{2}$$

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Add (*just necessary*) artificial diffusion $\widetilde{\boldsymbol{B}} = \boldsymbol{B} + \boldsymbol{D}$

$$d_{ij} = max\{-b_{ij}, 0, -b_{ji}\} \geq 0, \quad j \neq i \qquad \text{and} \quad d_{ii} = -\sum_{j \neq i} d_{ij}$$

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... at costs of accuracy (first order), [Godunov '59]

Flux correction

In order to correct the *over-diffusive* fluxes in eq. (3), we introduce limited *antidiffusive* fluxes.

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Some notes

- $\boldsymbol{f}_{ij} = -\boldsymbol{f}_{ji} \Rightarrow \alpha_{ij} = \alpha_{ji}$
- $\alpha_{ij} = 1 \Rightarrow$ Galerkin (2), $\alpha_{ij} = 0 \Rightarrow$ upwind (3)
- α_{ij} still need to be specified, we use Zalesak limiter, [Zalesak '79]

Details of flux correction

0. Pre-limiting step: cancel "flattening" fluxes

$$f_{ij} = 0, \quad \text{if } f_{ij}(u_j^L - u_i^L) > 0\,.$$

1. Calculate all antidiffusive fluxes into node i,

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

2. Calculate distace to local minima

$$Q_i^+ = \max\left\{0, \max_{j\neq i}(u_j^L - u_i^L)\right\}, \quad Q_i^- = \min\left\{0, \min_{j\neq i}(u_j^L - u_i^L)\right\}.$$

3. Calculate maximal correction factors

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

4. Finally

$$a_{ij} = \begin{cases} \min\{R_i^+, R_j^-\}, & \text{if } f_{ij} > 0\,, \\ \min\{R_i^-, R_j^+\}, & \text{otherwise.} \end{cases}$$

Explicit flux correction

Time discretisation of the AFC equation contribute nonlinearities even for $\theta = 0$

$$
\begin{aligned}
f_{ij}(\boldsymbol{u}^{n+1}, \boldsymbol{u}^{n}) \quad = \quad & m_{ij}(\boldsymbol{u}_i^{n+1} - \boldsymbol{u}_j^{n+1}) - m_{ij}(\boldsymbol{u}_i^{n} - \boldsymbol{u}_j^{n}) \\
& + \delta t \left[\theta d_{ij}^{n+1}(\boldsymbol{u}_i^{n+1} - \boldsymbol{u}_j^{n+1}) + (1-\theta) d_{ij}^{n}(\boldsymbol{u}_i^{n} - \boldsymbol{u}_j^{n}) \right]
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REMEDY: Linearisation via explicit AFC

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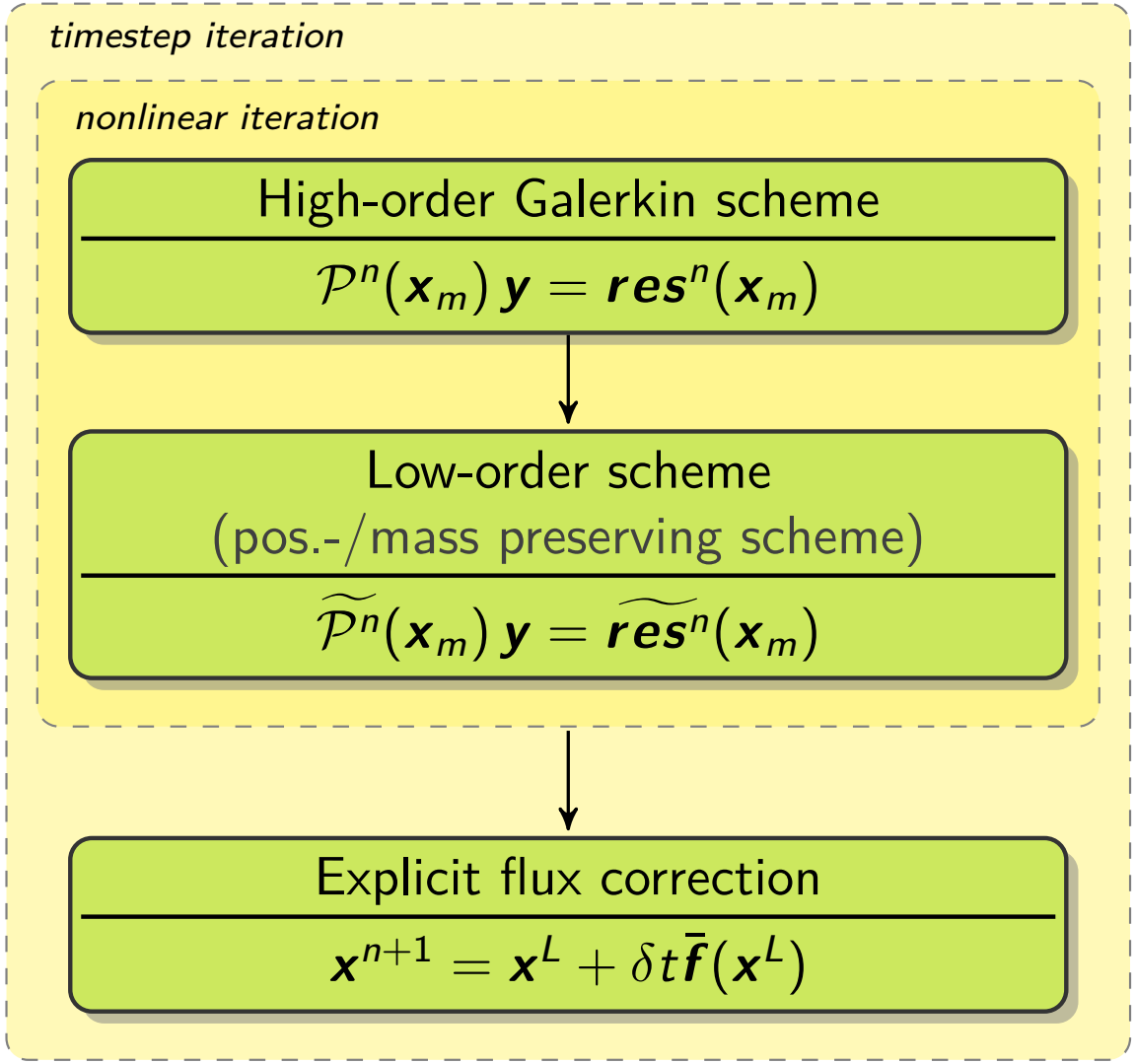
$$\boldsymbol{M}^L \boldsymbol{u}_{n+1} = \boldsymbol{M}^L \boldsymbol{u}^L + \delta t \bar{\boldsymbol{f}}(\boldsymbol{u}^L),$$

where we have

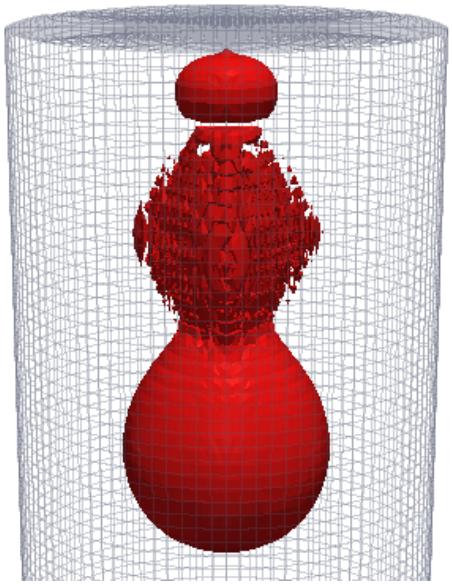
$$f_{ij}(\boldsymbol{u}^L) = m_{ij}(\dot{\boldsymbol{u}}_i^L - \dot{\boldsymbol{u}}_j^L) + d_{ij}^L(\boldsymbol{u}_i^L - \boldsymbol{u}_j^L).$$

Roadmap of explicit AFC

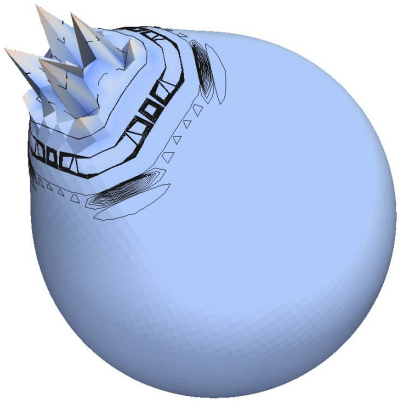


The need of AFC

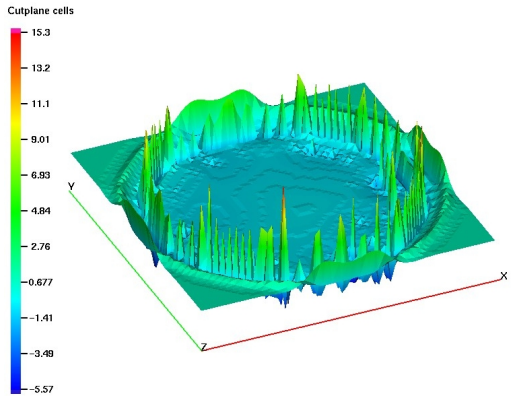
In generic situations, classical Galerkin schemes provide unphysical results, e.g. severe oscillations, negative densities, loss of characteristic profiles $\rightarrow$ possibly solver-breakdown



(a) blowup



(b) blowup

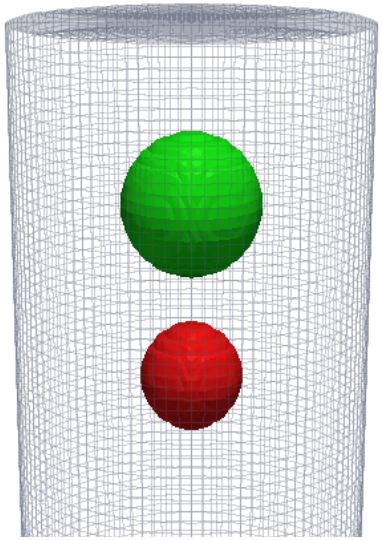


(c) pattern

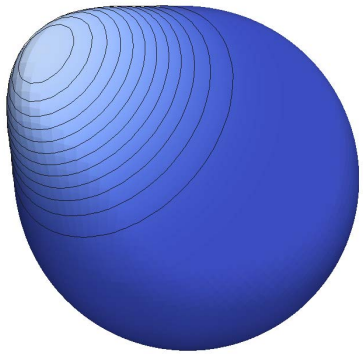
Figure : Challenges, blowup: Steep gradients, pattern: Maintenance of travelling waves/trailing spots

On AFC

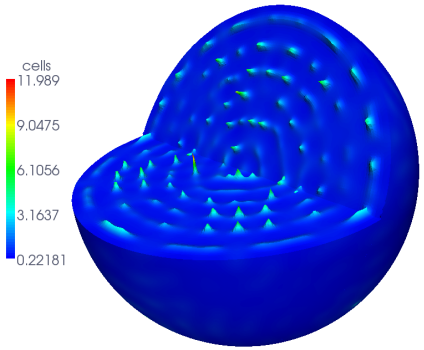
AFC stabilised schemes resolve the problem at costs linear in $\#DOF$ (per IT_{NL})



(a) blowup



(b) blowup



(c) pattern

Figure : No oscillations, no negative values, patterns are recaptured.

Outline

Take home messages

- Numerical studies offer validation and reshaping of underlying models and provide quantitative insights into complex dynamics
- Identification of proper num. scheme is a challenging task (user customisation), focus: accuracy, number of iterations, complexity of iterations, stability
- A first glimpse revealed the potential of elaborate solver strategies, particularly in case of large chemotaxis factors χ or poor (temporal) discretisations
- An AFC-like stabilisation counters chemotaxis-dominated num. artifacts and is highly flexible and inexpensive

Future interests

Numerical improvements

- jacobian-free Newton methods
- "global" AFC techniques
- adaptive schemes

Model considerations

- modeling aspects (variety and comparison of derivations, model assumptions, combination of models)
- possible patterns and steady states ($\rightarrow$ Winkler)
- multi species interactions ($\rightarrow$ Horstmann)
- follow signal transduction pathways up to the cell membranes
  $\rightarrow$ chemotaxis on surfaces (preliminary work by Sokolov exists)

go on

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Appendix: Gallery

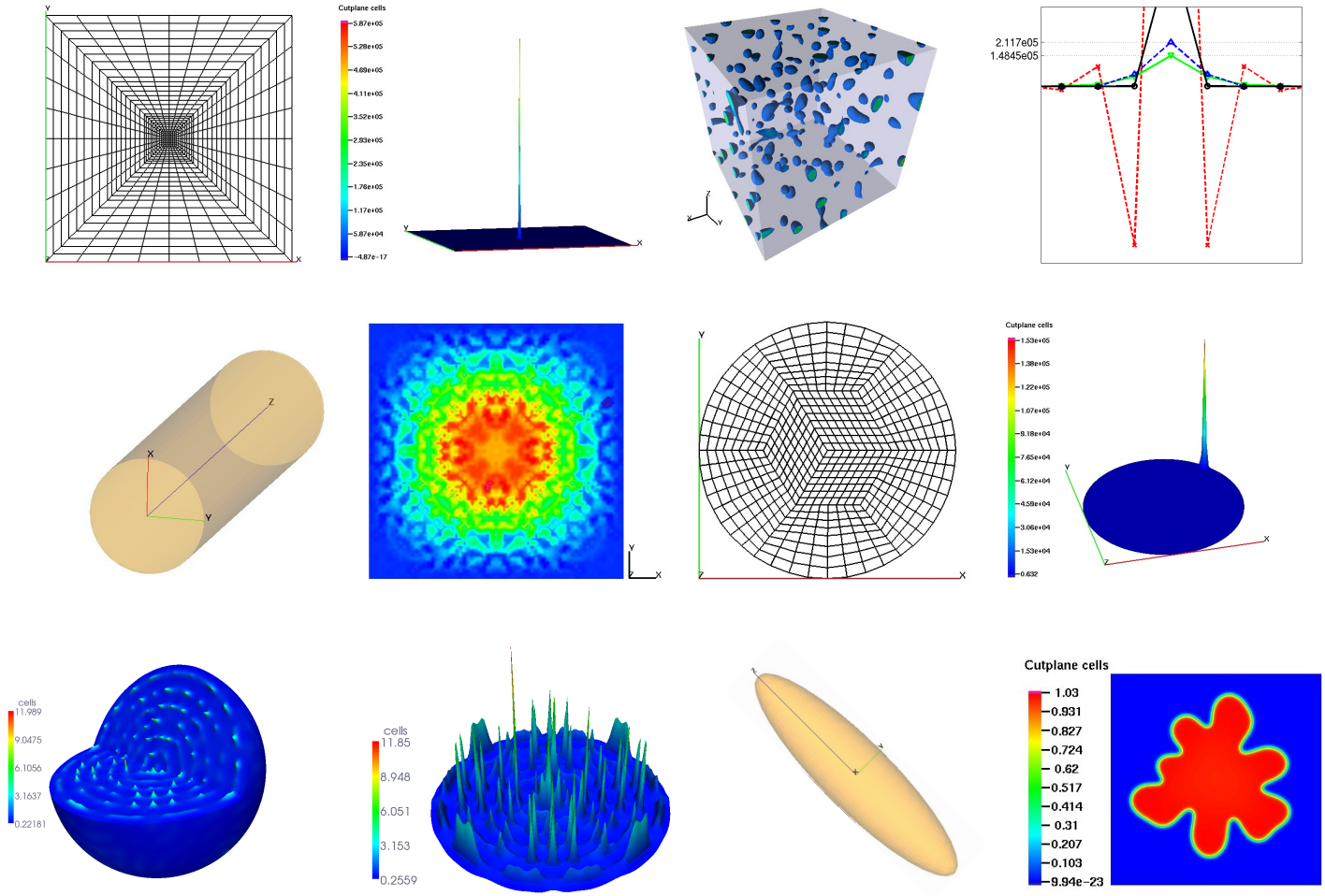

Figure : Some impressions.

Appendix: Modeling aspects

- Macroscopic derivation (e.g. [Keller & Segel '70]) require $\delta t/\delta h^2 = const$. Does it make sense to study chemotaxis-dominating scenarios (from the modeling pov)?
- Understand the motiviations for different microscopic approaches, space vs. velocity jump processes, [Othmer et al. '88, Othmer & Stevens '97]. What are their differences numerically, [Erban & Othmer, '04]? Is it perhaps numerically favorable to consider microscopic models?

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Appendix: Multi-Species

- higher coupling requires even more carefully chosen discretisations. Does a segregated approach still provide reasonable/reliable results?
- stabilisation techniques may also be required for Diffusion-like terms (in the presence of conflicts)
- consider (free-boundaries) multiphase-like scenarios. What about single species space posession, e.g. at most one species lives in designated areas?
- conditions for a blow-up are even less analysed, [Horstmann '11, Arenas et al., '09]. The results in [Arenas et al., '09] show that in the radial symmetric setting the blow-up for multispecies has to be simultaneous, but what happens for other initial symmetries?
- What effect does a new approach have to the receptor-based chemotactic sensitivity on the time asymptotic behavior and pattern forming mechanism?

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Appendix: PDEs on surfaces

- consider chemotaxis on the individual cell level: the chemo-gradient induces a polarisation of the cell in terms of localisation of membrane receptors $\rightarrow$ chemotaxis on surfaces
- coupling with surface PDEs promote a level-set ansatz (different scaling of grids)
- numerical and mathematical analysis for gradient-based slope limiters for PDEs on surfaces is desired (in context of AFC)

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Appendix: Gallery, Aggregation

Introducing Quorum-sensing-like terms protect the solution from blowing up, typical aggregation behaviour is still maintained.

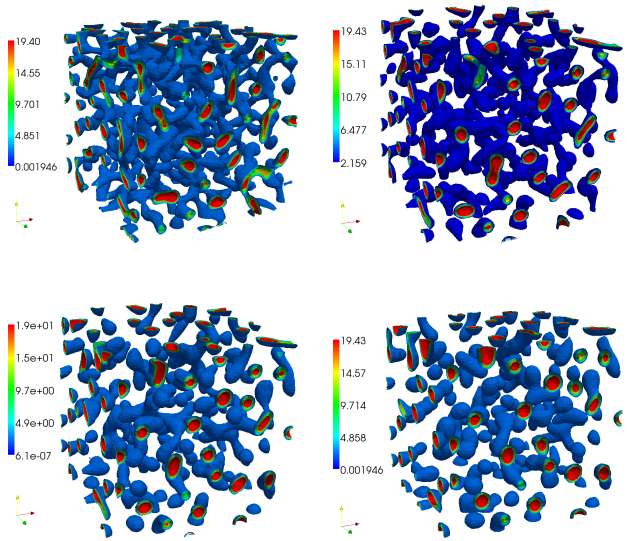

Figure : 3D simulation of an aggregation model with AFC. Note that aggregates grow moderately in concentration, however the total mass is preserved and neither a blow-up nor negative values are attained.

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Appendix: Gallery, AFC

Brief comparison of the pure Galerkin scheme, the low-order Upwinding and the high-order AFC scheme.

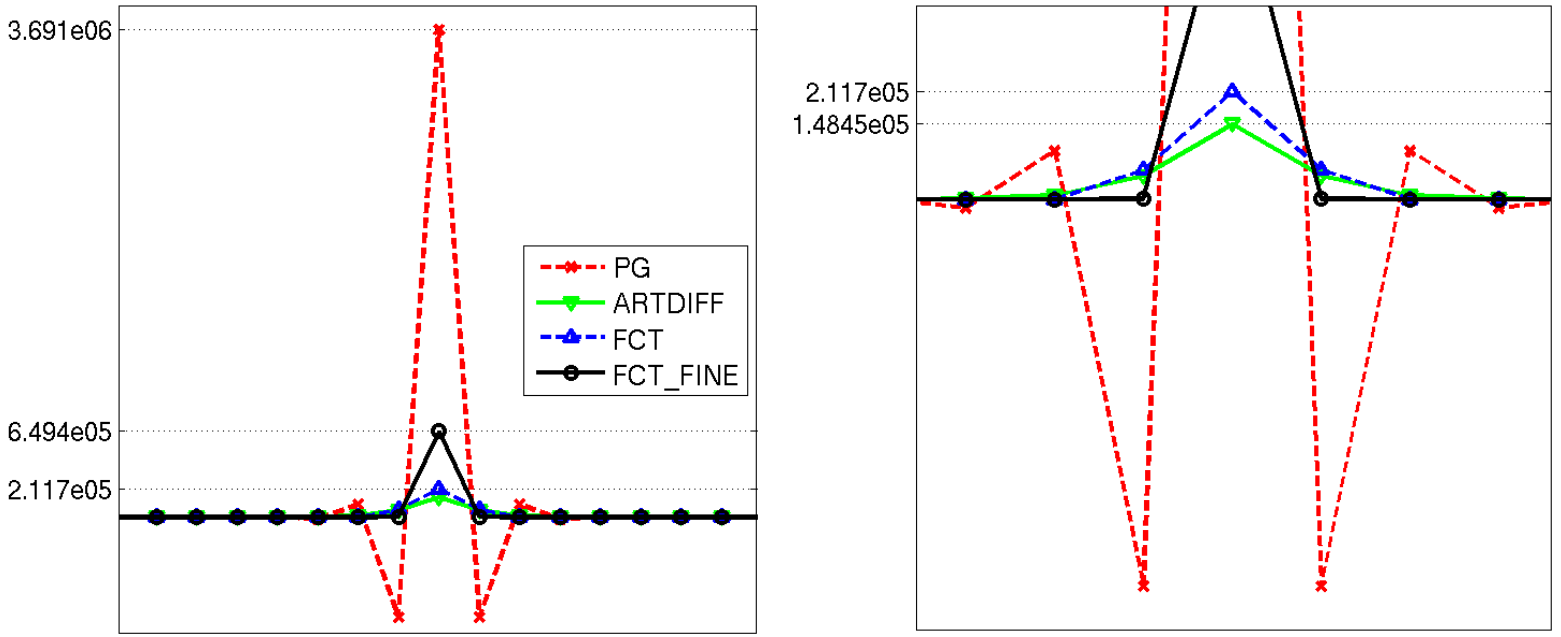

Figure : Observe the difference in height at the specified timeinstant near the blow-up time.

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Appendix: Gallery, BU

It was shown that in particular cases cells 'move' towards the boundary prior to a blow-up.

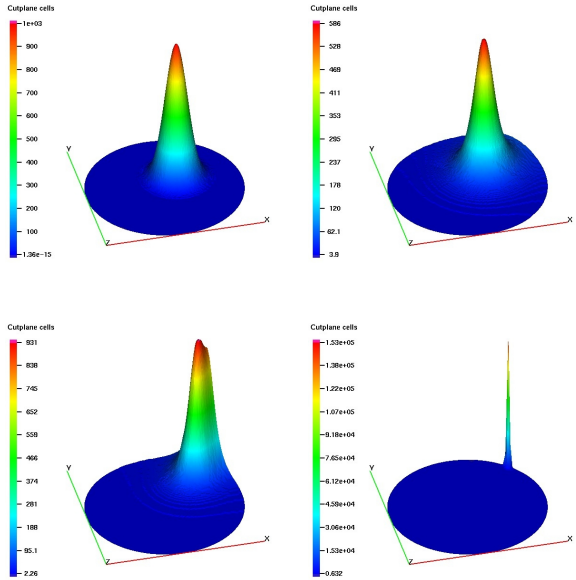

Figure : For a quadratic domain the solution prefers corners. Whether the curvature influences this behaviour is still an open question!

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Appendix: Gallery, Pattern 1

A simple logistic-like growth is added to the minimal model. This leads to travelling waves solutions.

Figure : 3D simulation of a pattern model with AFC. Note that the radial travelling wave converts into an unsteady chaotic straying of the 'cells'.

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Appendix: Gallery, Pattern 2

Mimura et al. introduced a pattern model with quadratic chemical gradient.

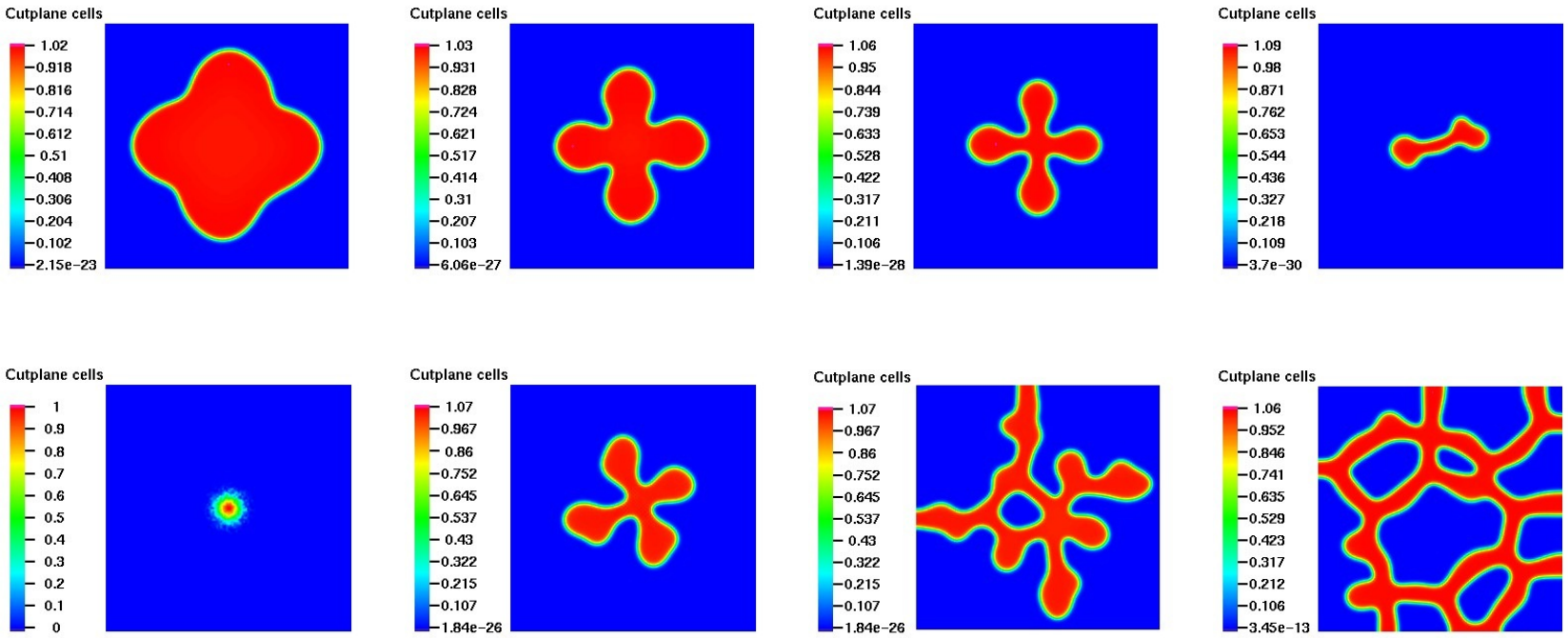

Figure : The pattern highly depend on χ, note that 'symmetry' breaks for large χ (top). Pattern spread, finally unsteady giraffe-like patches form (bottom).

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