Efficient, accurate and flexible Finite Element solvers for Chemotaxis

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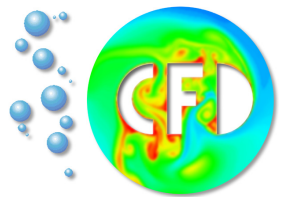

outline

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concept(1)

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.

http://dictybase.org/Multimedia/motility/motility.htm

concept(2)

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

Minimal Keller-Segel model (1970) for chemotaxis:

equation for motile species u:

$$\frac{\partial u}{\partial t} = \nabla \cdot \Big(\underbrace{\nabla u}_{\text{diffusion}} - \underbrace{\chi u \nabla c}_{\text{chemotaxis}} \Big)$$

equation for the chemical agent c:

$$\frac{\partial c}{\partial t} = \underbrace{\Delta c}_{\text{diffusion}} - \underbrace{c + u}_{\text{reaction}}$$

models(1)

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

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\end{aligned}$$

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

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$$\frac{\partial u_i}{\partial t} = \nabla \cdot \left[\left(\sum_{l=1}^{N} D^u_{i,l}(u_i) \nabla u_l \right) - \left(\sum_{k=1}^{M} \chi_{i,k}(u_i) \nabla c_k \right) \right] + f_i(u_i)$$

$$\frac{\partial c_j}{\partial t} = D^c_j \Delta c_j - \sum_{k=1}^{M} \alpha_{k,j} c_k + \sum_{l=1}^{N} \beta_{l,j} u_l$$

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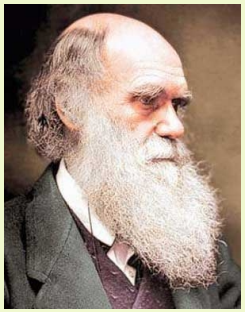
multispecies: e.g. species $u_1, \ldots, u_N$, chemical agents $c_1, \ldots, c_M$

models(2)

Biology



- models are well motivated
- all ingredients for their own are well understood

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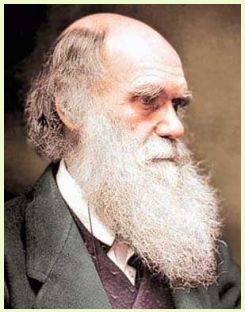

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Mathematics

- existence and uniqueness are nontrivial
- analysis revealed mathematical artifacts

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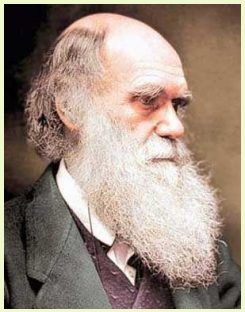

- models are well motivated
- all ingredients for their own are well understood

$\rightarrow$ numerical ansatz is highly desired to validate models and obtain more insights from mathematical point of view

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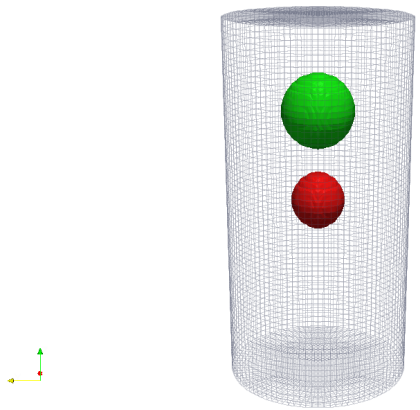
model examples(1)

1) the minimal model may lead to blowing up solutions. From biological point of view, those unbounded solutions do not make any sense.



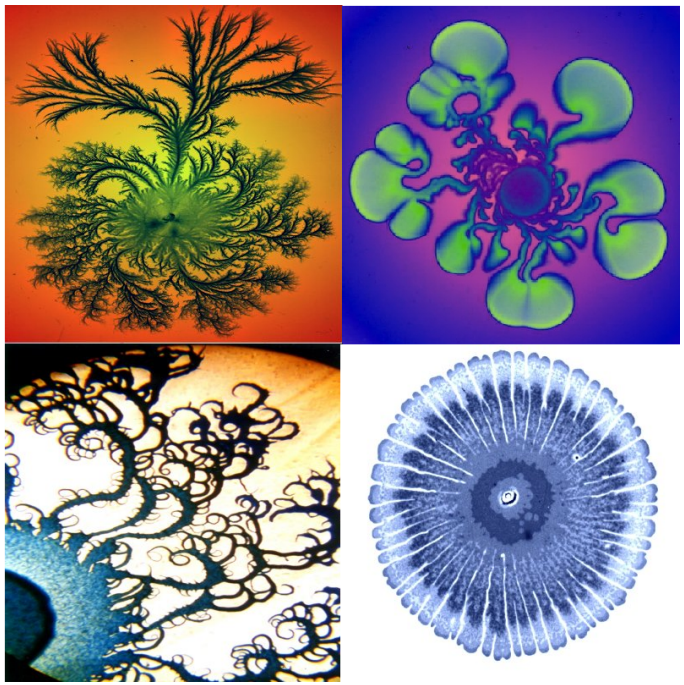
minimal model

$$\begin{aligned} \frac{\partial u}{\partial t} &= \nabla \cdot (\nabla u - \chi u \nabla c) \\ \frac{\partial c}{\partial t} &= \Delta c - c + u \end{aligned}$$

$\mathbb{R}^1$: 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

model examples(2)

2) Stunning results were obtained when biologists study certain mutated bacteria colonies. Their proliferation seems to follow certain patterns.



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

kinetic model

$$\frac{\partial u}{\partial t} = \nabla \cdot (Du - \chi u \nabla c) + \nu u(1-u)$$
$$\frac{\partial c}{\partial t} = \Delta c - \beta c + u$$

$\mathbb{R}^{1,2}$: unique global weak solution (at least for $\nu \gg 1$)
$\mathbb{R}^{\geq 3}$: far less is known
existence of nontrivial steady states

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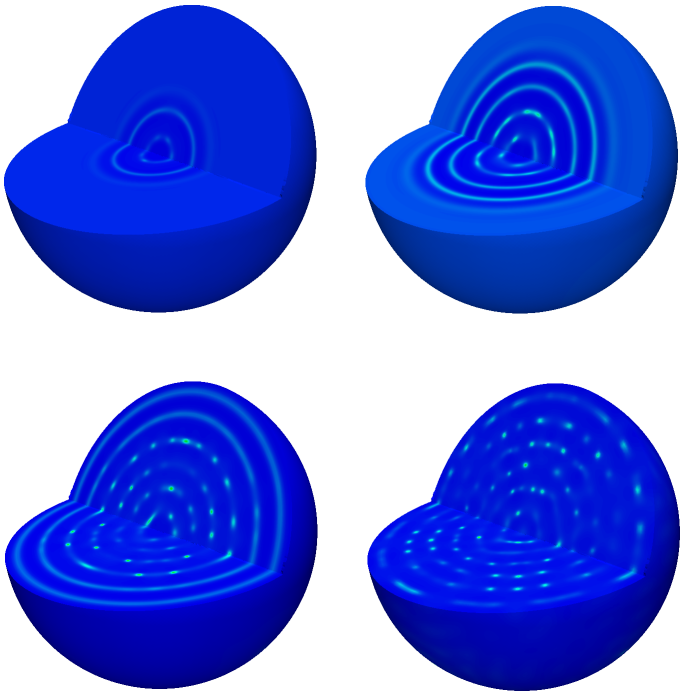

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existence of nontrivial steady states

outline

In order to obtain a reliable solver for chemotaxis PDEs many (numerical) concerns has to be tackled:

challenges

- high-order resolution (of sharp interfaces/steep gradients)
- fast solver techniques
- smart memory management
- robustness for a variety of parameters
- user interface (arbitrary coefficients)
- mass conservation (when applicable) and positivity preservation

overview

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Especially the last three are of particular interest in the presence of chemotaxis PDEs.

high-order vs. robustness

Applying standard (high-order) Finite Element Methods (FEM) on chemotaxis dominated PDEs lead to severe numerical instabilities.
When restricted to the minimal model, the troublemaker is the essential chemotaxis term $\nabla \cdot (\chi u \nabla c)$.

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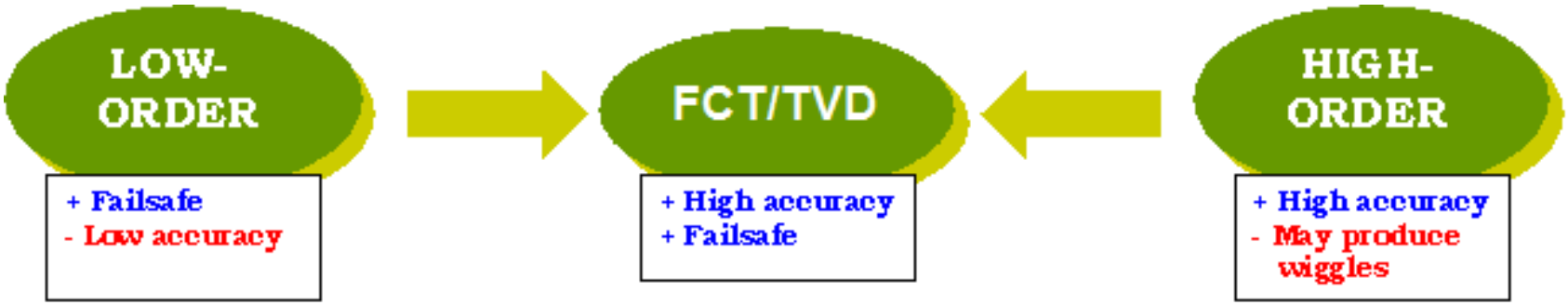
REMEDY: merging the two approaches leads to FCT/TVD which combines all desired properties



fast solver techniques

In the presence of more comprehensive models, the introduced nonlinearities also ask for a special treatment.
Common segregated linearization techniques converge very poorly when applied to ill-conditioned systemmatrices.

a segregated approach:

$$1.\ A_1(u_{n-1}, c_{n-1})\, c_n = b_1$$
$$2.\ A_2(u_{n-1}, c_n) \quad u_n = b_2$$

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set up a block system matrix (monolithic approach) and apply (damped) Newton-like or fixpoint methods

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a monolithic approach:

$$\underbrace{\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}}_{=:A(u_n, c_n)} \begin{pmatrix} u_n \\ c_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

user interface

When developing a software for solving a diversity of underlying models, an user-prescribed input is highly favorable.
Our software FEAST/FEATFLOW is designed in a module based fashion and allows for easy access via single 'stand-alone' objects.

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Our software `FEAST/FEATFLOW` is designed in a module based fashion and allows for easy access via single 'stand-alone' objects.

Generic super-model

The current underlying generic (single-species) model reads:

$$\begin{aligned} \frac{\partial u}{\partial t} &= \nabla \cdot (D(u)\nabla u - \chi(u,c)\,\nabla c) + f(u) \\ \frac{\partial c}{\partial t} &= \Delta c - \alpha\, c + \beta(u)\, u \end{aligned}$$

$\rightarrow$ all coefficients may be user-prescribed

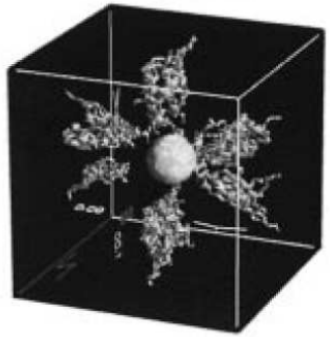
outline

going beyond academic models

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

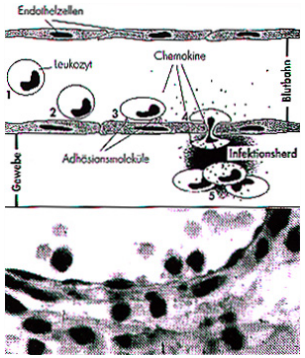
- proliferation of bacteria (not only in petri dishes)
- tumour growth/angiogenesis/haptotaxis
- breeding concerns (insemination of sea urchins)
- immunology (production of chemokines at infection sites)

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



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

C. Pietschmann, MPI



L. Kinzel, LMU

summary/features

The developed software embeds the following features:

- supported domains: $\Omega \subset \mathbb{R}^2, \mathbb{R}^3$ (reasonable mesh restrictions)
- spatial discretization via $Q_1, Q_2, \ldots$ elements
- temporal discretization: θ-scheme
- reasonable boundary conditions at will: Dirichlet, Neumann, periodic,...
- user-prescribed parameters/coefficients/callback functions (module-based Open Source Software)
- FCT/TVD stabilized solver (preservation of physical entities)
- embedded nonlinear solvers: (Deuflhard) damped Newton-like methods, fixpoint, Picard-linearization
- graphical output via `GMV`/`PARAVIEW`

extentions/outlook

Further aims for the software:

- extend the framework to multi-species systems
- implementation of fast multigrid-solvers
- spatial (h-, r-) and temporal (t-) adaptivity
- parallelization
- ...

Further informations:

- email: `robert.strehl@math.tu-dortmund.de`
- homepage: `http://www.mathematik.tu-dortmund.de/~rstrehl/downloads.html`
- software: `http://www.featflow.de`
- model organism: `http://dictybase.org`

list of figures: http://dictybase.org/Multimedia/motility/motility.htm ; http://www.youtube.com/watch?v=hpHpBHJZQvU ; http://star.tau.ac.il/ eshel/image-flow.html ; M. A. J. Chaplain, Mathematical modelling of angiogenesis, Journal of Neuro-Oncology, Vol. 50, pp. 37-51, 2000 ; Catarina Pietschmann, MaxPlanckForschung 2009 Heft 2, Wo, bitte, geht's denn hier zum Ei? ; Linda Kinzel, Seminar Autoimmunität, Einführung Chemokine, 24./25. Juni 2006