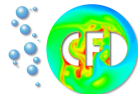# Efficient, accurate and flexible Finite Element solvers for Chemotaxis

Konrad Zuse Institut Berlin

Robert Strehl   Andriy Sokolov   Stefan Turek

Technische Universität Dortmund
Institut für Angewandte Mathematik/Numerik, LS III

June 21, 2011

underlying models
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numerical challenges
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applications
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1 underlying models

2 numerical challenges

3 applications

underlying models
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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

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

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Since 1970 various models have been proposed (especially in the recent decades).

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models(1)

Since 1970 various models have been proposed (especially in the recent decades).

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

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

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

Since 1970 various models have been proposed (especially in the recent decades).

$$
\begin{aligned}
\frac{\partial u}{\partial t} &= \nabla \cdot \big(\underbrace{D(u)\nabla u}_{\text{diffusion}} - \underbrace{\chi(u,c)\nabla c}_{\text{chemotaxis}} \big) + \underbrace{f(u)}_{\text{kinetics}} \\
\frac{\partial c}{\partial t} &= \underbrace{\Delta c}_{\text{diffusion}} - \underbrace{\alpha c + \beta(u)u}_{\text{reaction}}
\end{aligned}
$$

(nonlinear) coefficients modeling saturation effects:

e.g. $D(u), \chi(u,c), \beta(u) \overset{u\to\infty}{\to} 0$

introducing kinetics:

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

underlying models
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Since 1970 various models have been proposed (especially in the recent decades).

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

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

(nonlinear) coefficients modeling saturation effects:
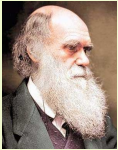
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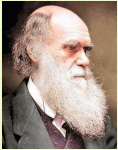
e.g. $f(u) = \nu u(1 - u)$ (logistic)

multispecies:

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

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Biology

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

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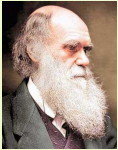○○○

models(2)

Biology

- models are well motivated
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Mathematics

- existence and uniqueness are nontrivial
- analysis revealed mathematical artifacts

Biology

- 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

Mathematics

- existence and uniqueness are nontrivial
- analysis revealed mathematical artifacts

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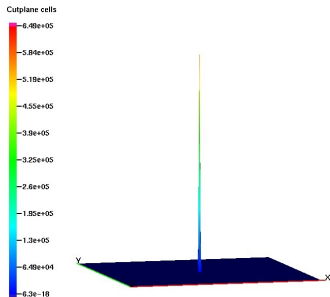
minimal model

$$\frac{\partial u}{\partial t} = \nabla \cdot \left(\nabla u - \chi u \nabla c \right)$$

$$\frac{\partial c}{\partial t} = \Delta c - c + u$$

$\mathbb{R}^1$: 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

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dortmund

2) Slime molds aggregate to form more energetic structures. The underlying regularized model introduces quorum-sensing alike nonlinearities.

regulated model

$$\frac{\partial u}{\partial t} = \nabla \cdot \left(D\nabla u - \chi \frac{u}{(1+c)^2} \nabla c \right)$$

$$\frac{\partial c}{\partial t} = \Delta c - c + \omega \frac{u^2}{\mu + u^2}$$

global existence is proven
$\rightarrow$ saturating signal production,
    signal-dependent sensitivity,
    quorum-sensing

T. Gregor, http://tglab.princeton.edu/

underlying models
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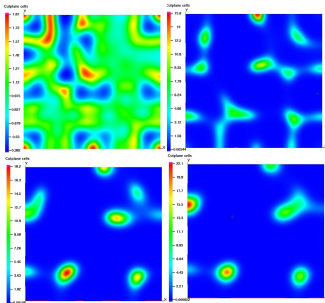

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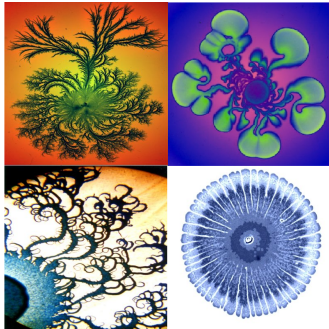
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3) Stunning results were obtained when biologists study certain mutated bacteria colonies. Their proliferation follow certain patterns.

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

kinetic model

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

$$\frac{\partial c}{\partial t} = \Delta c - \beta c + u$$

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

underlying models
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numerical challenges
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model examples(3)

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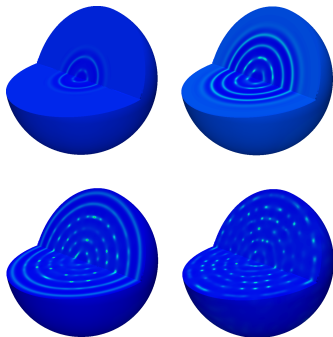bacteria colonies. Their proliferation follow certain patterns.

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outline

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2 numerical challenges

3 applications

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

challenges

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

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

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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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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 $\nabla \cdot (\chi u \nabla c)$.
$\rightarrow$ upwind schemes guarantee to 'smooth-out' instabilities and preserve physical entities

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underlying models
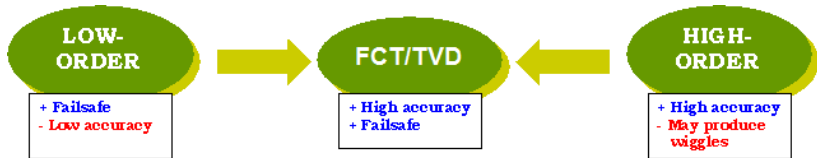○○○○○○○

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BUT: high-order is not anymore obtained.

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

LOW-ORDER
+ Failsafe
- Low accuracy

FCT/TVD
+ High accuracy
+ Failsafe

HIGH-ORDER
+ High accuracy
- May produce wiggles

underlying models
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numerical challenges
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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.

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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 segregate approach:

1. $A_1(u_{n-1}, c_{n-1})\, c_n = b_1$

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

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a monolithic approach:

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

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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 an object oriented fashion and allows for easy access via single modules.

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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 an object oriented fashion and allows for easy access via single modules.

Generic super-model

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

$$\frac{\partial u}{\partial t} = \nabla \cdot (D(u)\nabla u - \chi(u,c)\,\nabla c) + f(u)$$

$$\frac{\partial c}{\partial t} = \Delta c - \alpha\,c + \beta(u)\,u$$

$\rightarrow$ all coefficients may be user-prescribed

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Certainly, applied mathematicians look for practical benefits of their work. Since chemotaxis plays a key role for organisms, plenty applications come into mind.
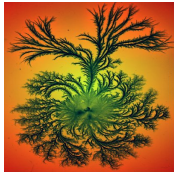
- proliferation of bacteria (not only in petri dishes)
- tumour growth/angiogenesis/haptotaxis
- breeding concerns (insemination of sea urchins)
- immunology (production of chemokines at infection sites)

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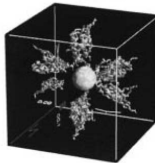- immunology (production of chemokines at infection sites)

E. Ben-Jacob,
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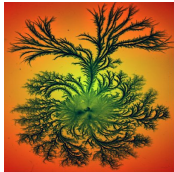- immunology (production of chemokines at infection sites)

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

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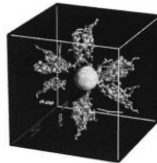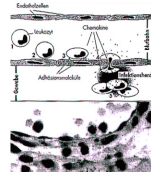http://star.tau.ac.il/~eshel/
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L. Kinzel, LMU

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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

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- 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

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Further aims for the software:

- extend the framework to multi-species systems
- implementation of fast multigrid-solvers
- spatial (h-, r-) and temporal (t-) adaptivity
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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
- next conference: http://www.biomath.bg

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

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