Efficient, accurate and flexible Finite Element solvers for Chemotaxis
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1 underlying models
2 numerical challenges
3 final notes
1. underlying models

2. numerical challenges

3. final notes
**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 → system of partial differential equations (PDE)

Minimal Keller-Segel model (1970) for chemotaxis:

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

equation for motile species \( u \):

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

equation for the chemical agent \( c \):
Since 1970 various models have been proposed (especially in the recent decades).

\[
\frac{\partial u}{\partial t} = \nabla \cdot (\nabla u - \chi u \nabla c) \\
\frac{\partial c}{\partial t} = \Delta c - c + u
\]

(diffusion) (chemotaxis) (diffusion) (reaction)

(e.g. $D(u)$, $\chi(u,c)$, $\beta(u)$)

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

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

(underlying models) (numerical challenges) (final notes)
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\[
\frac{\partial u}{\partial t} = \nabla \cdot \left( D(u) \nabla u - \chi(u, c) \nabla c \right)
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\[
\frac{\partial c}{\partial t} = \Delta c - \alpha c + \beta(u)u
\]

(nonlinear) coefficients modeling e.g. \( D(u), \chi(u, c), \beta(u) \xrightarrow{u \to \infty} 0 \)

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

\[
\frac{\partial u}{\partial t} = \nabla \cdot \left( D(u) \nabla u - \chi(u, c) \nabla c \right) + f(u)
\]

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

(nonlinear) coefficients modeling saturation effects:

introducing kinetics:

\[ u \to \infty \to 0 \]

\[ f(u) = \nu u (1 - u) \] (logistic)
Since 1970 various models have been proposed (especially in the recent decades).

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

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

(nonlinear) coefficients modeling saturation effects:

\begin{align*}
\lim_{u \to \infty} D(u), \chi(u, c), \beta(u) &= 0 \\
\text{e.g. } f(u) &= \nu u(1 - u) \text{ (logistic)} \\
\text{e.g. } \text{species } u_1, \ldots, u_N, \text{ chemical agents } c_1, \ldots, c_M
\end{align*}
Biology

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

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

\[
\begin{align*}
\frac{\partial u}{\partial t} &= \nabla \cdot (\nabla u - \chi u \nabla c) \\
\frac{\partial c}{\partial t} &= \Delta c - c + u
\end{align*}
\]

- \( \mathbb{R}^1 \): 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
2) Stunning results were obtained when biologists study certain mutated bacteria colonies. Their proliferation seems to follow certain patterns.

**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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- **\(\mathbb{R}^{1,2}\)**: unique global weak solution (at least for \(\nu \gg 1\))
- **\(\mathbb{R}^{\geq 3}\)**: far less is known

existence of nontrivial steady states
1 underlying models
2 numerical challenges
3 final notes
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
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- fast solver techniques
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- robustness for a variety of parameters
- user interface (arbitrary coefficients)
- mass conservation (when applicable) and positivity preservation

Especially the last three are of particular interest in the presence of chemotaxis PDEs.
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 $\nabla \cdot (\chi u \nabla c)$. 

BUT: upwind schemes guarantee to ‘smooth-out’ instabilities and preserve physical entities. 

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

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

a segregated approach:

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

a monolithic approach:

\[
\begin{pmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{pmatrix}
\begin{pmatrix}
u_n \\
c_n
\end{pmatrix} =
\begin{pmatrix}b_1 \\
b_2
\end{pmatrix}
\]

$= A(u_n, c_n)$
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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**Generic super-model**

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

\[
\begin{align*}
\frac{\partial u}{\partial t} &= \nabla \cdot \left( D(u) \nabla u - \chi(u, c) \nabla c \right) + f(u) \\
\frac{\partial c}{\partial t} &= \Delta c - \alpha c + \beta(u) u
\end{align*}
\]

→ all coefficients may be user-prescribed
1 underlying models

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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)
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: $\theta$-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
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