Parallel Adaptive Simulation of Processes from Science and Engineering

D. Logashenko, A. Nägel, S. Reiter, A. Vogel, G. Wittum

Presentation on ADVCOMP, IARIA Oct 2021
Short Bio

Gabriel Wittum holds professorships for Applied Mathematics, Computational Science, Computer Science and Bioengineering at KAUST, Saudi Arabia, and for Modelling and Simulation at Frankfurt University, Germany. He is an expert in modelling and simulation of problems from empirical sciences. He solves problems from the classical physical and engineering sciences like fluid mechanics, groundwater flow and transport, environmental science, energy research, reaching out to biology, pharmacy, medicine, finance and many more disciplines. Starting from numerical analysis, he develops advanced models, robust and scalable multi-grid methods and software systems for large scale computing. For his scientific work he has been honoured with the Heinz-Maier-Leibnitz price and the doIT Software Award. He authored over 200 scientific publications.
The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.

P.A.M. Dirac (1927)
Modelling Basics

- Morphology model
- Geometry
- Material properties
- Process model based on first principles (balance laws)

→ reliable model with prognostic quality
Modelling Basics

- A model is an answer, it needs a question.
- The model should be as detailed as necessary to answer the question and as simple as possible. „Man soll die Dinge so einfach machen wie möglich, aber nicht einfacher.” (Einstein)
- Complexity $\leftrightarrow$ Reliability
- Simulation technique is decisive for the complexity limit
# Modeling and Simulation

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<thead>
<tr>
<th>Mathematical Model</th>
<th>Applications, Mathematics (Analysis)</th>
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<tr>
<td>System of differential equations</td>
<td>Numerics</td>
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<table>
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<tr>
<th>Numerical approximation</th>
<th>Computer Science</th>
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<tr>
<td>Numerical methods</td>
<td></td>
</tr>
<tr>
<td>discretisation and solver</td>
<td></td>
</tr>
</tbody>
</table>

**Software Tools**

- Applications
- Mathematics (Analysis)
- Numerics
- Computer Science

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Modeling and Simulation

Mathematical Model
System of differential equations

Numerical approximation
Numerical methods
discretisation and solver

Software Tools

Applications,
Mathematics (Analysis)

Numerics

Computer Science

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Modeling and Simulation

Mathematical Model
System of differential equations

Numerical approximation
Numerical methods
discretisation and solver

Software Tools

Mapping Reality
Errors,
Complexity

Complexity,
Flexibility, ...

Hardware

Limiting Resource

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Adaptivity

- Refine grid where needed
Adptivity 3d

Peter Bastian

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Complexity - HPC Paradoxon

Algorithm complexity: Execution time $E = O(n^q)$, $q > 1$

Buying a new computer: On a new i.e. larger and faster computer, larger problems will be computed. Assume the new computer is a factor $\alpha > 1$ faster and larger than the old one. To compute a problem of size $\alpha \cdot n$, the new computer needs

$$O(\alpha^q \cdot n^q) = \alpha^{(q-1)} \alpha E.$$ 

The larger and faster the computer becomes, the longer the execution time will be!

Large scale computing needs $q=1$ i.e. optimal algorithms!
SIMULATION SYSTEM UG4

Adaptivity

Parallelism

Multigrid
Simulation System UG4

Engineering
- porous media flow
- CO₂ injection
- geothermal flows
- CFD
- struct. mechanics
- energy research
- chemical eng.
- process eng.
- biomass ferment.
- aeroacoustics

Medicine (Health)
- transdermal drug delivery
- signal processing in neurons
- HC virus replication
- infectious diseases

Finance
- option pricing
- credit risk estimation
- portfolio optimization

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UG 4  DEVELOPERS

New code UG4
≈ 200 person years for development

M. Breit
S. Grein
A. Grillo
M. Heisig
I. Heppner
M. Hoffer
S. Höllbacher
M. Knodel
M. Lampe
L. Larisch
B. Lemke
D. Logaschenko
I. Muha
A. Nägel
C. Poliwoda
R. Prohl
G. Queisser
S. Reiter
M. Rupp
P. Schröder
M. Stepniewski
S. Stichel
A. Vogel
C. Wehner
G. Wittum
K. Xylouris

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I. Heppner, A. Nägel, S. Reiter, M. Rupp, A. Vogel

- completely new code, strongly modularized
- hybrid unstructured grids, hanging nodes
- finite volumes of arbitrary order, finite elements
- parallel adaptive and robust multigrid
- highly scalable
- FAMG as separate module
• efficient parallel data migration via MPI-based Parallel Communication Layer (PCL) (Reiter et al 2015)
• Tool for gridding: ProMesh (Reiter 2017)
• GUI based on VRL (Hoffer, W. 2014)
\(\textbf{ug} 4 \textbf{GUI} \) (M. Hoffer)

- Based on VRL (Visual Reflection Library)
- allows graphical control of simulation
• Based on VRL (Visual Reflection Library)
• allows graphical control of simulation
Parallel Scaling

- *≈ 3 (1999):* Parallelization based on DDD, strongly limited parallelization ($\leq 4096$ cores)

- *≈ 4 (2014):* Parallelization based on PCL, perfect scaling up to $264\,144$ cores.
UG4: GMG Weak Scaling

- Laplacian 3d, GMG, structured

![Graph showing wall clock time in seconds for different numbers of processors (1, 8, 64, 512, 4.096, 32.768, 262.144). The graph compares total time, assembly time, and solver time. The total time remains relatively constant across different numbers of processors.]
Weak Scaling UG4

- Linear elasticity 3d uniform

<table>
<thead>
<tr>
<th>PE</th>
<th>level</th>
<th>DoF</th>
<th>$T_a(s)$</th>
<th>$T_s(s)$</th>
<th>$T_{a+s}(s)$</th>
<th>$E_{a+s}$(%)</th>
<th>$S_{a+s}$</th>
<th>$S_{ideal}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>14’739</td>
<td>2.347</td>
<td>4.987</td>
<td>7.334</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>8</td>
<td>4</td>
<td>107’811</td>
<td>2.352</td>
<td>5.070</td>
<td>7.422</td>
<td>98.8</td>
<td>7.9</td>
<td>8</td>
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<tr>
<td>64</td>
<td>5</td>
<td>823’875</td>
<td>2.368</td>
<td>5.212</td>
<td>7.580</td>
<td>96.8</td>
<td>62.0</td>
<td>64</td>
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<tr>
<td>512</td>
<td>6</td>
<td>6’440’067</td>
<td>2.375</td>
<td>5.414</td>
<td>7.789</td>
<td>94.2</td>
<td>482.3</td>
<td>512</td>
</tr>
<tr>
<td>4’096</td>
<td>7</td>
<td>50’923’779</td>
<td>2.400</td>
<td>5.502</td>
<td>7.902</td>
<td>92.8</td>
<td>3’801.1</td>
<td>4’096</td>
</tr>
<tr>
<td>32’768</td>
<td>8</td>
<td>405’017’091</td>
<td>2.371</td>
<td>5.711</td>
<td>8.082</td>
<td>90.7</td>
<td>29’720.6</td>
<td>32’768</td>
</tr>
<tr>
<td>262’144</td>
<td>9</td>
<td>3’230’671’875</td>
<td>2.391</td>
<td>5.816</td>
<td>8.207</td>
<td>89.4</td>
<td>234’356.7</td>
<td>262’144</td>
</tr>
</tbody>
</table>

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MODELING AND COMPUTATION OF THERMOHALINE FLOW IN HETEROGENEOUS POROUS MEDIA

S. Stichel, A. Grillo, M. Lampe, D. Logaschenko, S. Reiter, A Vogel, G. Wittum
in cooperation with S. Attinger, E. Fein, W. Kinzelbach, A. Schneider

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Density Driven Groundwater Flow

- Saltwater intrusion
- Upconing
- Flow around saltdomes
\[ \frac{\partial (n \rho(c))}{\partial t} + \nabla \cdot (\rho(c)\vec{v}) = Q_p(c), \]

\[ \frac{\partial (n \rho(c)c)}{\partial t} + \nabla \cdot (\rho(c)(c\vec{v} - D\nabla c)) = Q_c(c) \]

\[ + \text{ b.c.; with } \quad \vec{v} = -\frac{K}{\mu(c)}(\nabla p - \rho(c)\vec{g}), \]

\[ D(\vec{v}) := D_m \mathbb{I} + \alpha_t |\vec{v}| \mathbb{I} + (\alpha_t - \alpha_f) \frac{|\vec{v}|}{|\vec{v}|}, \]

\[ \frac{1}{\rho} := \left(1 - \frac{c}{c_{\text{max}}} \right) \frac{1}{\rho_f} + \frac{c}{c_{\text{max}} \rho_s} \]

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D³F

- complicated domains w. unstructured grids (UG)
D³F

- Full density dependent non-linear dispersion
- fully parallel adaptive
D³F Parallel Efficiency

- Uniform refinement
  weak scaling

- Adaptive refinement
  weak scaling

<table>
<thead>
<tr>
<th>$P$</th>
<th>$h$</th>
<th>UKN</th>
<th>NIT[#]</th>
<th>TIT[s]</th>
<th>$S_S$[#]</th>
<th>$E_S$</th>
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<td>45.83</td>
<td>5.4</td>
<td>0.67</td>
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<tr>
<td>64</td>
<td>1/32</td>
<td>8.414.978</td>
<td>35</td>
<td>54.12</td>
<td>24</td>
<td>0.37</td>
</tr>
<tr>
<td>512</td>
<td>1/64</td>
<td>66.602.498</td>
<td>22</td>
<td>58.54</td>
<td>282</td>
<td>0.55</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>$h$</th>
<th>UKN</th>
<th>TNLS[s]</th>
<th>TADAPT[s]</th>
<th>TLB[s]</th>
<th>TMIG[s]</th>
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<td>21.016</td>
<td>52.3</td>
<td>1.93</td>
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<td>1/32</td>
<td>102.280</td>
<td>224.</td>
<td>13.2</td>
<td>3.99</td>
<td>13.2</td>
</tr>
<tr>
<td>1/32</td>
<td>433.908</td>
<td>657.</td>
<td>44.6</td>
<td>11.2</td>
<td>41.8</td>
</tr>
<tr>
<td>1/64</td>
<td>1.750.708</td>
<td>2708.</td>
<td>160.</td>
<td>27.9</td>
<td>108.</td>
</tr>
</tbody>
</table>

Weak Scaling UG4

- Thermohaline flow in porous media, 2d Elder problem

\[
\begin{array}{cccccccccccc}
pe & L & DoFs & N_{iter} & T_{ass} & E_{ass} & T_{init} & E_{init} & T_{gmg} & E_{gmg} & T_{all} & E_{all} \\
32 & 8 & 2.102.274 & 11 & 6,15 & - & 4,93 & - & 8,62 & - & 37,96 & - \\
512 & 10 & 33.574.914 & 11 & 6,11 & 100,7 & 4,97 & 99,2 & 9,31 & 92,6 & 39,37 & 96,4 \\
2.048 & 11 & 134.258.690 & 11 & 6,18 & 99,5 & 5,09 & 96,9 & 9,45 & 91,2 & 40,18 & 94,5 \\
8.192 & 12 & 536.952.834 & 11 & 6,13 & 100,3 & 5,03 & 98,0 & 9,96 & 86,6 & 41,11 & 92,3 \\
32.768 & 13 & 2.147.647.490 & 10 & 6,17 & 99,6 & 6,22 & 79,3 & 10,84 & 79,6 & 48,45 & 78,3 \\
131.072 & 14 & 8.590.262.274 & 10 & 6,10 & 100,7 & 5,99 & 82,3 & 10,66 & 80,9 & 53,37 & 71,1 \\
\end{array}
\]

Table 5.6: Weak scaling study for porous medium flow on Juqueen.

- $T$: runtime [s], $E$: efficiency [%], $pe$: processes, $e$: grid level, $DoFs$: degrees of freedom, $N_{iter}$: multigrid iterations.
Thermohaline Flows

- Solving

\[
\phi_f \frac{\partial \hat{\rho}_f}{\partial t} + \nabla \cdot (\hat{\rho}_f \mathbf{q}_f) = 0,
\]

\[
\phi_f \frac{\partial (\hat{\rho}_f \omega_s)}{\partial t} + \nabla \cdot (\hat{\rho}_f \omega_s \mathbf{q}_f + \mathbf{J}_d) = 0,
\]

\[
\phi_f \hat{\rho}_f \Theta \frac{D_f \hat{S}_f}{Dt} + (1 - \phi_f) \rho_r \Theta \frac{\partial \hat{S}_r}{\partial t} + \nabla \cdot (\mathbf{J}_T - \hat{\mu}_{sw} \mathbf{J}_d) = 0,
\]

with \( \mathbf{q}_f = -\frac{k}{\nu_f} (\nabla p - \rho_f g) \) (Onsager)

\[
\mathbf{J}_d = -\phi_f \rho_f D \nabla \omega_s - \phi_f \rho_f D \frac{k_p}{p} \nabla p - \phi_f \rho_f D S \omega_s (1 - \omega_s) \nabla \Theta,
\]

\[
\mathbf{J}_T = -\phi_f \rho_f D Q \nabla \omega_s - \phi_f \rho_f D Q \frac{k_p}{p} \nabla p - \left[ L_{TT} - \phi_f \rho_f \frac{D Q h_{sw}}{\Theta \partial \hat{\mu}_{sw} / \partial \omega_s} \right] \nabla \Theta.
\]
Solving

\[ \phi_f \frac{\partial \hat{\rho}_f}{\partial t} + \nabla \cdot (\hat{\rho}_f \mathbf{q}_f) = 0, \]

\[ \phi_f \frac{\partial (\hat{\rho}_f \omega_s)}{\partial t} + \nabla \cdot (\hat{\rho}_f \omega_s \mathbf{q}_f + \mathbf{J}_d) = 0, \]

\[ \phi_f \hat{\rho}_f \Theta \frac{D_f S_f}{D_t} + (1 - \phi_f) \rho_r \Theta \frac{\partial S_r}{\partial t} + \nabla \cdot (\mathbf{J}_T - \hat{\mu}_{sw} \mathbf{J}_d) = 0, \]

---

THERMOHALINE FLOWS

• opposite effects of temperature and salt concentration

Temperature $\uparrow$

salt water $\downarrow$

• connection of mass flux with temperature gradient (Ludwig–Soret effect)

• connection of heat flux with concentration gradient (Dufour effect)
Example

- Moving parcel, benchmark problem from Oldenburg, Pruess, 1999 (2d)
Thermohaline Flows

- Dufour effect – negative buoyancy
THERMOHALINE FLOWS

- Ludwig effect – positive buoyancy
**GRID DEPENDENCE**

Symmetry breaking due to grid refinement  
The number of fingers depends on grid size and time.
FRACTURED MEDIA

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FRACTURED MEDIA

- Low dimensional formulation
  Multiphase flow
  R. Helmig; O. Kolditz; V. Reichenberger; ...

- Multiscale modeling and numerics:
  Dynamic coupling between micro and macroscales
Flow in Fractured Media

- low dimensional <-> full dimensional

Representation of fractures:

1. Polyhedral faces + pointwise thickness
2. expand to volume

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Fracture Extrusion in 3D

Extrusion of a triangle and a quadrilateral.

Extrusion of a 2d fractured geometry.
Left: 2d source, Middle: boundary surfaces, Right: Volume geometry.
Created with ProMesh3.

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Flow in Fractured Media

- Grid follows the anisotropic direction rectangularly

![Image](image_url)

successful treatment of anisotropy possible: ARTE

Fuchs, W., 2003, Feuchter, 2007
Low Dimensional Model

- Density driven flow model
  average across fracture

\[ \langle F \rangle(t, x, y) := \frac{1}{\epsilon} \int_{-\epsilon/2}^{\epsilon/2} F(t, x, y, z) dz. \]

+ transmission conditions

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TRANSMISSION CONDITIONS

- Full dimensional:

Continuity of normal fluxes

\[-\rho(c_f) \frac{K_f}{\mu} \left( \frac{\partial p_f}{\partial n} - \rho(c_f)g_n \right) = -\rho(c_m) \frac{K_m}{\mu} \left( \frac{\partial p_m}{\partial n} - \rho(c_m)g_n \right)\]

\[-D_f \left(1 - \frac{\rho'}{\rho_p c_f}\right) \frac{\partial c_f}{\partial n} = -D_m \left(1 - \frac{\rho'}{\rho_p c_m}\right) \frac{\partial c_m}{\partial n}.\]

Continuity of pressure and concentration

\[p_f = p_m, \quad \text{and} \quad c_f = c_m\]
Transmission Conditions (Grillo)

- Low dimensional

the auxiliary vector fields

\[ Q_\alpha := \rho^{pW} q_\alpha - \rho' J_\alpha, \quad \text{and} \quad P_\alpha := c_\alpha q_\alpha + J_\alpha; \]

with

\[ q_\alpha = -\frac{K_\alpha}{\mu} [\nabla p_\alpha - \rho_\alpha(c_\alpha) g], \]

\[ J_\alpha = -\left(\frac{\rho^{pW}}{\rho^{pW} + \rho' c_\alpha} D_\alpha\right) \nabla c_\alpha \]

are continuous across the fracture interfaces

\[ Q_{fn}^{(k)} = Q_{mn}^{(k)}, \quad \text{and} \quad P_{fn}^{(k)} = P_{mn}^{(k)} \]

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Lower Dim. Representation

\[
\begin{align*}
\frac{\partial (\phi \Sigma \rho_f c_f)}{\partial t} + \nabla \Sigma \cdot (\rho_f c_f q_{\Sigma} - \rho_f D_{\Sigma} \nabla \Sigma c_f) + \frac{1}{\epsilon} (\rho_f c_m q_{\perp} - \rho_f D_{\perp} \delta c_m)|^a_b = 0 \\
\frac{\partial (\phi \Sigma \rho_f)}{\partial t} + \nabla \Sigma \cdot (\rho_f q_{\Sigma}) + \frac{1}{\epsilon} (\rho_f q_{\perp})|^a_b = 0
\end{align*}
\]

\[
q_{\Sigma} = -\frac{K_{\Sigma}}{\mu_f} (\nabla \Sigma p_f - \rho_f g_{\Sigma})
\]

\[
q_{\perp} = -\frac{K_{\perp}}{\mu_f} (\delta p - \rho_f g_{\perp})
\]

\[
(\delta c_m)|_a := \frac{c_a - c_f}{\epsilon/2}, \quad (\delta p)|_a := \frac{p_a - p_f}{\epsilon/2}
\]
**Henry’s Problem (2D)**

Intrusion of saltwater into freshwater aquifer

\[
\frac{\partial c}{\partial n} = 0 , \quad \frac{\partial p}{\partial n} = 0
\]

\[
c = 0 \quad \text{in} \quad \frac{\partial c}{\partial n} = 0 , \quad \frac{\partial p}{\partial n} = 0
\]

\[
c = 1 \quad \text{on} \quad \frac{\partial c}{\partial n} = 0 , \quad \frac{\partial p}{\partial n} = 0
\]

Parameters in fracture: \( \phi_\Sigma = 2\phi_m , \quad K_\Sigma = 10^3 \cdot K_m \)
Henry’s Problem

- Parameters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Quantity</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_d$</td>
<td>Diffusion coefficient</td>
<td>$18.8571 \cdot 10^{-6}$</td>
<td>$[m^2 s^{-1}]$</td>
</tr>
<tr>
<td>$D_m = \phi_m D_d$</td>
<td>Diffusion coefficient in the medium</td>
<td>$6.6 \cdot 10^{-6}$</td>
<td>$[m^2 s^{-1}]$</td>
</tr>
<tr>
<td>$D_f = \phi_f D_d$</td>
<td>Diffusion coefficient in the fracture</td>
<td>$13.2 \cdot 10^{-6}$</td>
<td>$[m^2 s^{-1}]$</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravity</td>
<td>$9.81$</td>
<td>$[m s^{-2}]$</td>
</tr>
<tr>
<td>$K_m$</td>
<td>Permeability of the medium</td>
<td>$1.019368 \cdot 10^{-9}$</td>
<td>$[m^2]$</td>
</tr>
<tr>
<td>$K_f$</td>
<td>Permeability of the fracture</td>
<td>$1.019368 \cdot 10^{-5}$</td>
<td>$[m^2]$</td>
</tr>
<tr>
<td>$\phi_m$</td>
<td>Porosity of the medium</td>
<td>$0.35$</td>
<td>$-$</td>
</tr>
<tr>
<td>$\phi_f$</td>
<td>Porosity of the fracture</td>
<td>$0.7$</td>
<td>$-$</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Viscosity</td>
<td>$10^{-3}$</td>
<td>$[kg m^{-1} s^{-1}]$</td>
</tr>
<tr>
<td>$\rho_w$</td>
<td>Density of water</td>
<td>$1 \cdot 10^3$</td>
<td>$[kg m^{-3}]$</td>
</tr>
<tr>
<td>$\rho_s$</td>
<td>Density of brine</td>
<td>$1.025 \cdot 10^3$</td>
<td>$[kg m^{-3}]$</td>
</tr>
<tr>
<td>$a_{t\alpha}$</td>
<td>Transversal dispersivity length</td>
<td>$0$</td>
<td>$[m]$</td>
</tr>
<tr>
<td>$a_{l\alpha}$</td>
<td>Longitudinal dispersivity length</td>
<td>$0$</td>
<td>$[m]$</td>
</tr>
</tbody>
</table>

The main results of Henry’s problem in the absence of fractures were summarized for examples in [x6]. Three main factors can be recognized. Since the incoming brine is heavier than pure waters it tends to “fall” down and occupy the lower part of the domain. This alters the initial density of freshwaters and generates a density-driven flow. This is a nontpotential flow characterized by the presence of vortices due to the inhomogeneity of the fluid phase mass density. In the presence of fractures vortices are also generated by the discontinuity of the permeability field in the domain. Both the flow and the concentration profile are strongly affected for fixed values of physical parameters by the geometrical properties and the location of the fractures. In order to investigate these effects we propose the following four numerical experiments that were computed for both the full and the equivalent low-dimensional case:

- Thin fracture placed at $z = 0.5$ m (cf. Fig. 4).

The fundamental result is that the velocity in the fracture produces a deflection of the concentration isolines. The deflection is maximal when the right end of the fracture (sea side) is approached. We observed that the magnitude and the direction of the velocity in the fracture hinders the spreading of the brine in the fracture. This occurs because of the...
Henry's Problem w. Fracture

\[ \varepsilon = 3 \, \text{mm}, \, T = 5 \, \text{h} \]

- full dim. rep.
- low dim. rep.

\[ x = 1.5 \, \text{m} \]
HENRY’S PROBLEM W. FRACTURE

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HENRY'S PROBLEM W. FRACTURE

\[ \varepsilon = 24 \text{ mm}, \ T = 5h \]

full dim. rep.  

low dim. rep.  

\[ x = 1.5m \]

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COMPARISON D-1 AND D DIM

averaged \( c \)

\[ \epsilon = 0.006 \text{ fixed} \]

\[ K_f = 10^{-6} \text{ fixed} \]
Rotational Flow

\[ |\nabla \times \mathbf{q}| \]

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THIN FRACTURE

$\varepsilon = 0.006$

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Rotational Flow

$\varepsilon = 0.024$
Vorticity

\[ \omega = \nabla \times \mathbf{q} = \frac{\rho'K}{\mu} \nabla c \times \mathbf{g} \]

with \[ \mathbf{q} = -\frac{K}{\mu} (\nabla p - \rho \mathbf{g}) \]

and \[ \rho_\alpha(c_\alpha) = \rho^{pW} + \rho' c_\alpha, \]

Vorticity is maximum, if the concentration gradient is perpendicular to gravity (i.e. isolines are parallel)
Henry in 3D

\[ \omega = 0 \]
\[ q_x = 3.3 \cdot 10^{-6} \text{ m s}^{-1} \]
\[ \partial_n \omega = 0 \quad q_n = 0 \]
\[ \omega = 1 \]
\[ p = (-10055.25z) \text{ Pa} \]
3D

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Comparison 3d

d-dim.

(d-1)  
-dim.

\[ \varepsilon = 0.003 \quad \varepsilon = 0.024 \]

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PROFILE

Full dimensional
$\epsilon = 0.024$
Observations

- For very thin fractures a low dim. model suffices
- In wider fractures, rotational flow can occur
FLOW CHARACTERIZATION

\[ \theta_f := \frac{|q_f|}{|q_{rot}|} \quad q_{rot} := \frac{\epsilon}{2} \frac{K_f}{K_m} \frac{\omega_f}{\omega_\theta} (\nabla \times q_f) \]

\( q_{rot} \) rotational flow velocity
\( \theta_f \) is dimensionless, characterizes flow
\[ |q_f| > |q_{rot}| \] rotational flow can be neglected
\[ \theta_\mathcal{F} := \max_{\mathcal{F}} \{\theta_f\} \]

\[ \theta_\mathcal{F} < 1 - \delta \quad \text{d-dimensional} \]
\[ \theta_\mathcal{F} > 1 + \delta \quad (d - 1)\text{-dimensional} \]
CRITERION

\[ \theta = \frac{\epsilon |\omega_f|}{\|v_\theta\|} \frac{K_f}{K_m} \frac{c_f}{c_\theta} \]

max \( \theta > \theta_0 \) \implies \text{full dimensional}

max \( \theta \leq \theta_0 \) \implies \text{low dimensional}
Dimensional Adaptivity

- The fracture representation is adapted during the computation
- Full-dimensional resolution is used only, if necessary
- We need:
  - 2 grids (low and full dimensional)
  - Transfer operators between these grids
  - Criterion, when to use which formulation
TRANSFER OPERATORS

„Full -> Low“:
• Copy values on the interface (p corrected)
• Value on the interface is mean value across the fracture

„Low -> Full“:
• We assume quadratic behaviour of the function in the fracture. Values on the interface with corrected p and mean values are given.
Transfer Operators

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DIMENSIONAL ADAPTIVITY

$\varepsilon = 0.006$

Massenbruch $\omega$

Zeit $t$ [min]

- d-dim.
- (d-1)-dim.
- dim.-adaptiv

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Dimensional Adaptivity

\( \epsilon = 0.024 \)

Sprung Massenbruch \((\omega_2 - \omega_1)\)

Zeit \(t\) [min]
Comparison in 3d

\[ \epsilon = 0.003 \]

\[ c \]

\[ cl - cu \]
Comparison in 3d

\[ \epsilon = 0.024 \]

\[ \begin{array}{c}
\text{Massenbruch} \\
\text{d-dimensional} \\
\text{(d-1)-dimensional}
\end{array} \]

\[ \begin{array}{c}
\text{Sprung Massenbruch} \\
\text{d-dimensional} \\
\text{(d-1)-dimensional}
\end{array} \]
Test Example

- Variation of
  - Thickness and length of fracture
  - Angle with gravity
  - Parameters (Conductivity,...)
  - Boundary conditions
Test Example

- 3 simulation runs for each configuration:
  - d-dimensional
  - (d-1)-dimensional
  - dimensional-adaptive

- Comparison of results:
  - d-dim. is reference solution
  - max. rel. error
Test Example: Results

Relativer Fehler $E$ (d−1)-dim. \( \text{dim.adaptiv} \)

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### Test Example: Results

<table>
<thead>
<tr>
<th></th>
<th>( \frac{E_{\text{rel}}(\omega_f)}{(d-1)\text{-dim.}} )</th>
<th>( \frac{E_{\text{rel}}(\omega_m^{(2)} - \omega_m^{(1)})}{\text{dim.-adaptiv}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum</td>
<td>( \max_{i=1, \ldots, N} E_i ) \quad 87 \quad 31 \quad &gt; 100 \quad 76</td>
<td></td>
</tr>
<tr>
<td>Mean value</td>
<td>( \bar{E} = \frac{1}{N} \sum_{i=1}^{N} E_i ) \quad 12 \quad 2 \quad 24 \quad 4</td>
<td></td>
</tr>
<tr>
<td>Mean dev.</td>
<td>( \frac{1}{N} \sum_{i=1}^{N}</td>
<td>E_i - \bar{E}</td>
</tr>
<tr>
<td>0.75-Quantil</td>
<td>( F^{-1}(0.75) ) \quad 16 \quad 1 \quad 0 \quad 0</td>
<td></td>
</tr>
<tr>
<td>0.9-Quantil</td>
<td>( F^{-1}(0.9) ) \quad 34 \quad 5 \quad 28 \quad 3</td>
<td></td>
</tr>
</tbody>
</table>

Statistics of \( N = 1261 \) test problems
Comparison in 3d

\[
\epsilon = 0.024
\]

\[c\]

\[c_l - c_u\]

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Results Criterion

\[ \theta_f \]

Zeit \( t \) [min]

\( \epsilon=0.024 \text{ m} \)
\( \epsilon=0.003 \text{ m} \)

\[ (d-1)\text{-dim.} \]

\[ d\text{-dim.} \]
Selected Publications


Transdermal Drug Delivery


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Skin Anatomy

Primary Barrier: Stratum Corneum (SC)

Goals:
• Characterize Barrier (Permeability, Lag Time)
• Prediction of behavior in an exposure scenario
Aims

• Quantitative understanding of diffusion through stratum corneum and of permeation pathways
• Influence of corneocyte permeability
• Are corneocytes permeable?
• Influence of layer offset
• Deriving reduced models
Detailed SC Models

Brick-and-mortar: Ribbon (2D), Cuboid (3D)
(Heisig et al, 1996; Wang et al., 2006; Rim et al., 2007; ...)

Cell-like morphology: Tetrakaidekahedra (3D)
(Feuchter et al., 2006)

Micrograph of mouse ear SC

Gabriel Wittum
AMCS, CEMSE, KAUST
G-CSC, University of Frankfurt
Grid Problem

• highly anisotropic (aspect ratio: 150/1)
• => large approximation error
• remedy:
• anisotropic (“blue”) refinement! (Kornhuber, 1990)
2d Brick and Mortar
Base Grid

Gridlines follow jumps of coefficients
Grid Problem

- highly anisotropic (aspect ratio: 150/1)
- => large approximation error
- remedy:
- anisotropic ("blue") refinement! (Kornhuber, 1990)
Geometry Models

• 3d Cuboid Model

Cuboid modeller (C. Wagner, 2007)
Tetrakaidekahedron (TKD)
Geometry Models

- 3d Tetrakaidekahedral Model

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G-CSC, University of Frankfurt
Tetrakaidekahedra Model

• Basic Element:
  • Tetrakaidekahedron (14 faces)
Cluster of TKDs

- 3d Tetrakaidekahedra Model

Dirk Feuchter

Gabriel Wittum
AMCS, CEMSE, KAUST
G-CSC, University of Frankfurt
Tetrakaidekahedra Model

- Theory of densest packing (Kepler 1611)
- What space-filling arrangement of regular polyhedra has minimal surface area?
- W. Thompson (Kelvin) 1885: Tetrakaidekahedron
TKD for cells in tissue

- Cells fill tissue => polyhedral form except for special functions (neuron, hepatocyte, …)
- Cell membrane is from lipid bilayers, a special material quite costly for the cell => surface minization
Tetrakaidekahedra Model

- Flattening of Corneocytes
Tetrakaidekahedra Model

Dirk Feuchter

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Process Model: Diffusion

\[
\frac{\partial c(x, t)}{\partial t} = \nabla^T \cdot (D(x)\nabla c(x, t)) \quad \text{in } \Omega \subset \mathbb{R}^d
\]

with \(D(x) = \begin{cases} 
D_{\text{Lip}}(x) & \text{for } x \in \text{Lipid} . \\
D_{\text{Cor}}(x) & \text{for } x \in \text{Corneocyte} . 
\end{cases}\)
Process Model: Diffusion

Boundary and initial conditions

$$\frac{\partial c(x, t)}{\partial \vec{n}} = 0 \text{ on } \partial \Omega_l, \partial \Omega_r$$

and $c(x, t) = \begin{cases} 0 & \text{for } x \in \Omega_u \\ 1 & \text{for } x \in \Omega_o \end{cases}$

Transmission conditions on internal interfaces

$$D_{Lip} \nabla c_{Lip}(x, t) \cdot \vec{n} = D_{Cor} \nabla c_{Cor}(x, t) \cdot \vec{n}$$

$$K_{Cor/Lip} c_{Lip}(x, t) \bigg|_{n-} = c_{Cor}(x, t) \bigg|_{n+}$$

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Simulation Results $T = T_\infty / 3$

$\varepsilon = 10^{-4}$

$\varepsilon = 10^{-6}$
Simulation Results $T = 2T_\infty/3$

\[ \varepsilon = 10^{-4} \]

\[ \varepsilon = 10^{-6} \]

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Simulation Results $T = T_\infty$

$\varepsilon = 10^{-4}$

$\varepsilon = 10^{-6}$
Characterization

- Flux across upper boundary

\[ F_{\Gamma_0}(t) = \int_{\mathcal{T}_0} D \frac{du}{dt} d\sigma = f_\infty + \sum_j \alpha_j e^{-\lambda_j t} \]

- Mass transported across upper boundary

\[ M_{\Gamma_0}(T') = \int_0^T F_{\Gamma_0}(t) dt = f_\infty T + m_0 + \sum_j \beta_j e^{-\lambda_j t} \]
Experiment (schematic)
Characterization Lag Time
Analytical Solutions

1. $\varepsilon = 1$ (homogeneous membrane): $T_{\text{lag}} = 20 \text{ sec}$
2. $\varepsilon = 0$ (impermeable corneocytes): $T_{\text{lag}} \approx 1 \text{ h}$

$$T_{\text{lag},\infty} = \frac{L^2}{6D}$$
Computed Lag Times

$K_{\text{cor/lip}} = 1$

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Computed Lag Times

\[ K_{\text{cor/lip}} = 1 \]

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$T_{\text{lag}}$ vs. $\varepsilon$ and $K_{\text{cor/lip}}$
$T_{\text{lag}}$ vs. $\varepsilon$ and $\omega$
Simulation: 2D Brick Model


- Intra cellular pathways matter
- Nearly optimum barrier design,
- Robust w.r.t. insensitivity against shift and corneocyte permeability.

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Simulation: 2D Brick Model


- Intra cellular pathways matter
- Nearly optimum barrier design,
- Robust w.r.t. insensitivity against shift and corneocyte permeability.
- Experimentally confirmed in 2003!

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Tetrakaidekahedra based model

\[ \partial_t (Ku) + \partial_x [-DK \partial_x u] = 0 \]

Transport equation
(w/ diffusion and partition coefficients)

Morphology & Process = Effect

Corneocyte sponge effect

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Weak Scaling UG4

- Robust GMG solver for skin problem (transdermal drug delivery)

![Graph showing wall clock time vs. number of processes for Assembly, Solver, and Total.]

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Weak Scaling UG4

- Robust GMG solver for transdermal drug delivery problem (JuQueen)
  > $10^9$ unknowns

**Graph:**
- **Assembly**
- **Solver**
- **Total**

**Axes:**
- Wall clock time [s]
- #Procs

**Legend:**
- Gabriel Wittum
- ECRC, CEMSE, KAUST
- G-CSC, University of Frankfurt
Skin Problem: TKD

- Base solver UG4: Parallel adaptive multigrid
  - acceleration from $10^2$ to $10^6$ by adaptivity
Parallel Adaptivity

- Base solver UG4: Parallel adaptive mg
  - acceleration by 512 by adaptivity

- Importance of adaptivity increases with problem size!

Resolution [nm]
uniform 25,91
adaptive 2,70

uniform L13: 33,554,432 cores
adaptive L13: 65536 cores
factor 512 (99.5%) in computational resources and power consumpt.

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Parallel Adaptivity

- Key strategy for
  - saving CPU time (99.5%),
  - saving power (99.5%),
  - improving accuracy
    (uniform needs 3 more levels to reach same error)

- Higher order effect without additional smoothness

- Importance of adaptivity increases with problem size!

- Multi-scale modeling necessary.

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Thank you!

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