Parallel Adaptive Simulation of Processes from Science and Engineering

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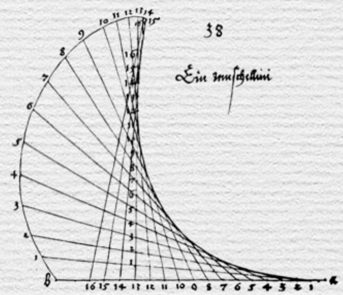
Presentation on ADVCOMP, IARIA Oct 2021

IARIA



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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.

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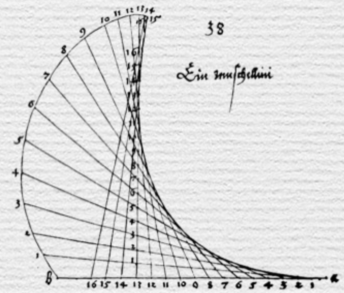

The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.

P.A.M. Dirac (1927)

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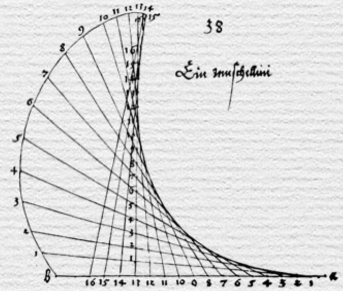

Modelling Basics

- Morphology model
  - Geometry
  - Material properties
- Process model

based on first principles (balance laws)

➡ reliable model with prognostic quality

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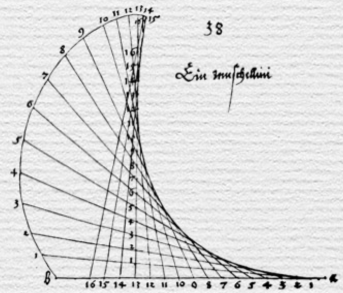

Modelling Basics

- 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 <–> Reliability
- Simulation technique is decisive for the complexity limit

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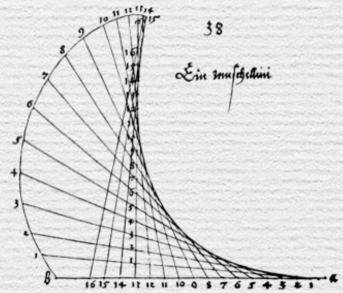

Modeling and Simulation

Mathematical Model
System of differential equations

Applications, Mathematics (Analysis)

Numerical approximation
Numerical methods
discretisation and solver

Numerics

Software Tools

Computer Science

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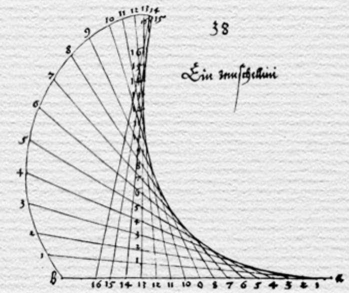

Modeling and Simulation

Mathematical Model
System of differential equations

Numerical approximation
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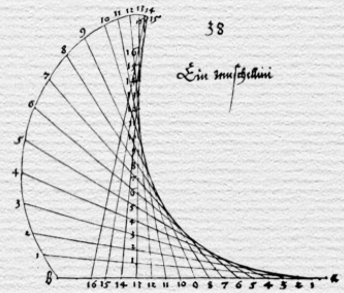
discretisation and solver

Software Tools

Applications,
Mathematics (Analysis)

Numerics

Computer Science



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Modeling and Simulation

Mathematical Model
System of differential equations

Mapping Reality

Numerical approximation
Numerical methods
discretisation and solver

Errors,
Complexity

Software Tools

Complexity,
Flexibility, ...

Hardware

Limiting Resource

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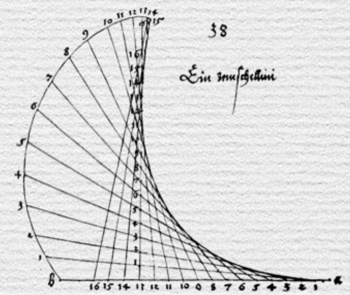
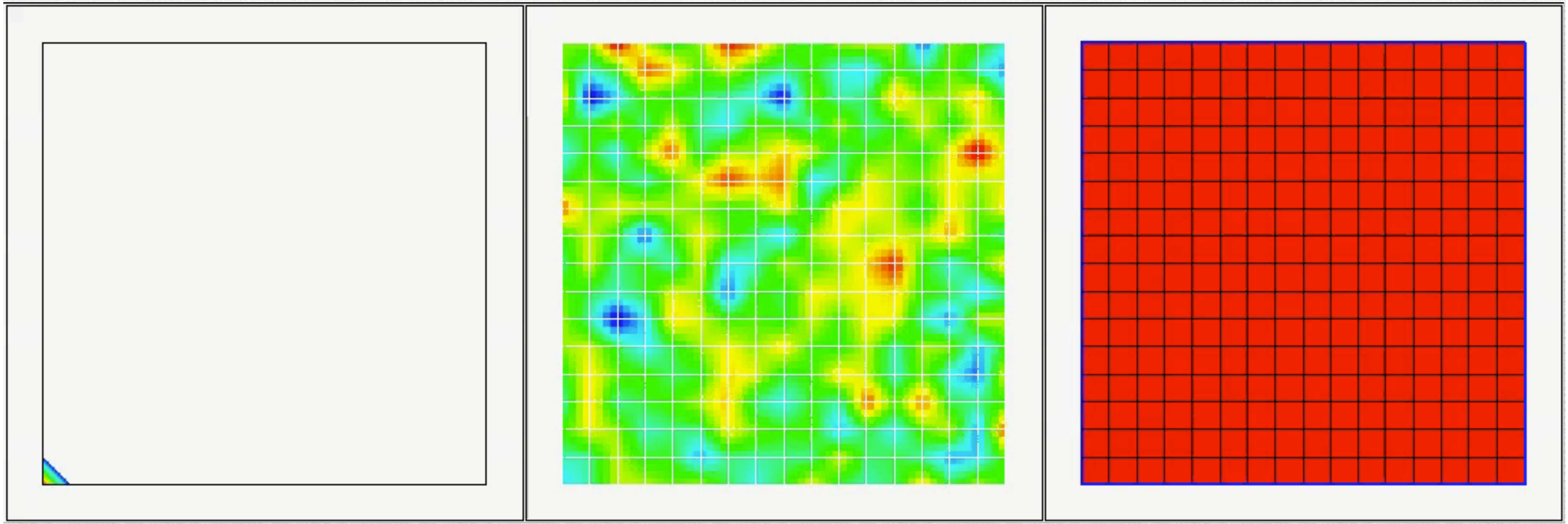
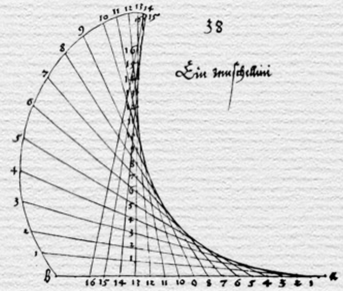


Adaptivity

- Refine grid where needed



Stefan Lang



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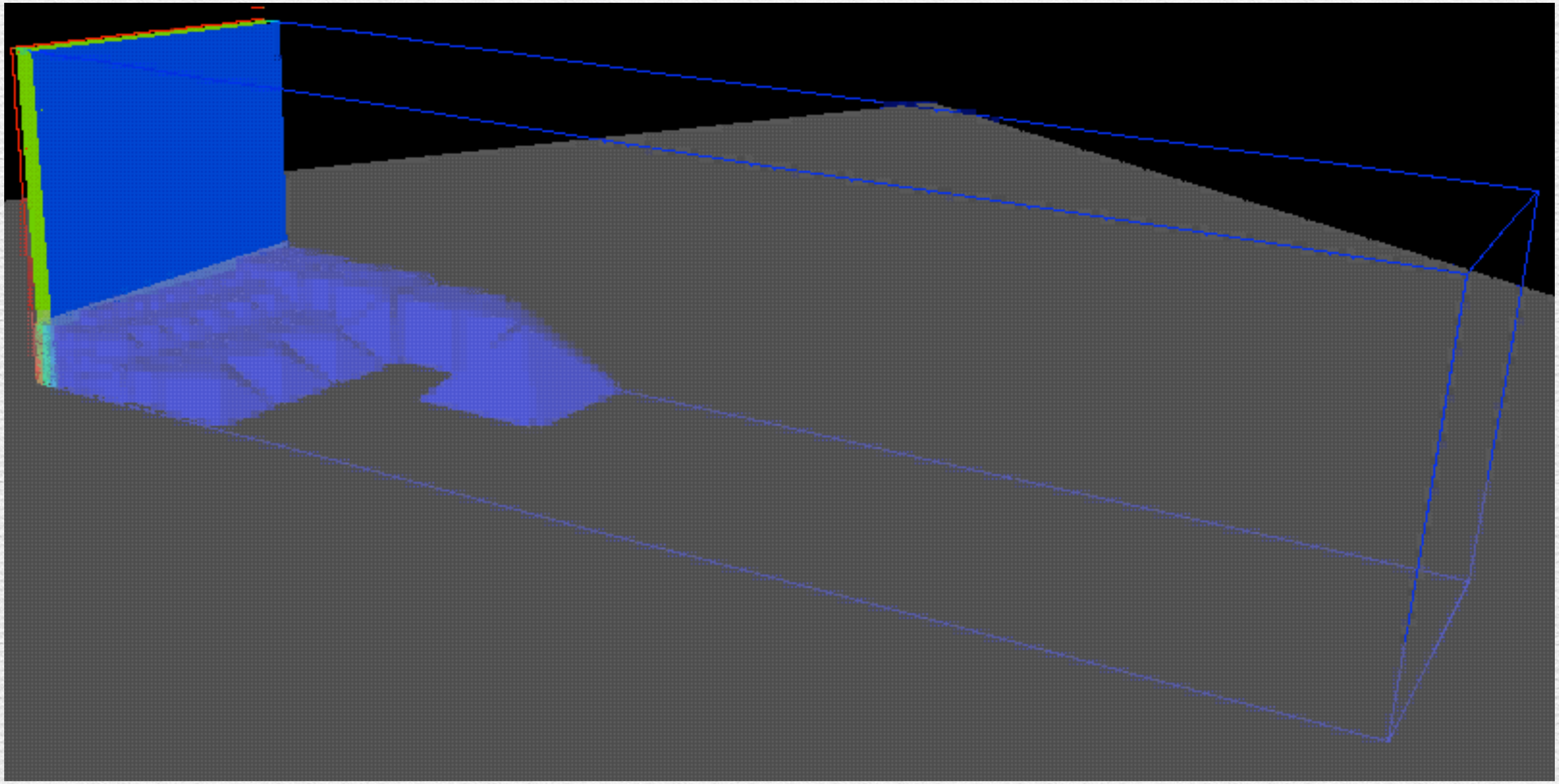
Adptivity 3d



Peter Bastian

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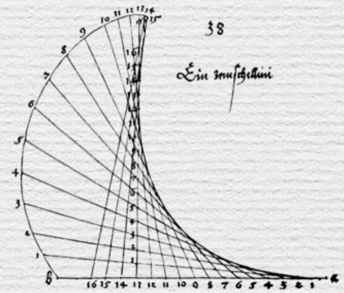

Complexity - HPC Paradoxon

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

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

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

Large scale computing needs q=1 i.e. optimal algorithms!

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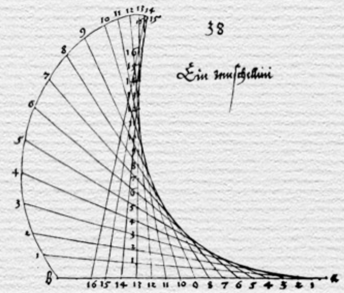

Simulation System UG4

Adaptivity

Parallelism

Multigrid

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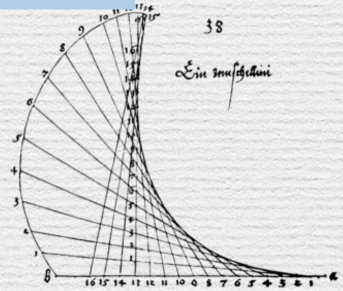
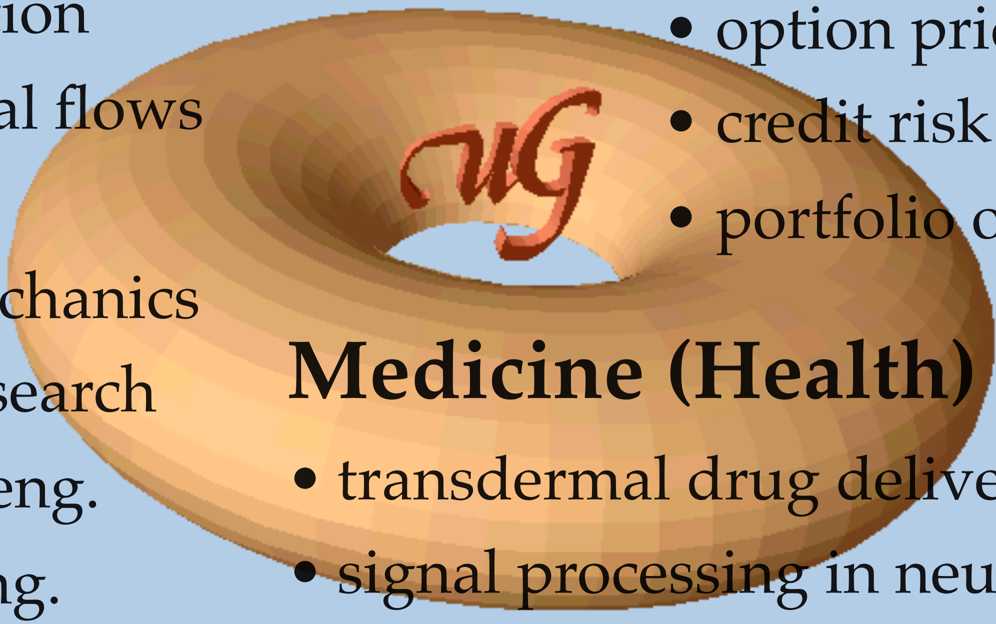


Simulation System UG4

Engineering

- porous media flow
- CO_2 injection
- geothermal flows
- CFD
- struct. mechanics
- energy research
- chemical eng.
- process eng.
- biomass ferment.
- aeroacoustics



Finance

- option pricing
- credit risk estimation
- portfolio optimization

Medicine (Health)

- transdermal drug delivery
- signal processing in neurons
- HC virus replication
- infectious diseases

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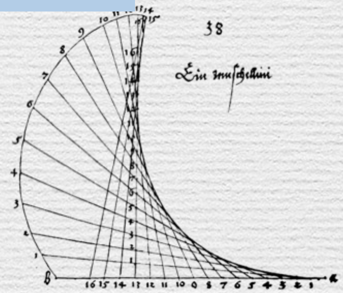

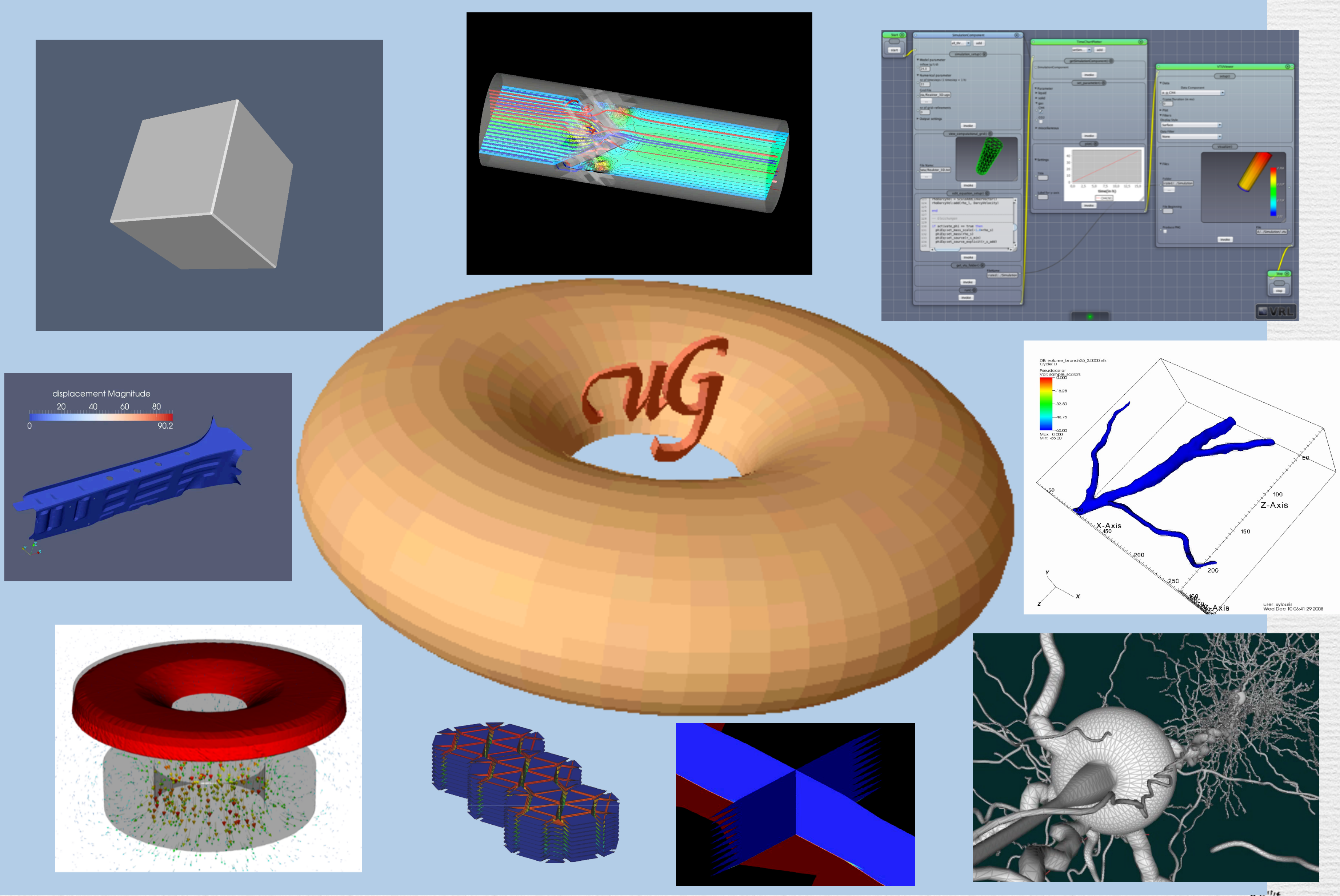

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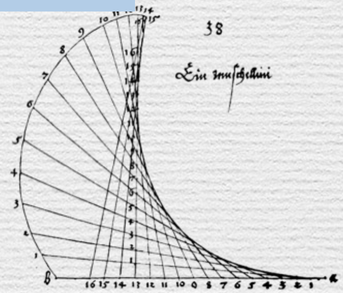

uG 4 DEVELOPERS

New code *uG* 4

≈ 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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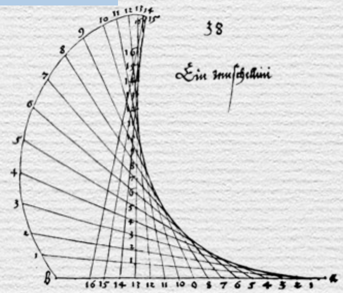

uG4 I. Heppner, A. Nägel, S. Reiter, M. Rupp, A. Vogel

- 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

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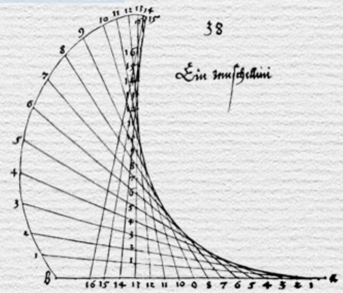
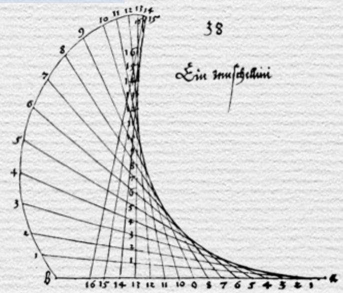


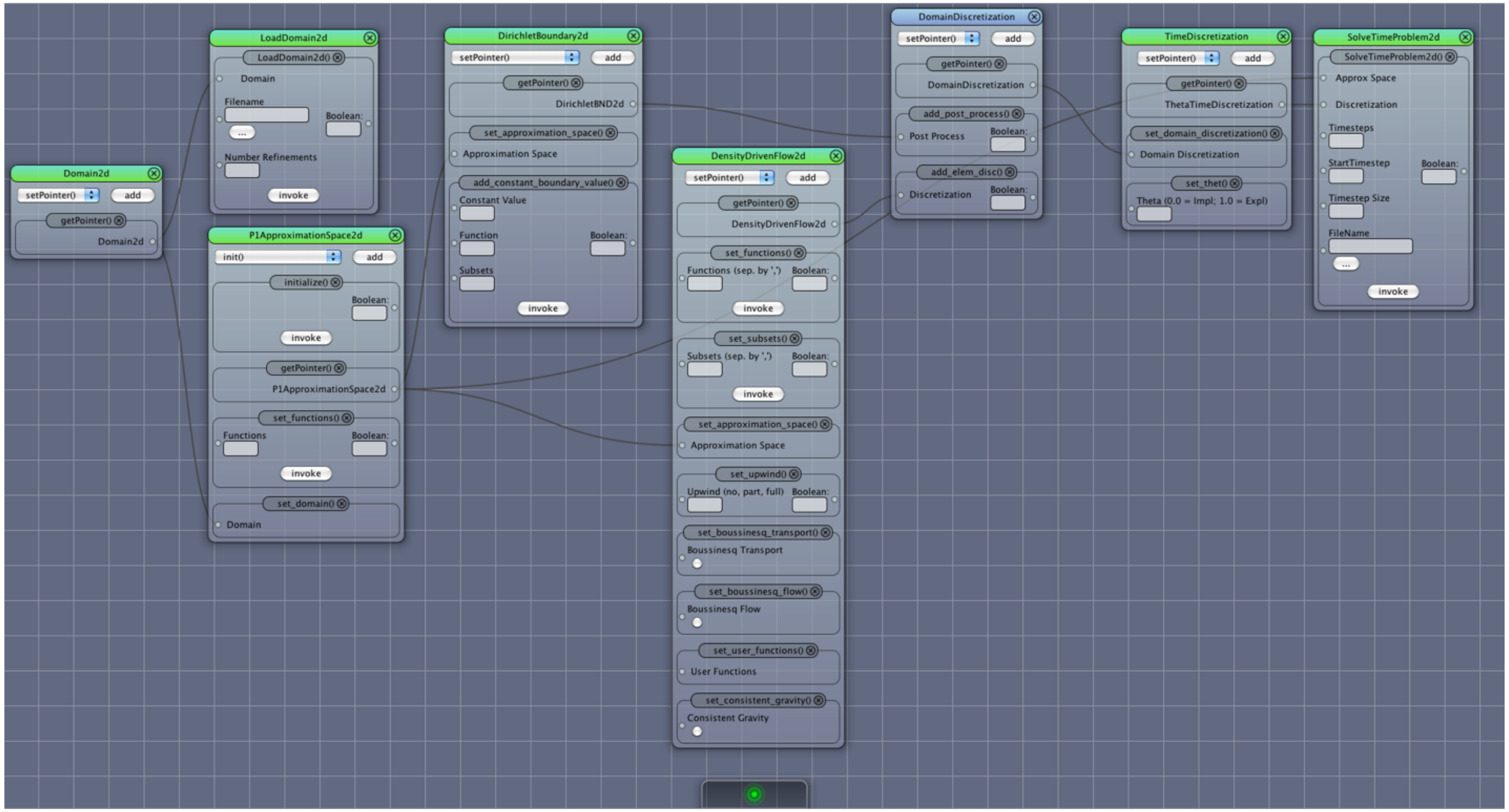
uG4 I. Heppner, M. Hoffer, A. Nägel, S. Reiter, M. Rupp, A. Vogel

- 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)



uG 4 GUI (M. Hoffer)

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



ug 4 GUI (M. Hoffer)

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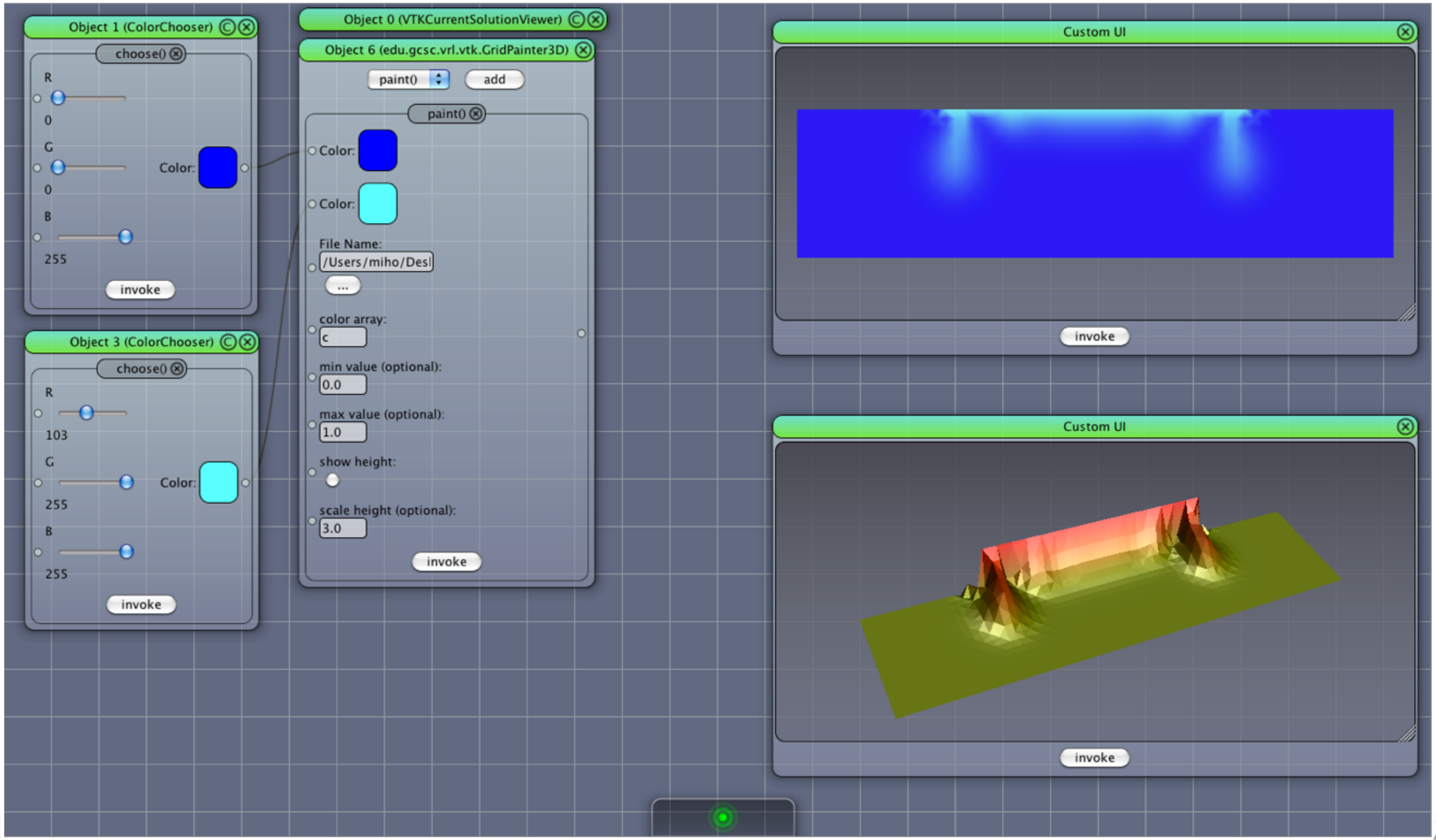

Parallel Scaling

- **uG 3 (1999):**
  Parallelization based on DDD, strongly limited parallelization (≤ 4096 cores)

- **uG 4 (2014):**
  Parallelization based on PCL, perfect scaling up to 264144 cores.

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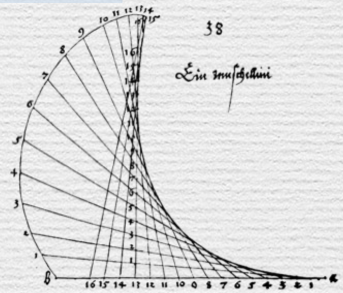
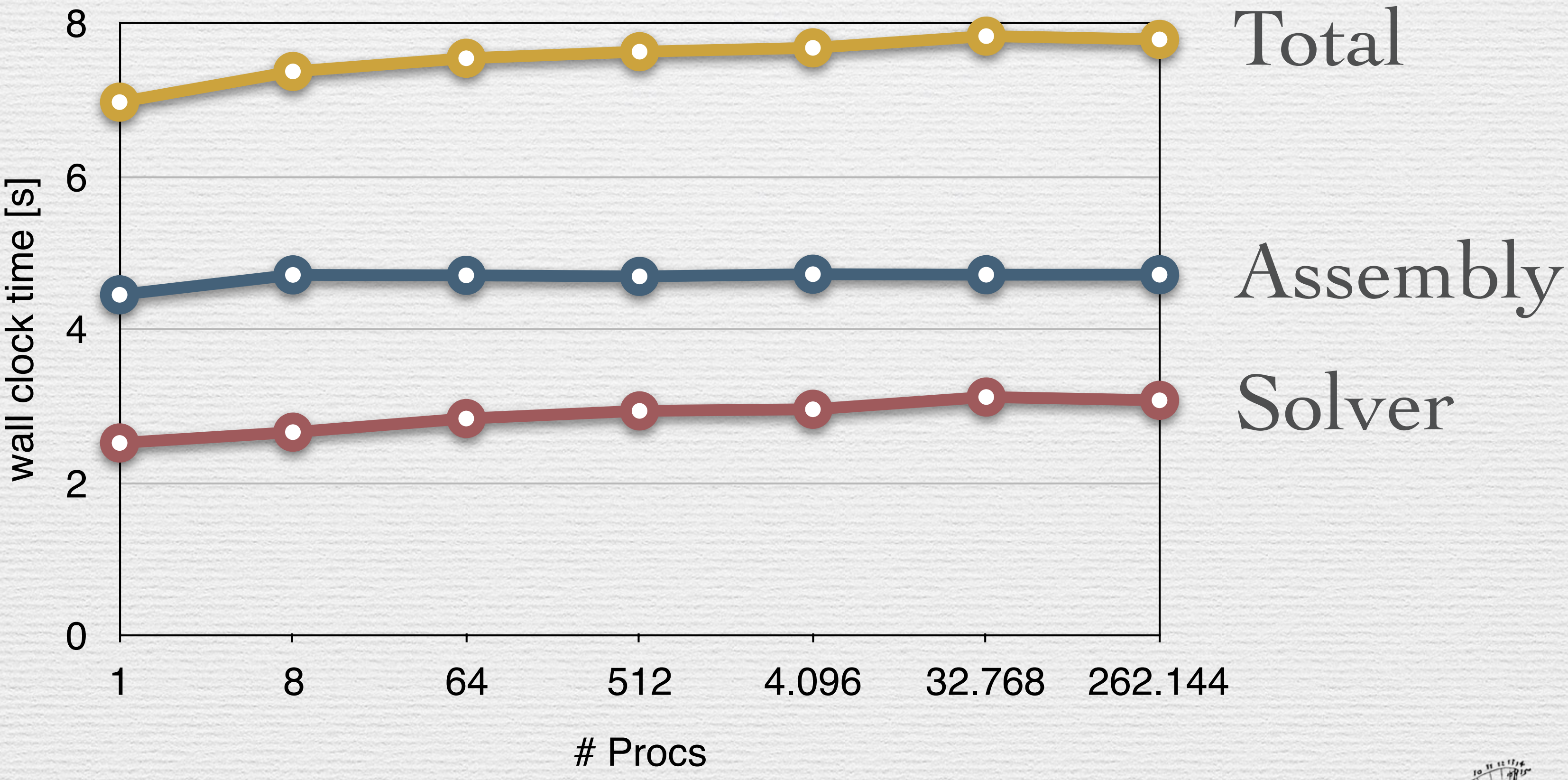


UG4: GMG Weak Scaling

- Laplacian 3d, GMG, structured



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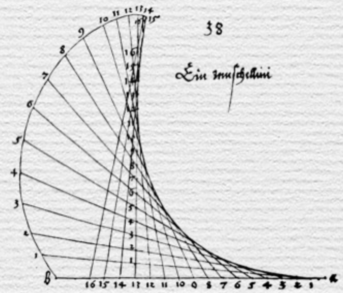
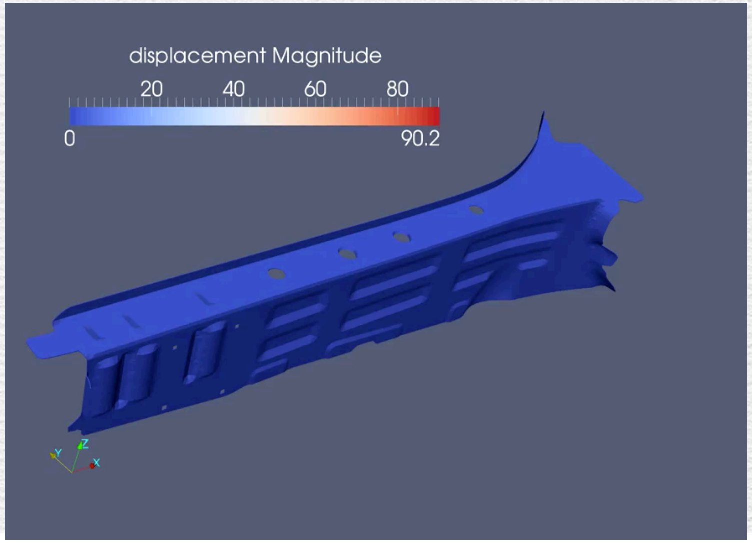
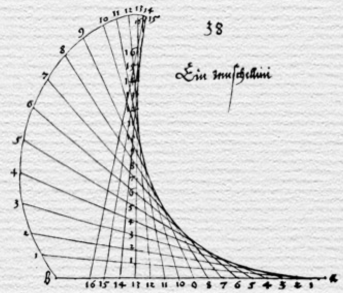


Weak Scaling UG4



- Linear elasticity 3d uniform

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



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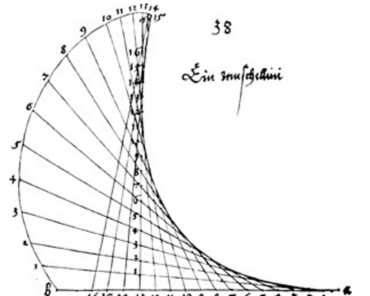
Modeling and Computation of Thermohaline Flow in Heterogenous porous media

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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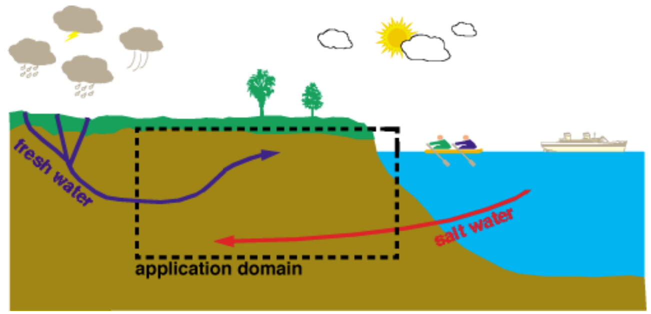
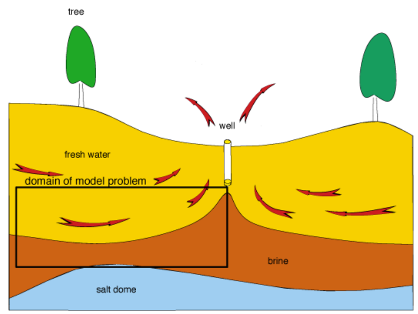
Density Driven Groundwater Flow

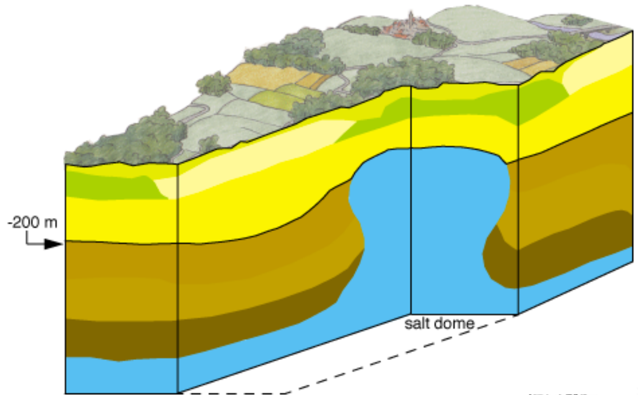
- Saltwater intrusion

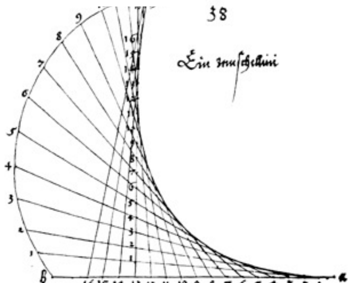


- Upconing



- Flow around saltdomes





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D³F

- Distributed Density Driven Flow

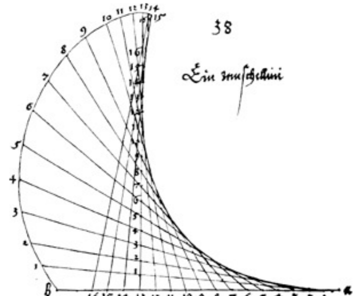
$$\frac{\partial(n\rho(c))}{\partial t} + \nabla \cdot (\rho(c)\vec{v}) = Q_p(c),$$

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

+ b.c.; with $\vec{v} = -K/\mu(c)(\nabla p - \rho(c)\vec{g}),$

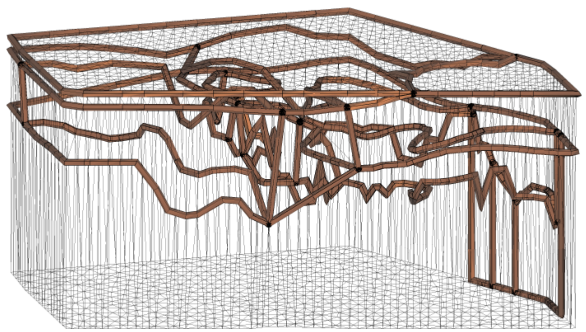
$$\mathbb{D}(\vec{v}) := D_m\mathbb{I} + \alpha_t|\vec{v}|\mathbb{I} + (\alpha_l - \alpha_t)\vec{v}\vec{v}/|\vec{v}|,$$

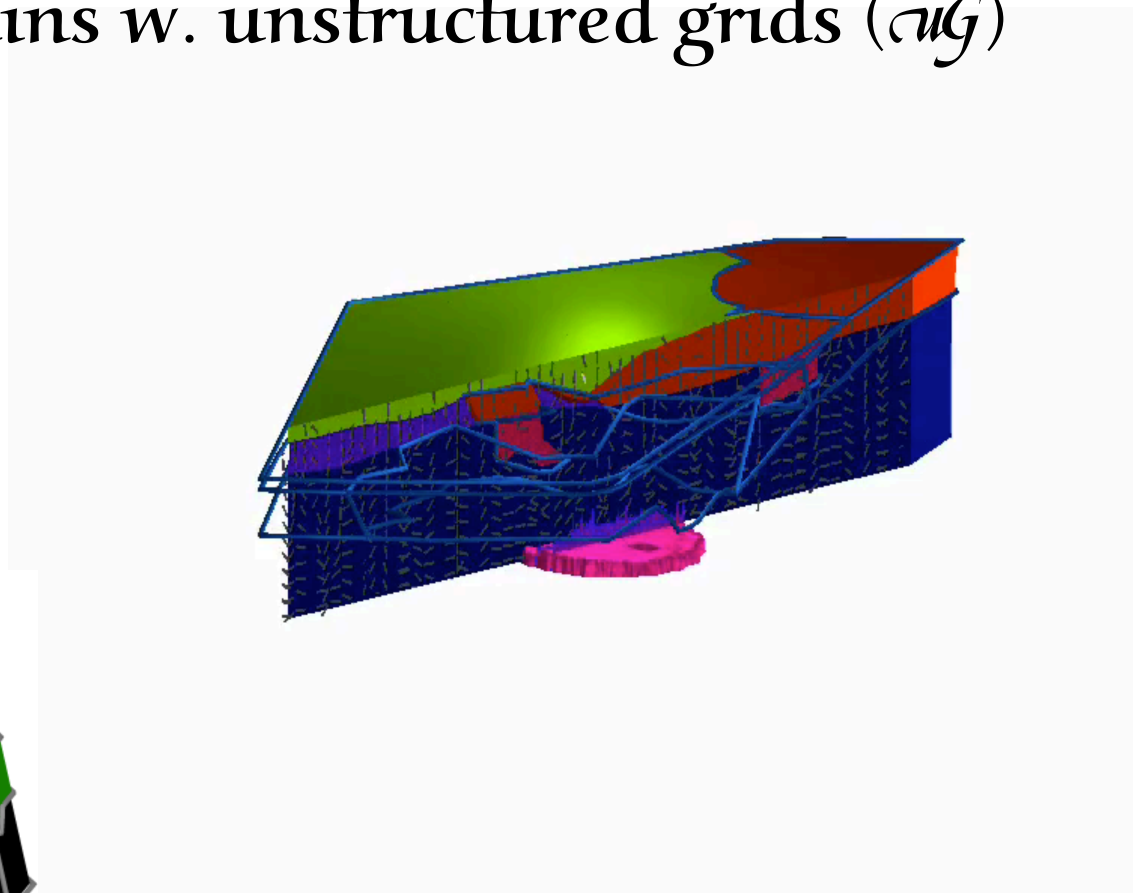
$$\frac{1}{\rho} := \left(1 - \frac{c}{c_{\max}}\right)\frac{1}{\rho_f} + \frac{c}{c_{\max}}\frac{1}{\rho_s}$$

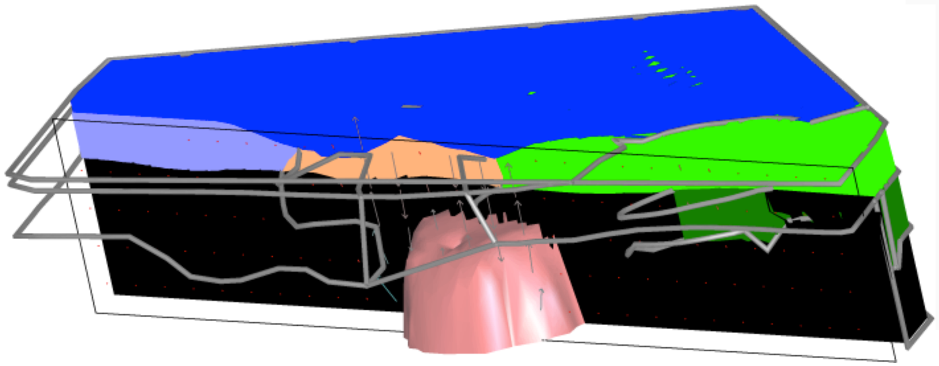


D^{3}F

- complicated domains w. unstructured grids (*uG*)







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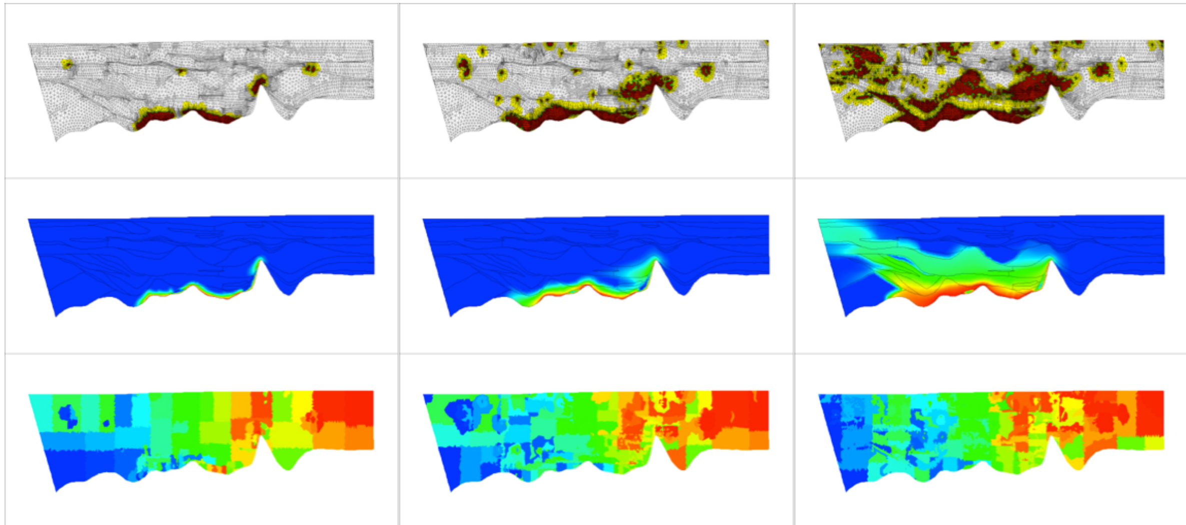
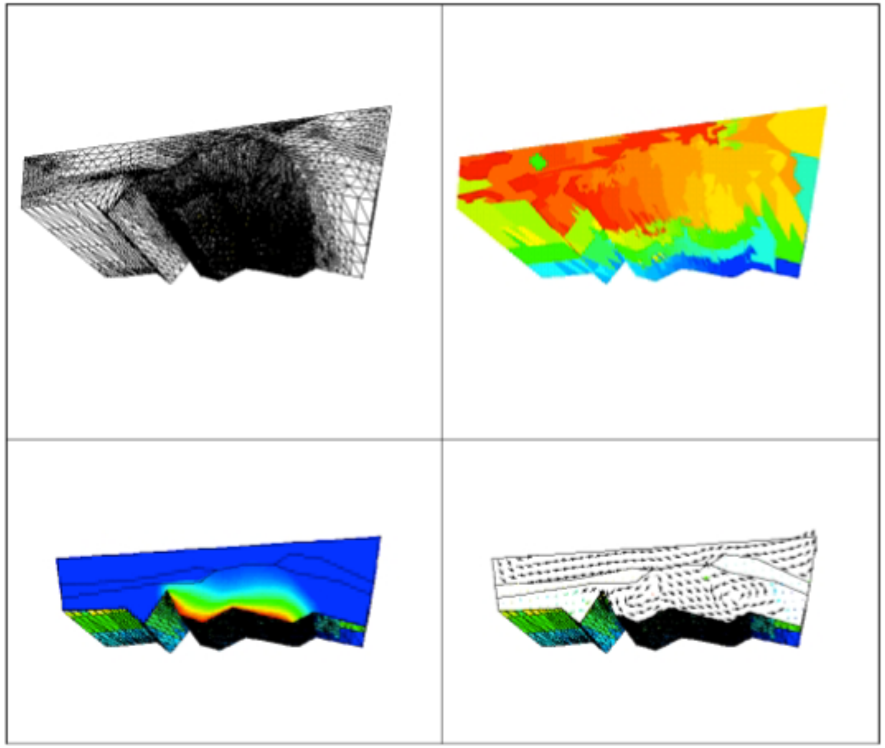
D^3F

- Full density dependent non-linear dispersion
- fully parallel adaptive





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D³F Parallel Efficiency

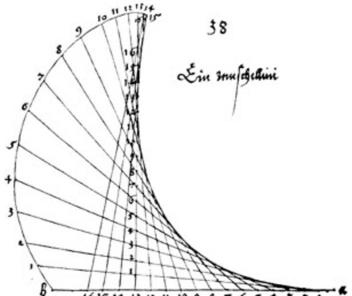
- Uniform refinement
  weak scaling

P	h	UKN	NIT[#]	TIT[s]	S_S[#]	E_S
1	1/8	147.074	19	37.31	1	1.0
8	1/16	1.082.498	23	45.83	5.4	0.67
64	1/32	8.414.978	35	54.12	24	0.37
512	1/64	66.602.498	22	58.54	282	0.55

- Adaptive refinement
  weak scaling

h	UKN	TNLS[s]	TADAPT[s]	TLB[s]	TMIG[s]
1/16	21.016	52.3	1.93	0.97	3.57
1/32	102.280	224.	13.2	3.99	13.2
1/32	433.908	657.	44.6	11.2	41.8
1/64	1.750.708	2708.	160.	27.9	108.

- Lang, S., Wittum, G.: Large scale density driven flow simulations using parallel unstructured grid adaptation and local multigrid methods. Concurrency Computat., 17, 11, 1415 - 1440, Oct. 2005.



Weak Scaling UG4

- Thermohaline flow in porous media, 2d Elder problem

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	-
128	9	8.398.850	11	6,16	99,8	4,86	101,4	8,70	99,1	38,15	99,5
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

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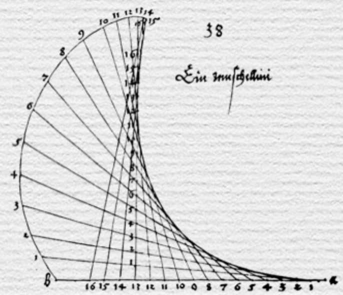

Thermohaline Flows

- Solving

$$
\begin{aligned}
\phi_f \frac{\partial \widehat{\rho}_f}{\partial t} + \nabla \cdot (\widehat{\rho}_f \mathbf{q}_f) &= 0, \\
\phi_f \frac{\partial (\widehat{\rho}_f \omega_s)}{\partial t} + \nabla \cdot (\widehat{\rho}_f \omega_s \mathbf{q}_f + \mathbf{J}_d) &= 0, \\
\phi_f \widehat{\rho}_f \Theta \frac{\mathrm{D}_f \widehat{S}_f}{\mathrm{D}t} + (1-\phi_f)\rho_r \Theta \frac{\partial \widehat{S}_r}{\partial t} + \nabla \cdot (\mathbf{J}_T - \widehat{\mu}_{sw} \mathbf{J}_d) &= 0,
\end{aligned}
$$

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

$$
\begin{aligned}
\mathbf{J}_d &= -\phi_f \rho_f D \nabla \omega_s - \phi_f \rho_f D \frac{k_p}{p} \nabla p - \phi_f \rho_f D S \omega_s (1-\omega_s) \nabla \Theta, \\
\mathbf{J}_T &= -\phi_f \rho_f D Q \nabla \omega_s - \phi_f \rho_f D Q \frac{k_p}{p} \nabla p - \left[L_{TT} - \phi_f \rho_f \frac{D Q h_{sw}}{\Theta \frac{\partial \widehat{\mu}^i_{sw}}{\partial \omega_s}} \right] \nabla \Theta,
\end{aligned}
$$

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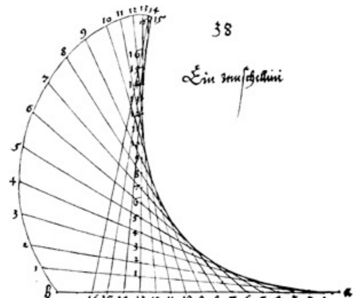
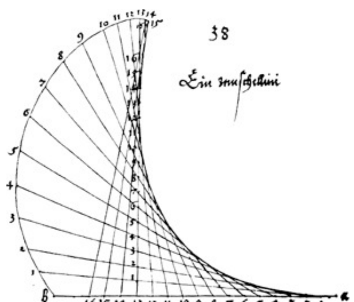


Thermohaline Flows

Solving

$$
\begin{aligned}
\phi_f \frac{\partial \widehat{\rho}_f}{\partial t} + \nabla \cdot (\widehat{\rho}_f \mathbf{q}_f) &= 0, \\
\phi_f \frac{\partial (\widehat{\rho}_f \omega_s)}{\partial t} + \nabla \cdot (\widehat{\rho}_f \omega_s \mathbf{q}_f + \mathbf{J}_d) &= 0, \\
\phi_f \widehat{\rho}_f \Theta \frac{\mathrm{D}_f \widehat{S}_f}{\mathrm{D}t} + (1-\phi_f)\rho_r \Theta \frac{\partial \widehat{S}_r}{\partial t} + \nabla \cdot (\mathbf{J}_T - \widehat{\mu}_{sw} \mathbf{J}_d) &= 0,
\end{aligned}
$$

Alfio Grillo, Michael Lampe, Gabriel Wittum: Modelling and Simulation of temperature-density-driven flow and thermodiffusion in porous media. Journal of Porous Media, 2010.



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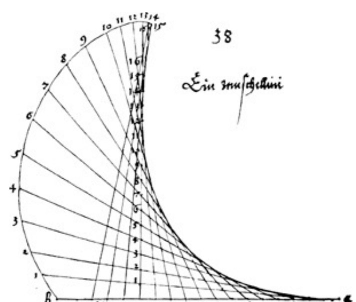
Thermohaline Flows

- opposite effects of temperature and salt concentration

  Temperature ↑

  salt water ↓

- connection of mass flux with temperature gradient (Ludwig-Soret effect)
- connection of heat flux with concentration gradient (Dufour effect)



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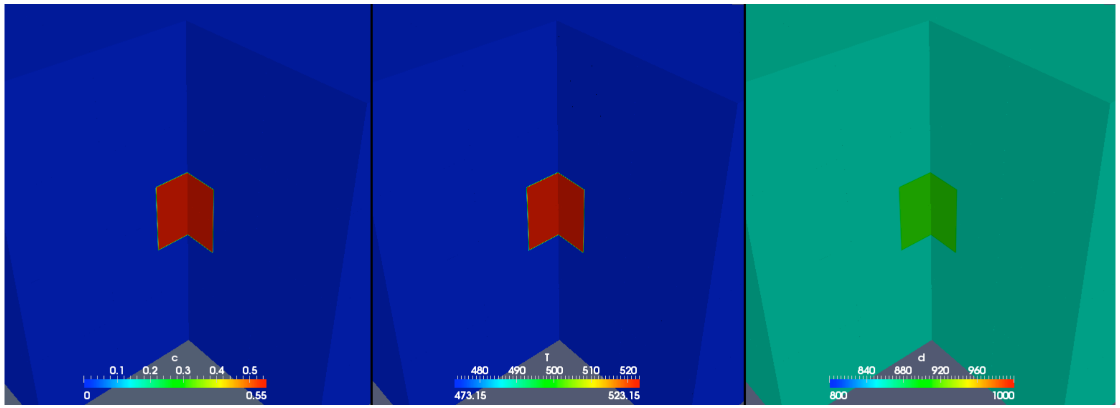
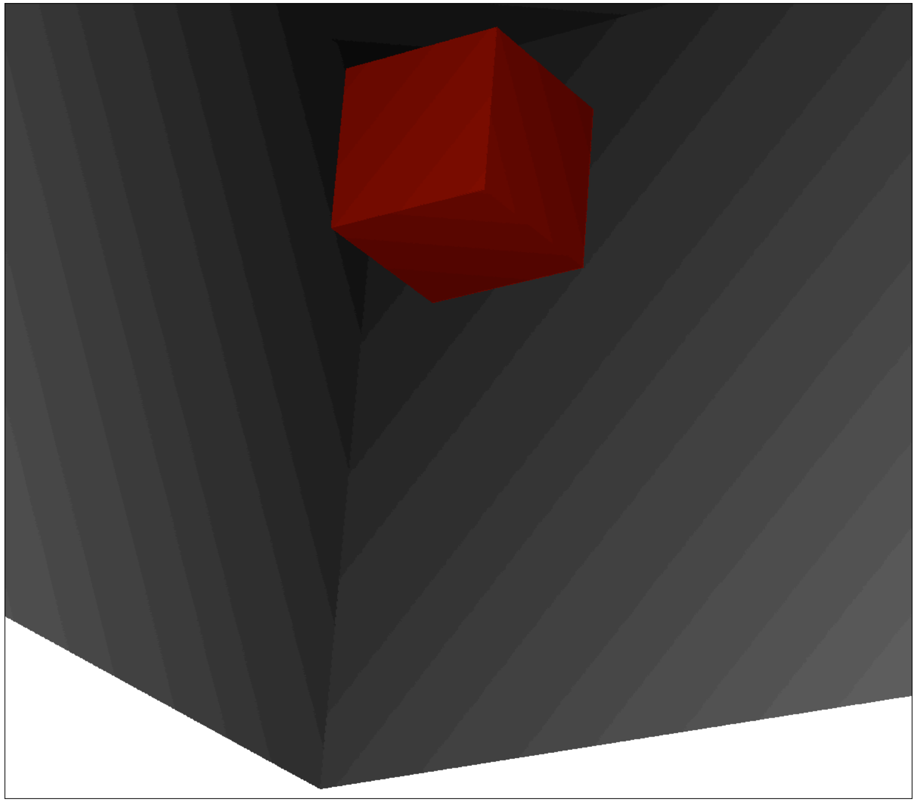
Example

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

Thermohaline Flows

- Dufour effect – negative buoyancy





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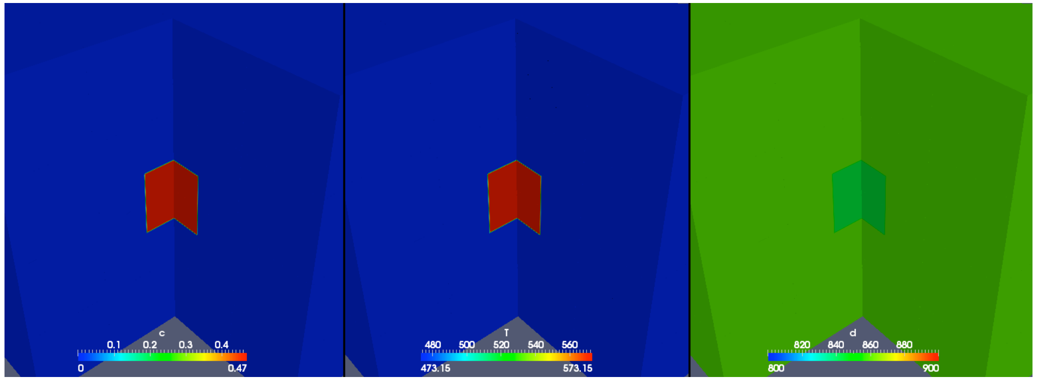
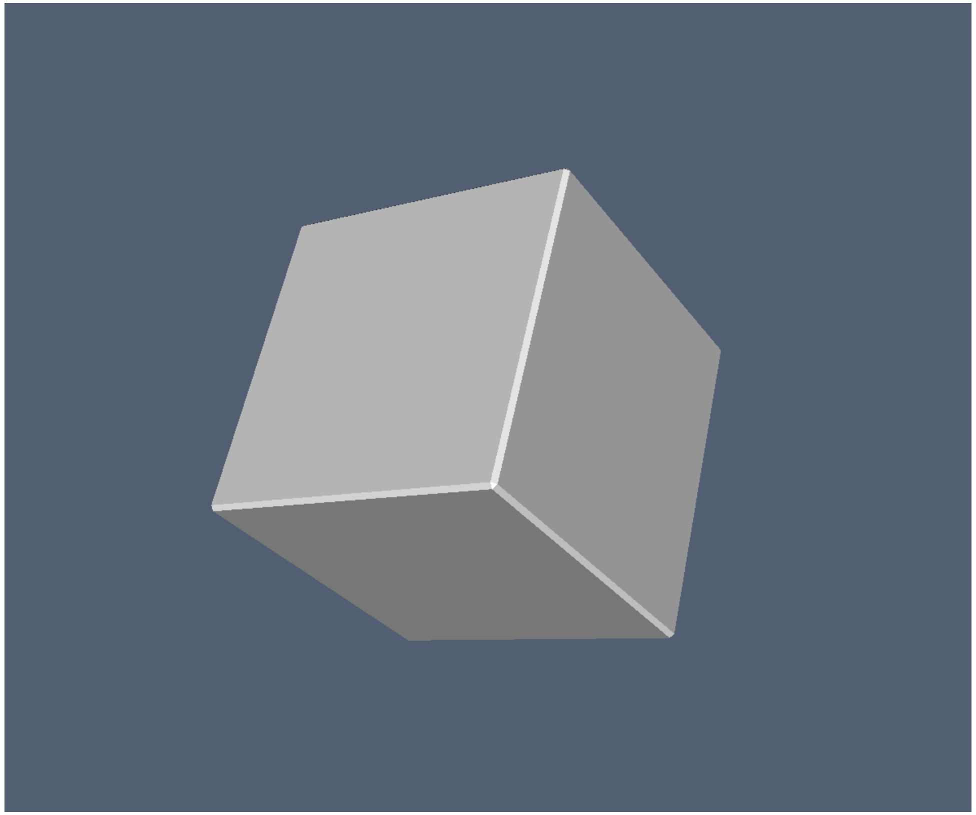
Thermohaline Flows

- Ludwig effect – positive buoyancy





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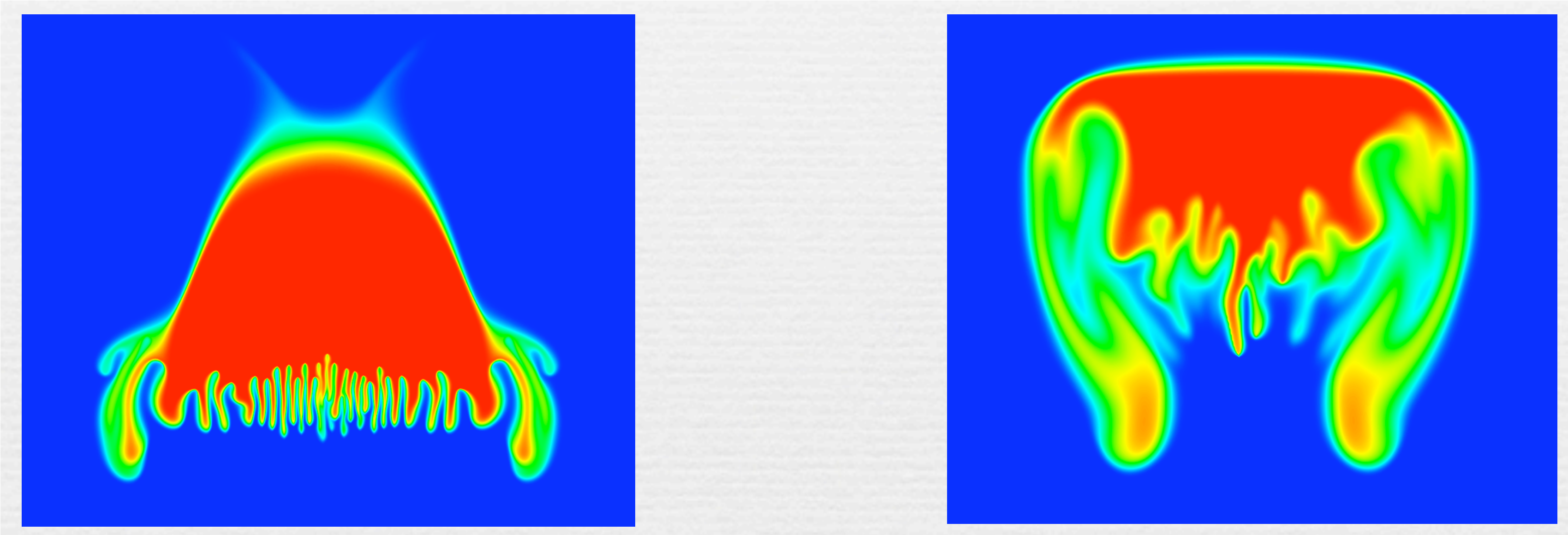
Grid Dependence



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

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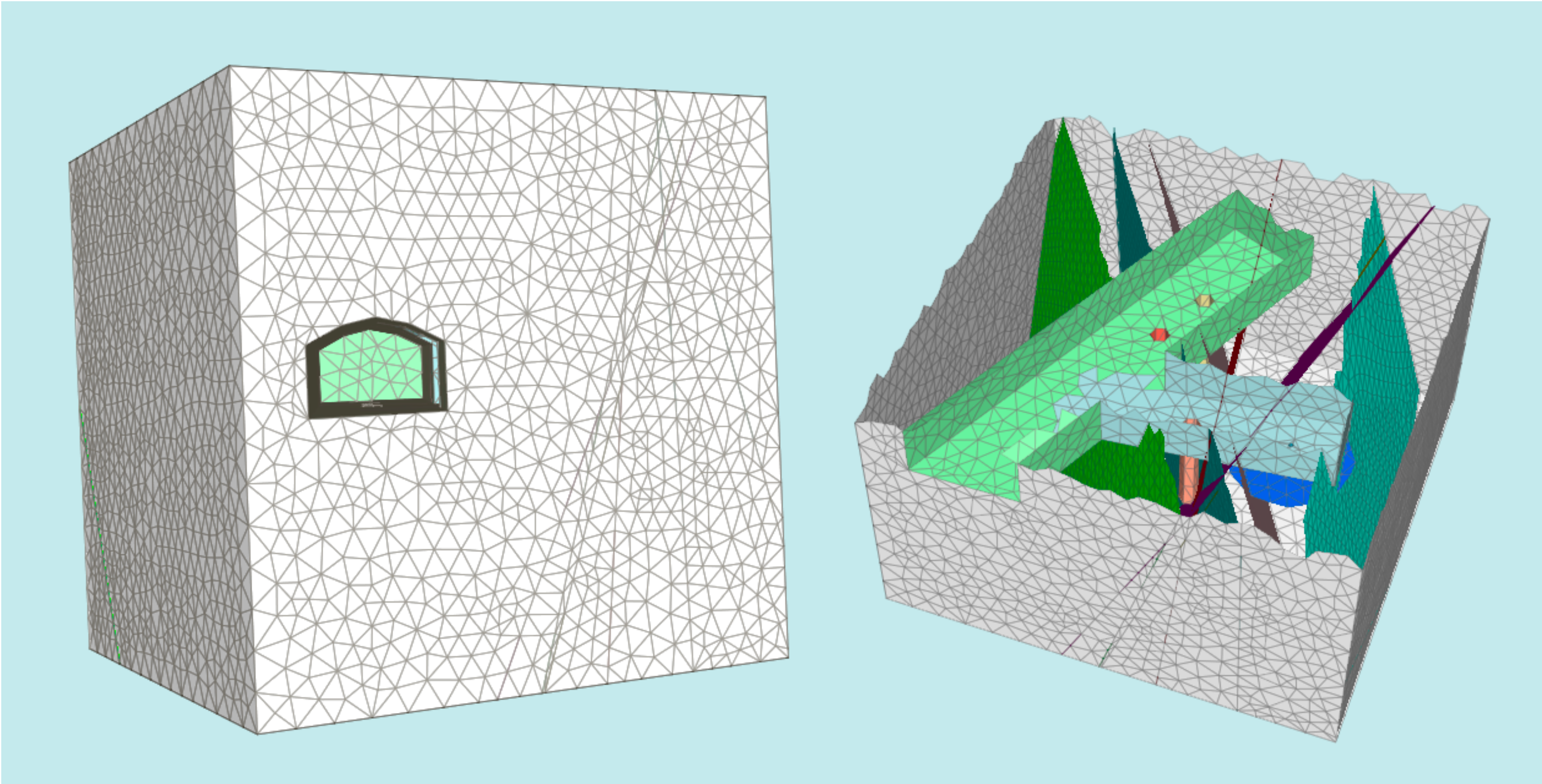
Fractured Media



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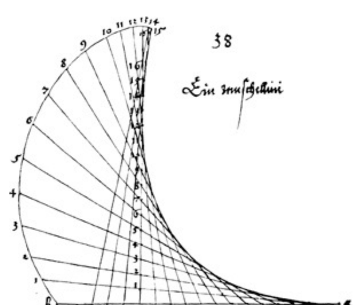
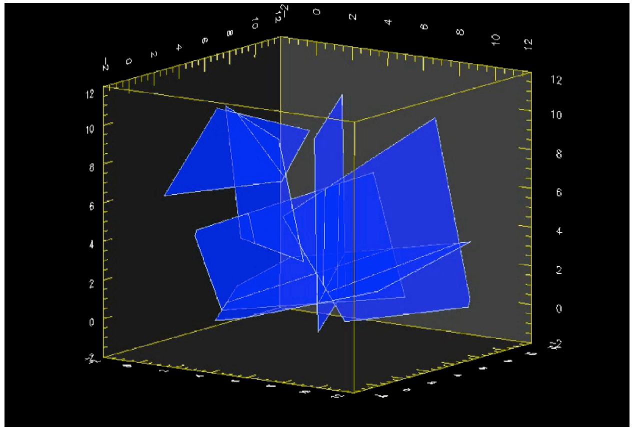


Fractured Media



- Low dimensional formulation

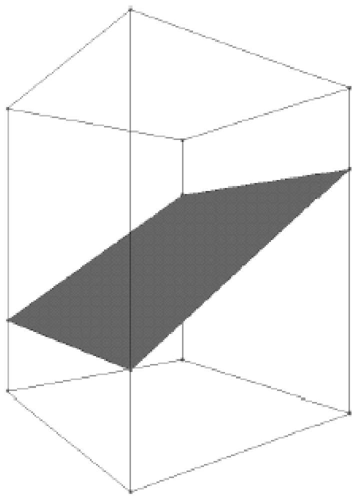
  Multiphase flow

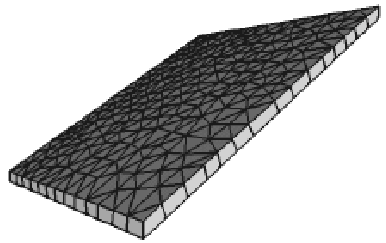
  R. Helmig; O. Kolditz; V. Reichenberger; …

- Multiscale modeling and numerics: Dynamic coupling between micro and macroscales

Flow in Fractured Media

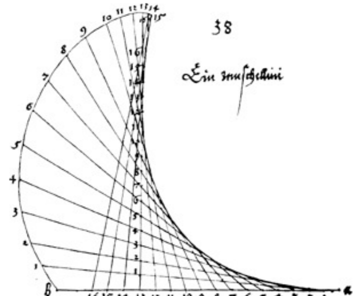
- low dimensional <-> full dimensional



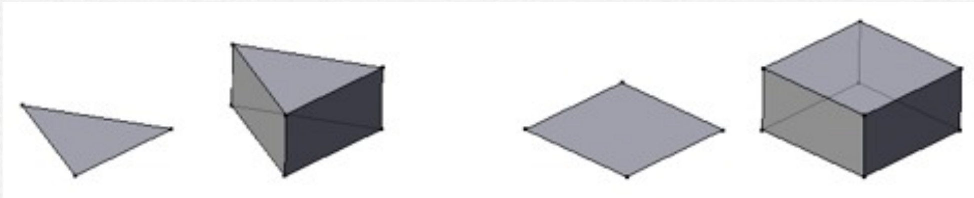


Representation of fractures:

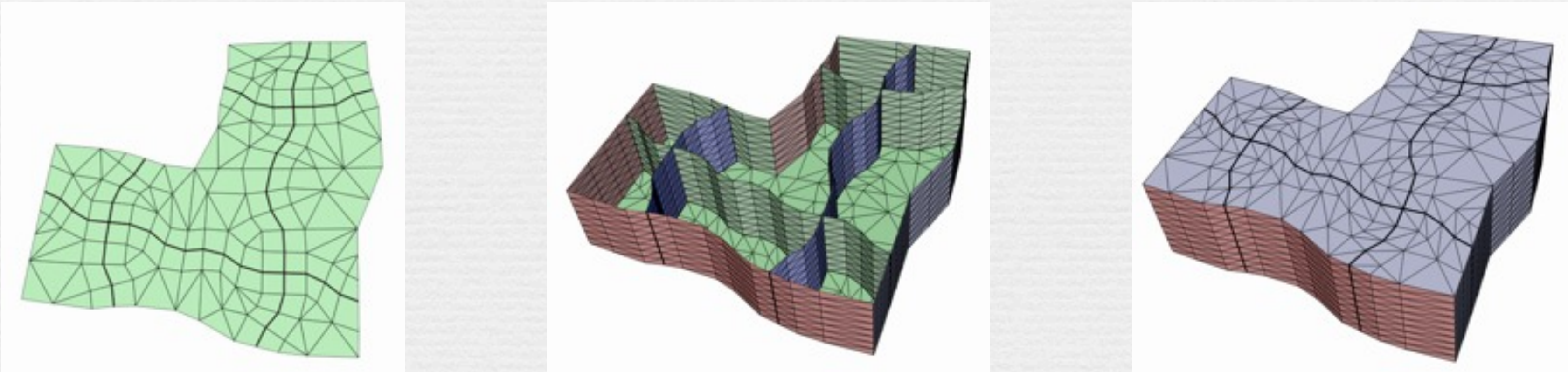
1. Polyhedral faces + pointwise thickness
2. expand to volume



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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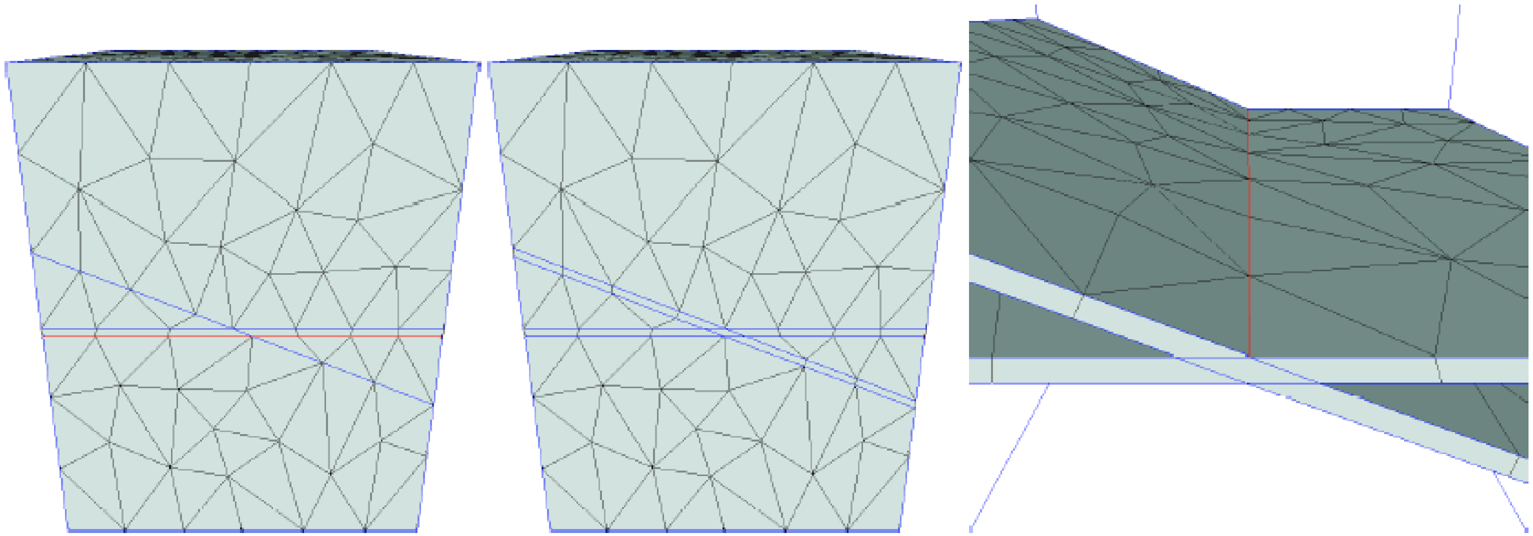
Flow in Fractured Media

- Grid follows the anisotropic direction rectangularly



successful treatment of anisotropy possible: ARTE

Fuchs, W., 2003, Feuchter, 2007

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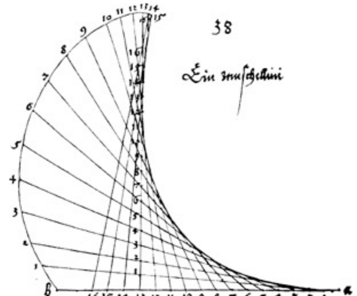


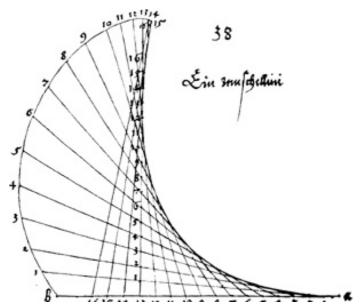
Low Dimensional Model

- Density driven flow model

  average across fracture

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

+transmission conditions



Transmission Conditions

- Full dimensional:

Continuity of normal fluxes

$$\begin{aligned} -\rho(c_f)\frac{K_f}{\mu}\left(\frac{\partial p_f}{\partial n} - \rho(c_f) g_n\right) &= -\rho(c_m)\frac{K_m}{\mu}\left(\frac{\partial p_m}{\partial n} - \rho(c_m) g_n\right) \\ -D_f\left(1 - \frac{\rho'}{\rho^{pW}} c_f\right)\frac{\partial c_f}{\partial n} &= -D_m\left(1 - \frac{\rho'}{\rho^{pW}} c_m\right)\frac{\partial c_m}{\partial n}. \end{aligned}$$

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

$$\mathbf{Q}_\alpha := \rho^{pW}\,\mathbf{q}_\alpha - \rho'\mathbf{J}_\alpha, \quad \text{and} \quad \mathbf{P}_\alpha := c_\alpha \mathbf{q}_\alpha + \mathbf{J}_\alpha\,;$$

with

$$\begin{aligned} \mathbf{q}_\alpha &= -\frac{\mathbf{K}_\alpha}{\mu}[\nabla p_\alpha - \rho_\alpha(c_\alpha)\mathbf{g}], \\ \mathbf{J}_\alpha &= -\left(\frac{\rho^{pW}}{\rho^{pW} + \rho'\,c_\alpha}\mathbf{D}_\alpha\right)\nabla c_\alpha \end{aligned} \qquad \rho' = \frac{\rho^{pB} - \rho^{pW}}{\rho^{pB}}$$

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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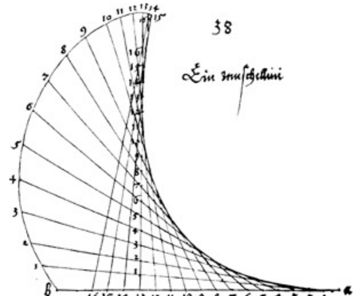
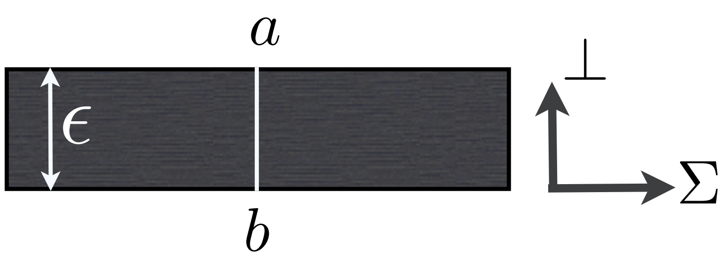


Lower Dim. Representation

$$\frac{\partial(\phi_\Sigma \rho_f c_f)}{\partial t} + \nabla_\Sigma \cdot (\rho_f c_f \mathbf{q}_\Sigma - \rho_f \mathbf{D}_\Sigma \nabla_\Sigma c_f) + \frac{1}{\epsilon}(\rho_f c_m \mathbf{q}_\perp - \rho_f D_\perp \delta c_m)|_b^a = 0$$

$$\frac{\partial(\phi_\Sigma \rho_f)}{\partial t} + \nabla_\Sigma \cdot (\rho_f \mathbf{q}_\Sigma) + \frac{1}{\epsilon}(\rho_f \mathbf{q}_\perp)|_b^a = 0$$



$$\begin{aligned} \mathbf{q}_\Sigma &= -\frac{K_\Sigma}{\mu_f}(\nabla_\Sigma p_f - \rho_f \mathbf{g}_\Sigma) \\ \mathbf{q}_\perp &= -\frac{K_\perp}{\mu_f}(\delta p - \rho_f \mathbf{g}_\perp) \\ (\delta c_m)|_a &:= \frac{c_a - c_f}{\epsilon/2} \quad , \quad (\delta p)|_a := \frac{p_a - p_f}{\epsilon/2} \end{aligned}$$

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Henry's Problem (2d)

Intrusion of saltwater into freshwater aquifer

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

$$\begin{aligned} c &= 0 \\ \mathbf{q}_{in} &= 6.6 \cdot 10^{-5} \end{aligned}$$

$$\begin{aligned} c &= 1 \\ p &= 10055.25 \cdot z \end{aligned}$$

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

Parameters in fracture: $\phi_\Sigma = 2\phi_m, \; K_\Sigma = 10^3 \cdot K_m$

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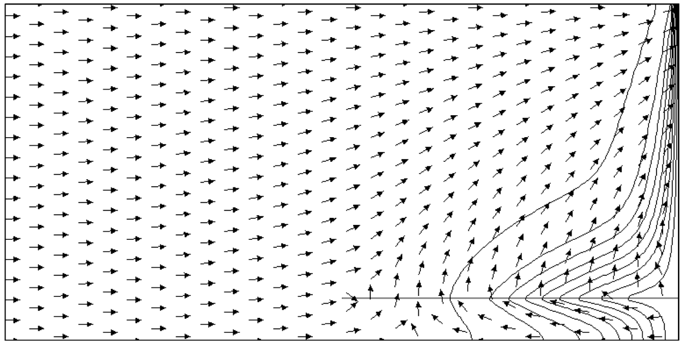
Henry's Problem

- Parameters

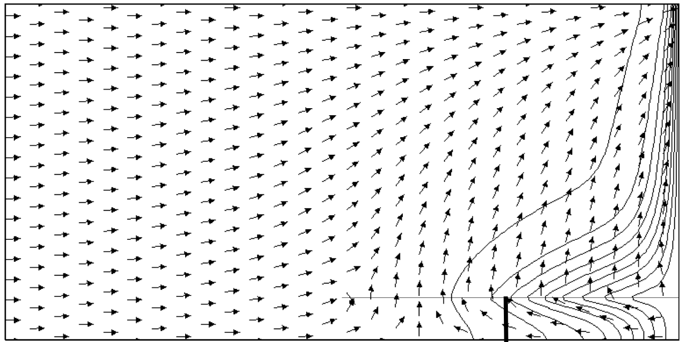
Symbol	Quantity	Value	Unit
D_d	Diffusion coefficient	$18.8571 \cdot 10^{-6}$	$[\mathrm{m}^2\ \mathrm{s}^{-1}]$
$D_m = \phi_m\ D_d$	Diffusion coefficient in the medium	$6.6 \cdot 10^{-6}$	$[\mathrm{m}^2\ \mathrm{s}^{-1}]$
$D_f = \phi_f\ D_d$	Diffusion coefficient in the fracture	$13.2 \cdot 10^{-6}$	$[\mathrm{m}^2\ \mathrm{s}^{-1}]$
$\mathbf{g}$	Gravity	9.81	$[\mathrm{m}\ \mathrm{s}^{-2}]$
K_m	Permeability of the medium	$1.019368 \cdot 10^{-9}$	$[\mathrm{m}^2]$
K_f	Permeability of the fracture	$1.019368 \cdot 10^{-5}$	$[\mathrm{m}^2]$
ϕ_m	Porosity of the medium	0.35	-
ϕ_f	Porosity of the fracture	0.7	-
μ	Viscosity	10^{-3}	$[\mathrm{kg}\ \mathrm{m}^{-1}\ \mathrm{s}^{-1}]$
ρ_w	Density of water	$1 \cdot 10^3$	$[\mathrm{kg}\ \mathrm{m}^{-3}]$
ρ_s	Density of brine	$1.025 \cdot 10^3$	$[\mathrm{kg}\ \mathrm{m}^{-3}]$
a_α^t	Transversal dispersivity length	0	$[\mathrm{m}]$
a_α^l	Longitudinal dispersivity length	0	$[\mathrm{m}]$

Henry's Problem w. Fracture

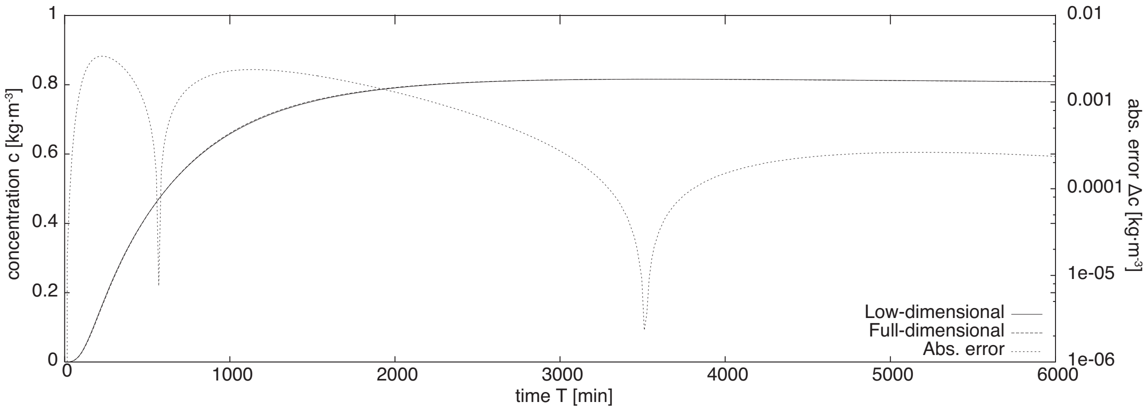
ε = 3 mm, T = 5h



full dim. rep.



low dim. rep.



x = 1.5 m

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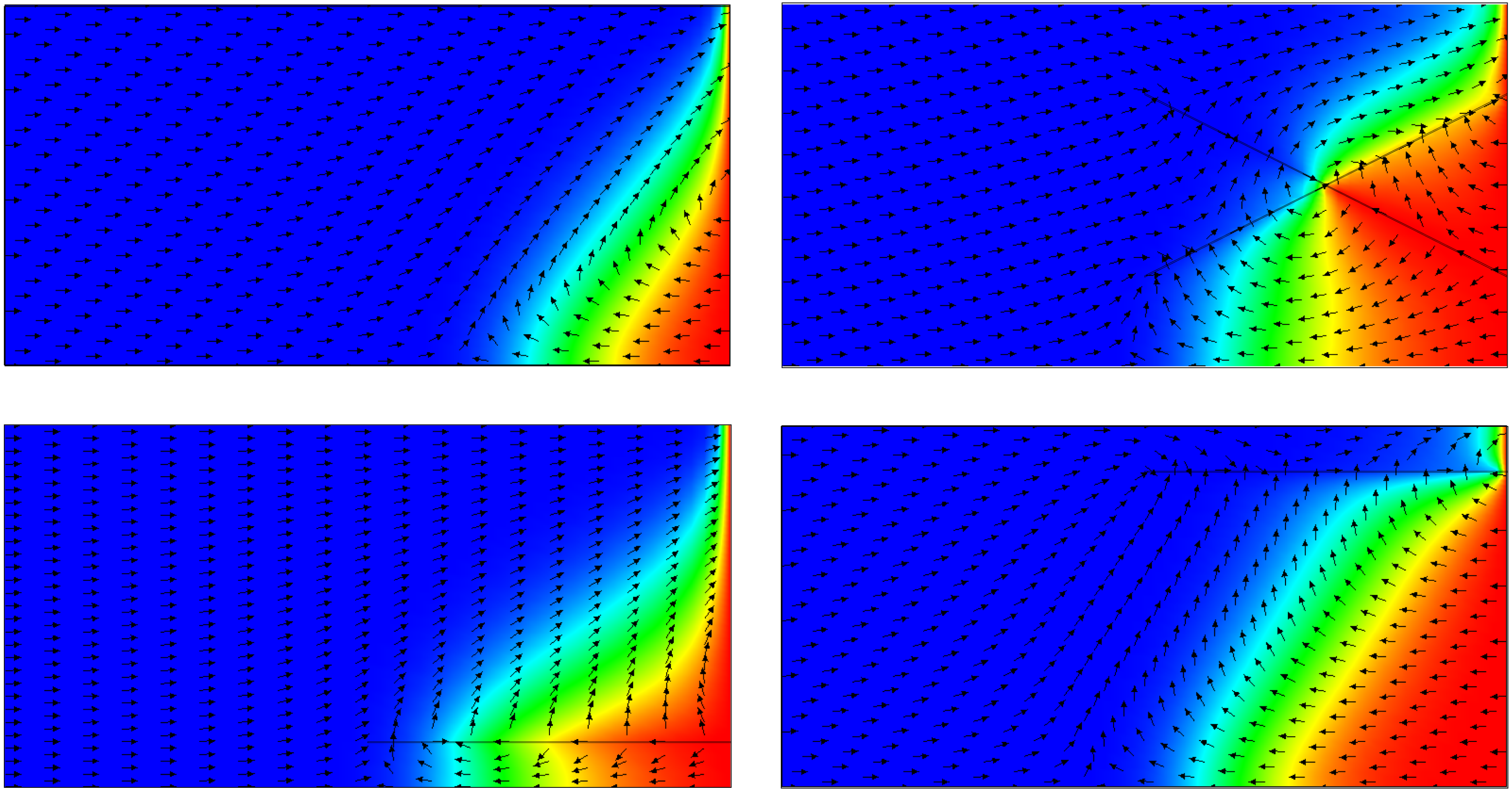
Henry's Problem w. Fracture



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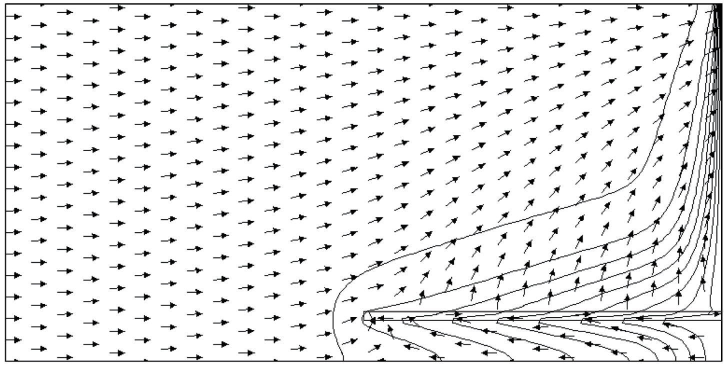
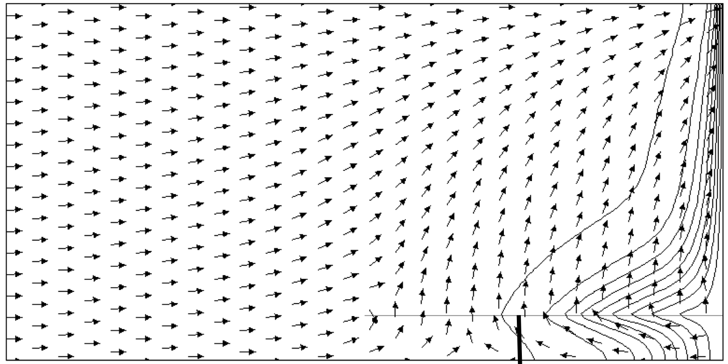
Henry's Problem w. Fracture

$\varepsilon = 24$ mm, $T = 5$h

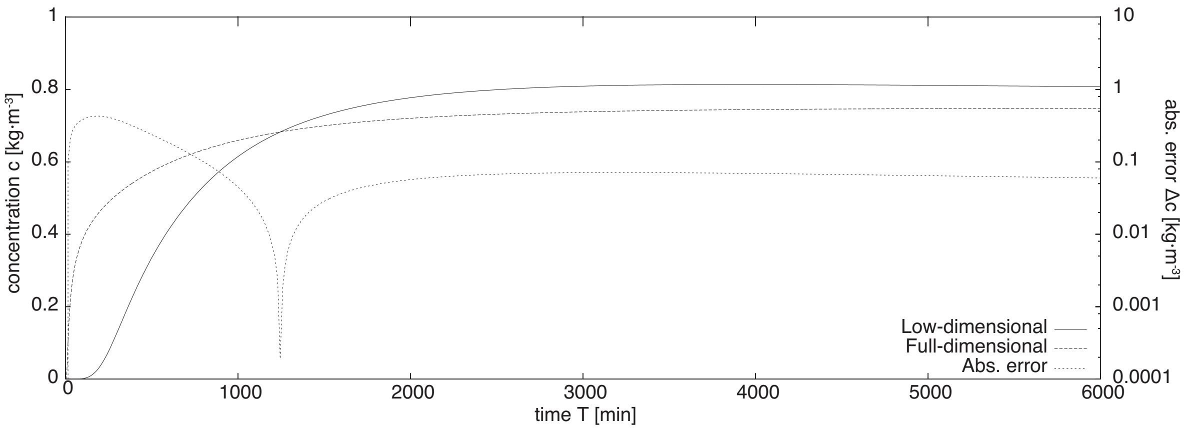


full dim. rep.



low dim. rep.

x = 1.5m



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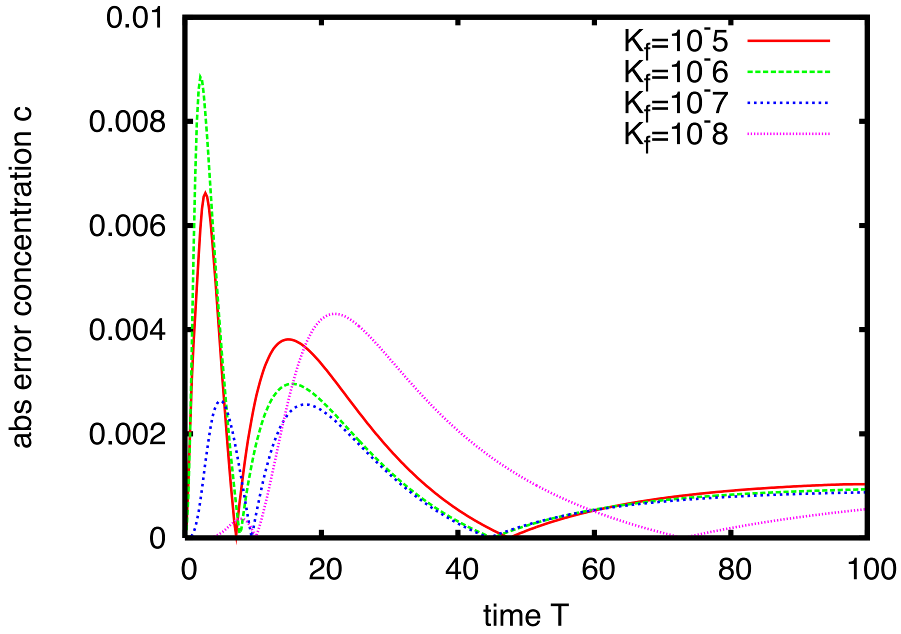
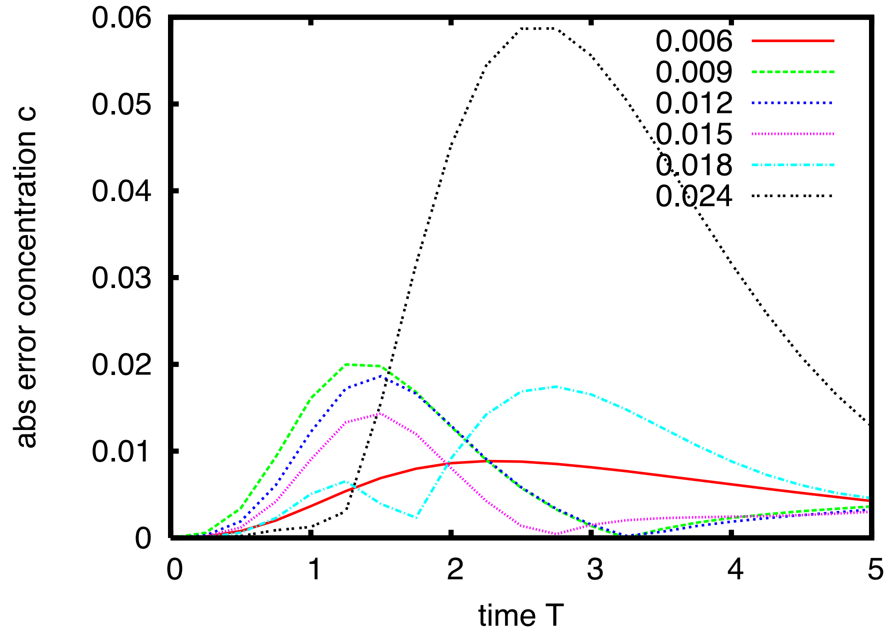
Comparison d-1 and d dim

averaged c



$\epsilon = 0.006$ fixed



$K_f = 10^{-6}$ fixed

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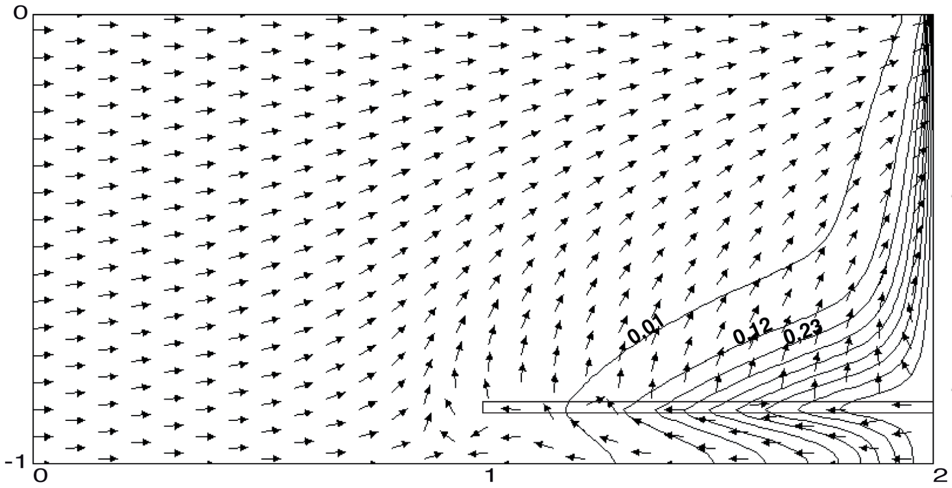
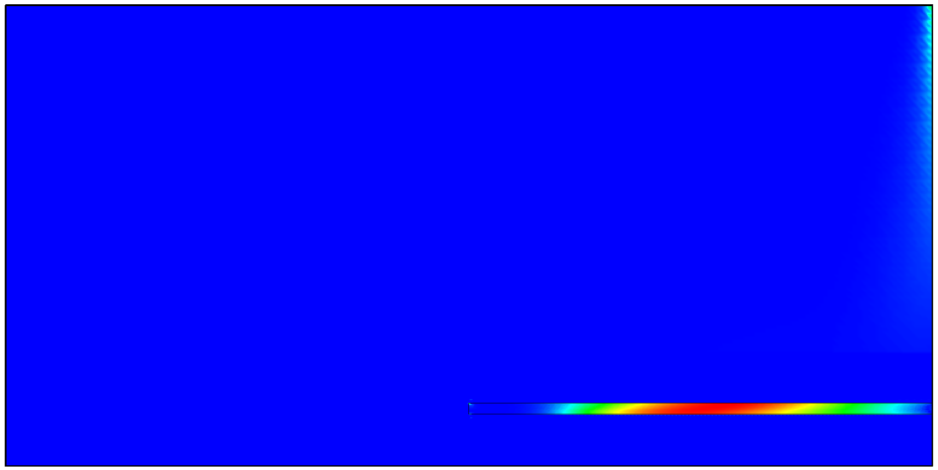
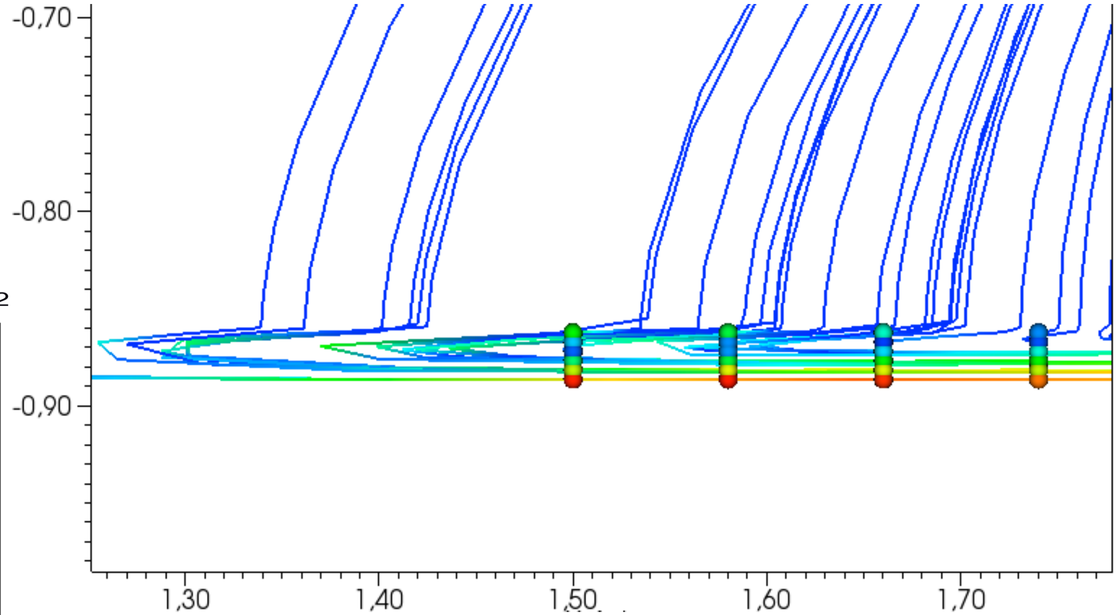
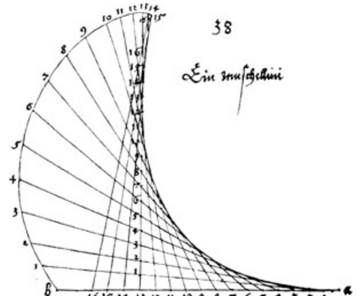
Rotational Flow





$$|\nabla \times \mathbf{q}|$$





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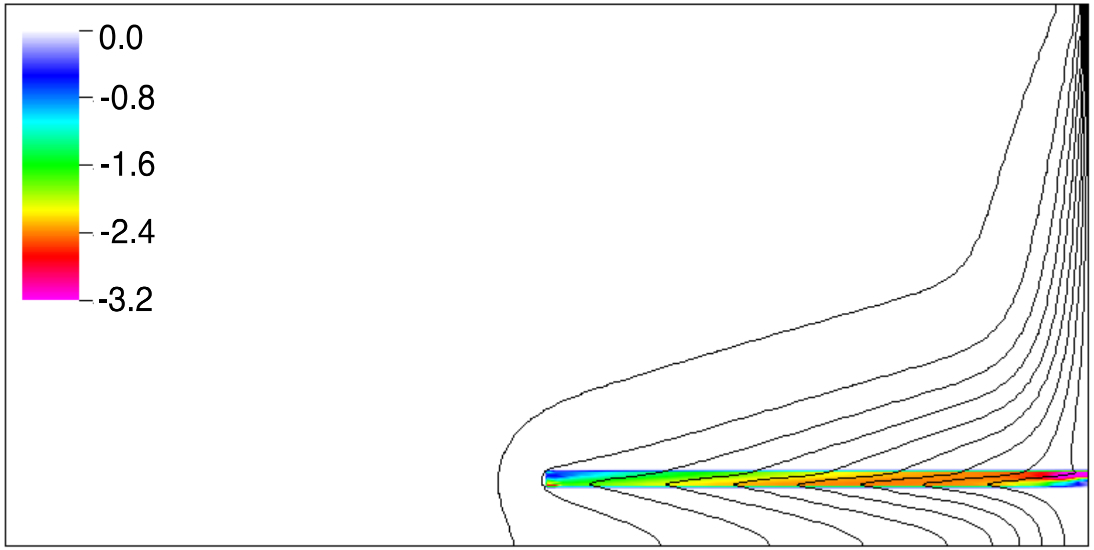
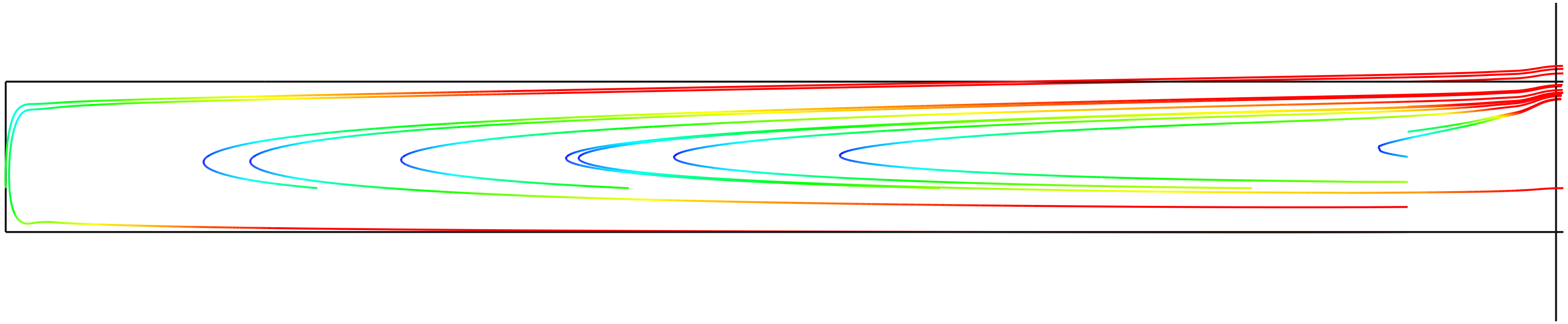
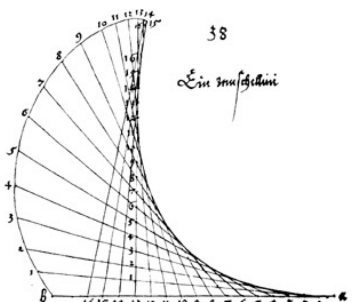
Thin Fracture

$\varepsilon = 0.006$







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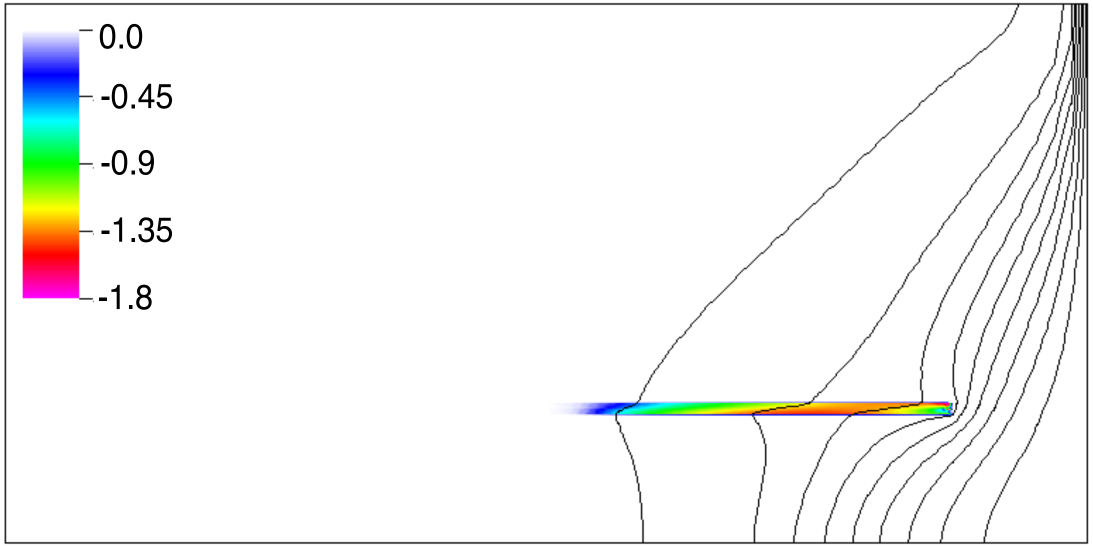
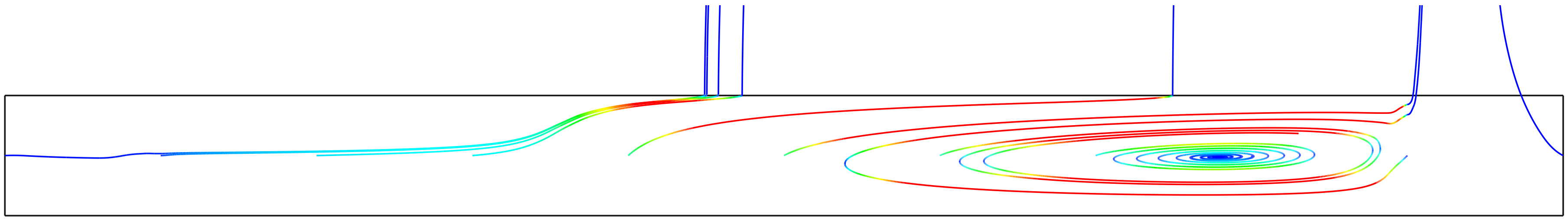
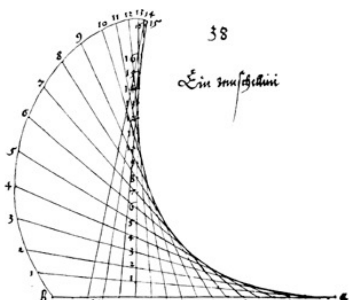
Rotational Flow

$\varepsilon = 0.024$







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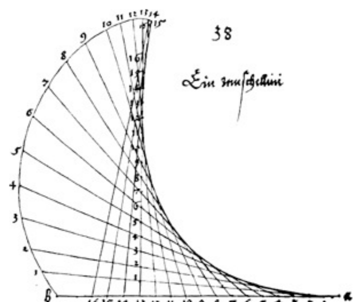
Vorticity

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

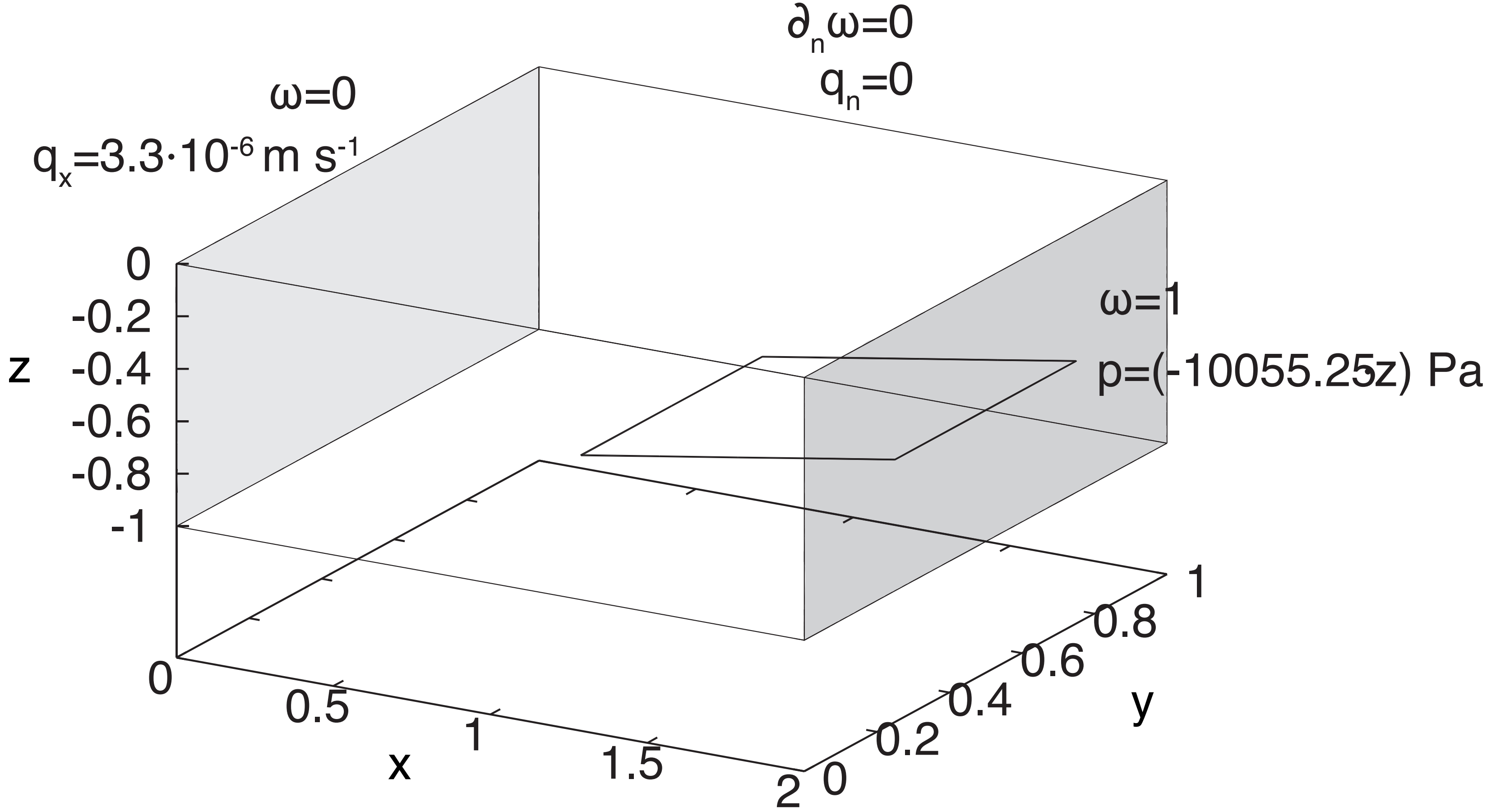
with $$\mathbf{q} = -\frac{K}{\mu}(\nabla p - \rho \mathbf{g})$$

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



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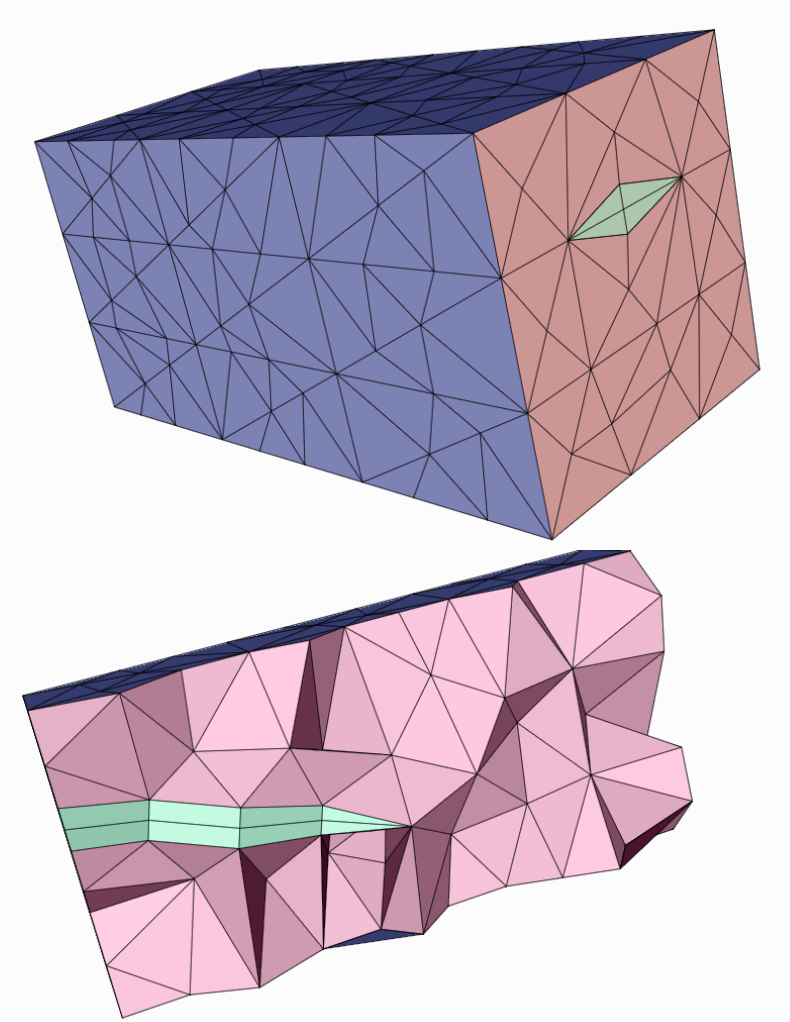
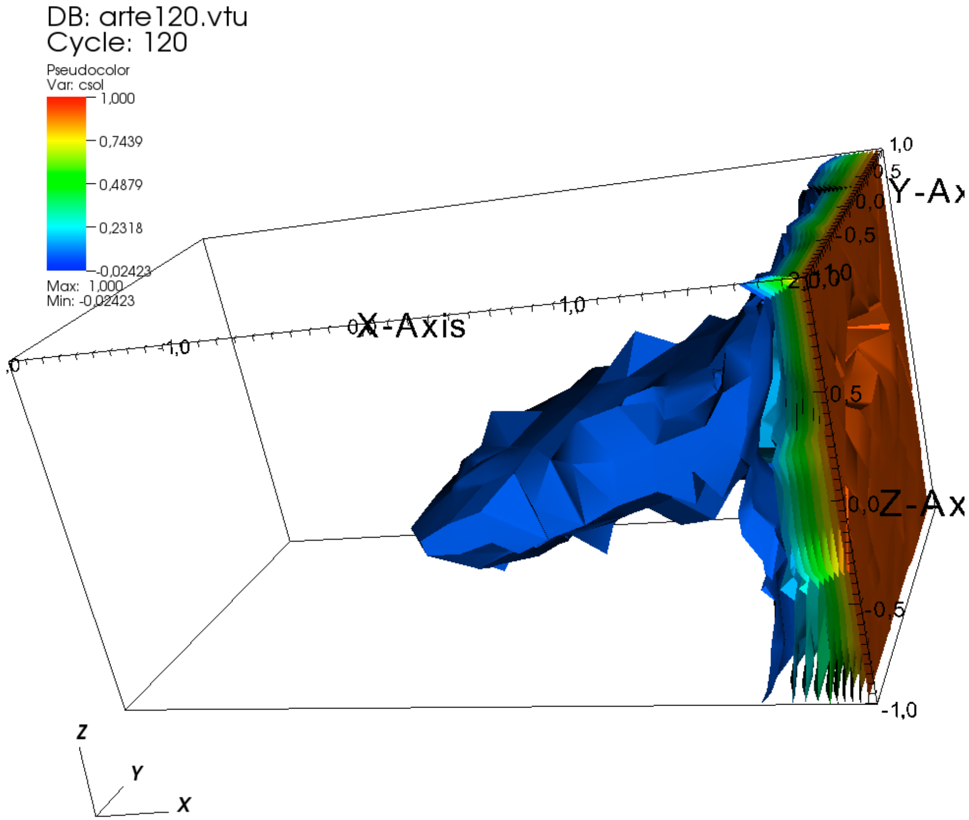
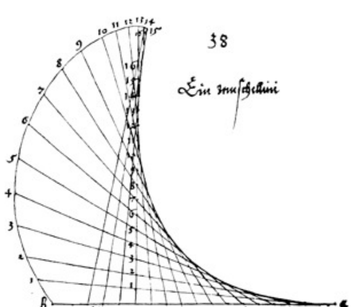
3D







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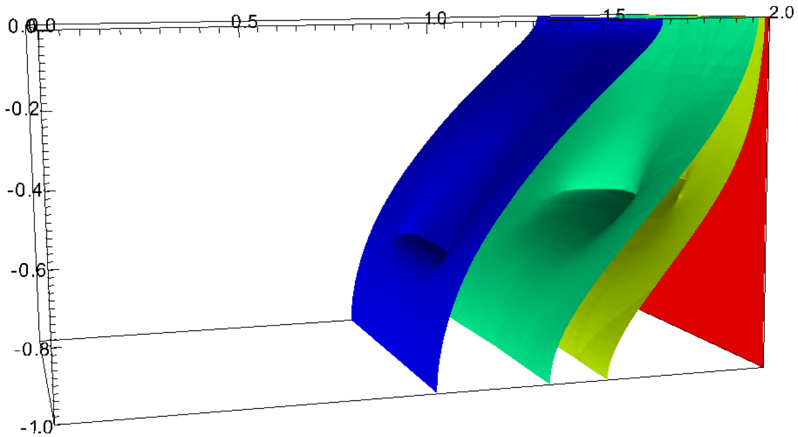
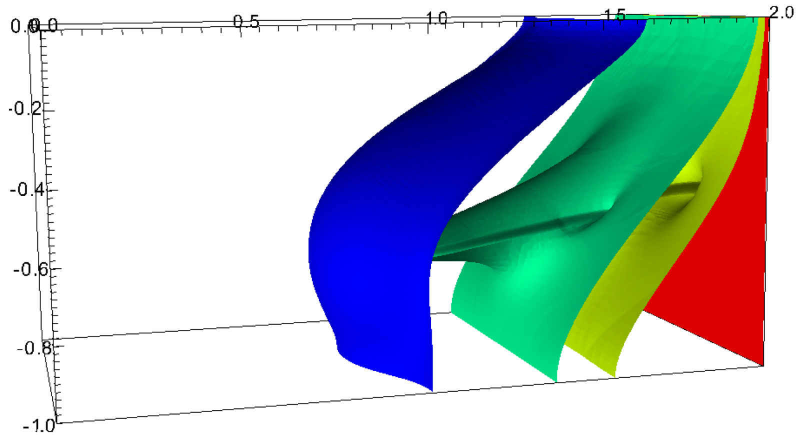
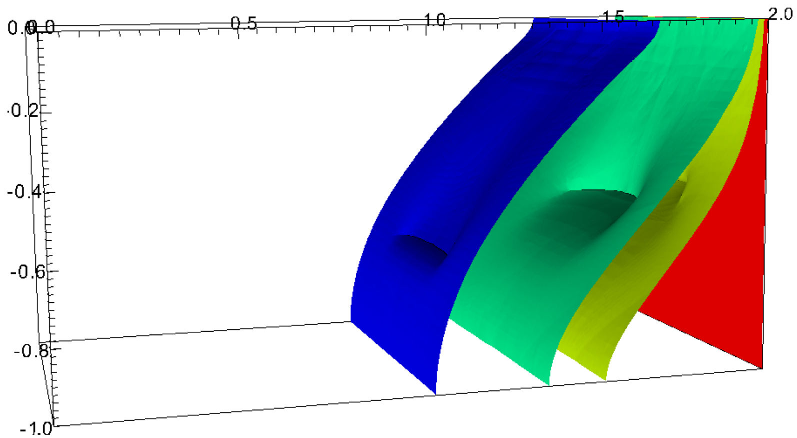
Comparison 3d

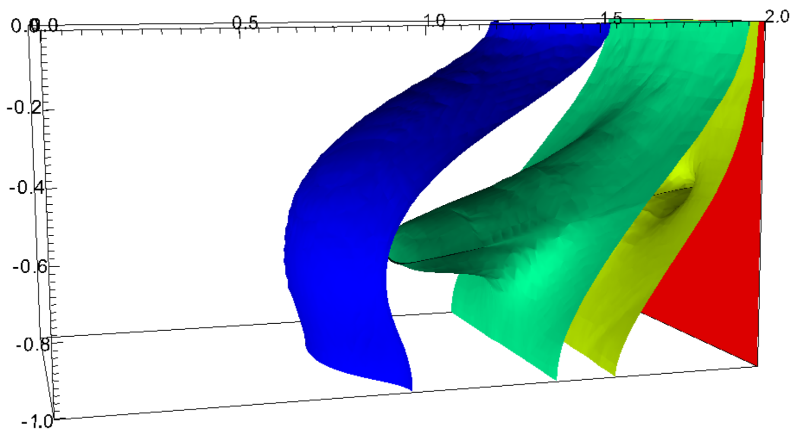
d-dim.





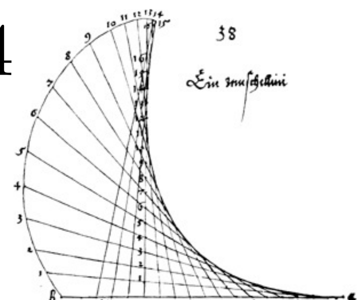
(d-1)
-dim.





$\epsilon = 0.003$

$\epsilon = 0.024$



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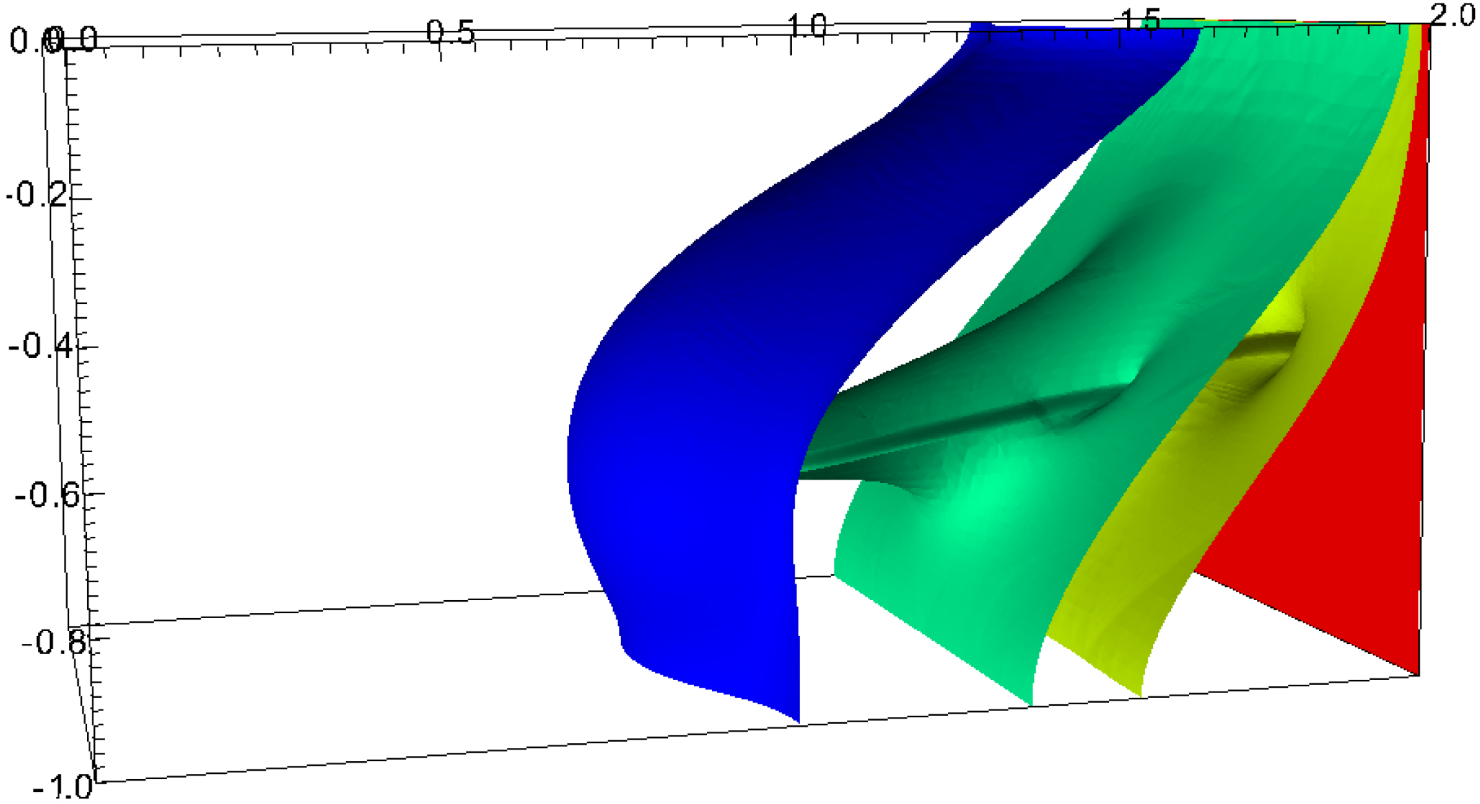
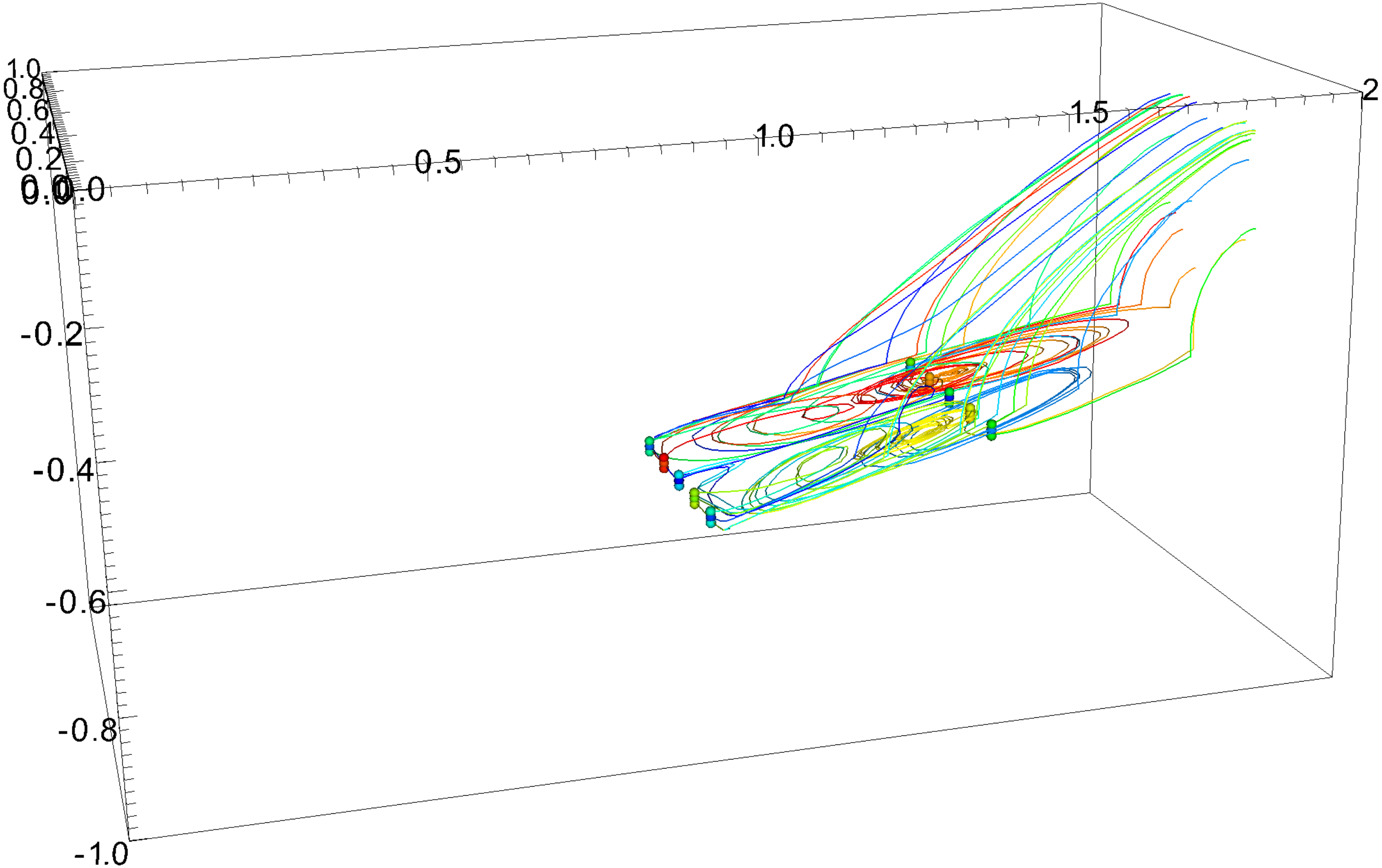
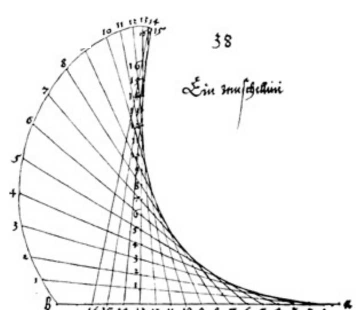
Profile

Full dimensional



$\epsilon = 0.024$





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Observations

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

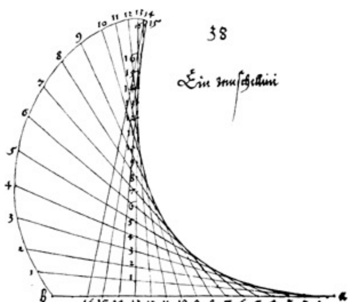
Flow Characterization

$$\theta_f := \frac{|\mathbf{q}_f|}{|\mathbf{q}_{\mathrm{rot}}|} \qquad\qquad \mathbf{q}_{\mathrm{rot}} := \frac{\epsilon}{2}\frac{K_f}{K_m}\frac{\omega_f}{\omega_\theta}(\nabla \times \mathbf{q}_f)$$

$\mathbf{q}_{\mathrm{rot}}$ rotational flow velocity

θ_f is dimensionless, characterizes flow

$|\mathbf{q}_f| > |\mathbf{q}_{\mathrm{rot}}|$ rotational flow can be neglected



Criterion

$$\theta_{\mathscr{F}} := \max_{\mathscr{F}}\{\theta_f\}$$

$$\begin{array}{llll} \theta_{\mathscr{F}} & < & 1-\delta & \quad d\text{-dimensional} \\ \theta_{\mathscr{F}} & > & 1+\delta & \quad (d-1)\text{-dimensional} \end{array}$$

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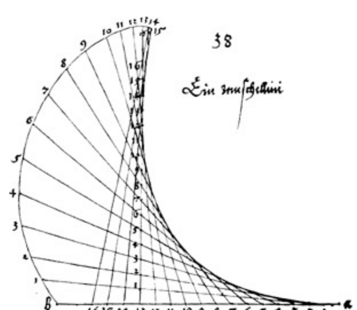
Criterion

$$\theta = \frac{\epsilon \, |\omega_f|}{\|v_\theta\|} \frac{K_f}{K_m} \frac{c_f}{c_\theta}$$

max $\theta > \theta_0$ => full dimensional
max $\theta \le \theta_0$ => low dimensional



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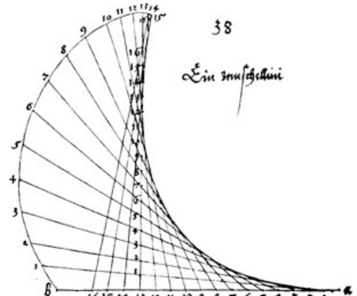
Dimensional Adaptivity

- 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

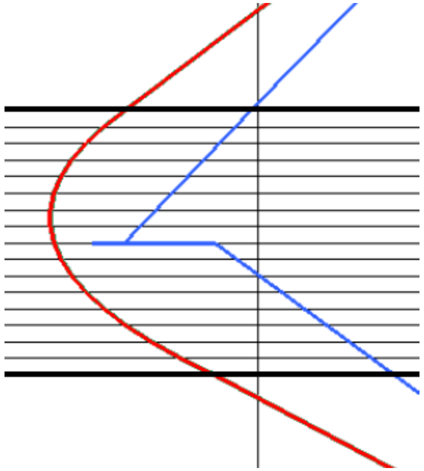
„Full -> Low“:

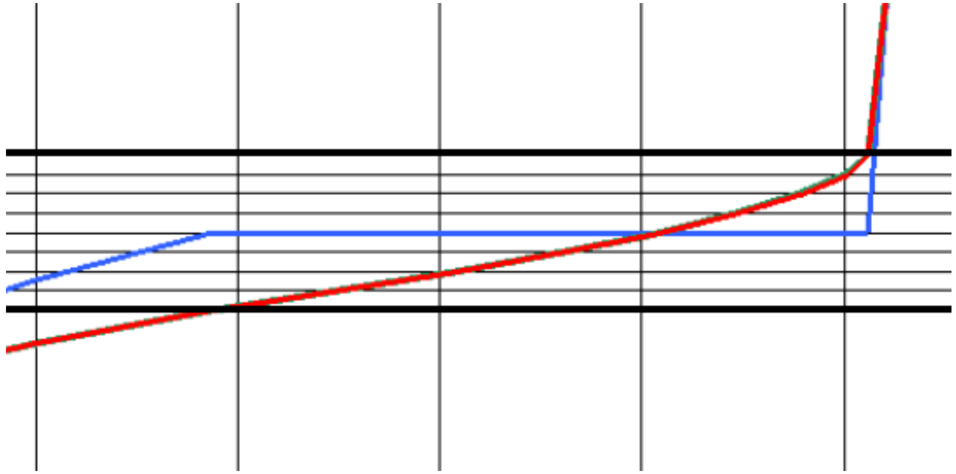
- Copy values on the interface (p corrected)
- Value on the interface is mean value across the fracture

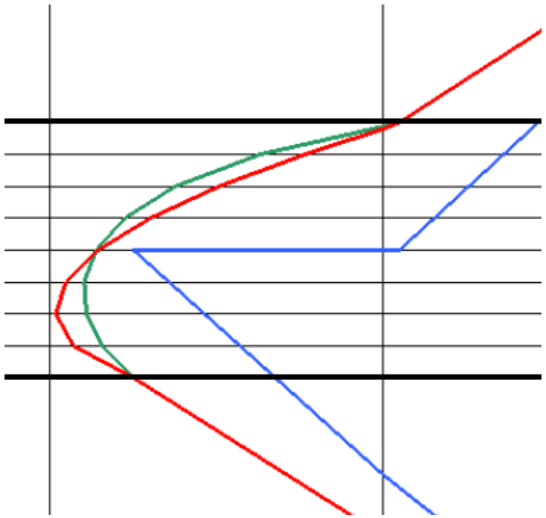
„Low -> Full“:

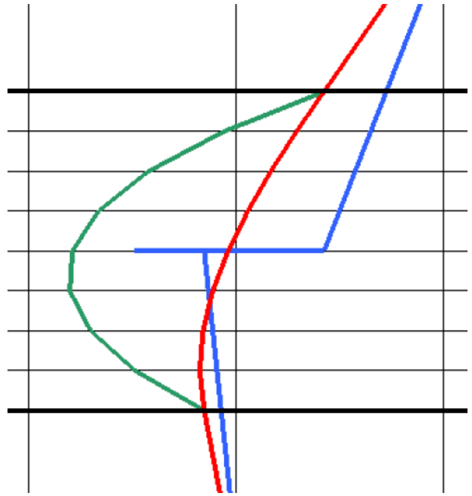
- We assume quadratic behaviour of the function in the fracture. Values on the interface with corrected p and mean values are given.

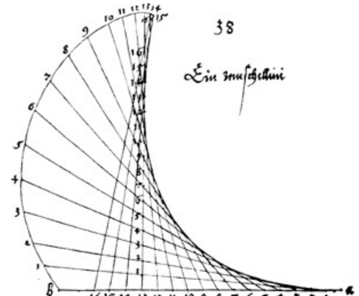
Transfer Operators











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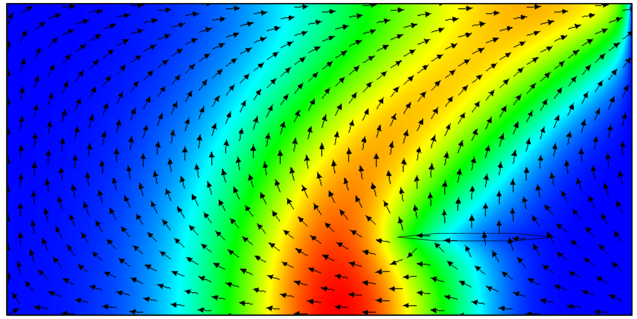
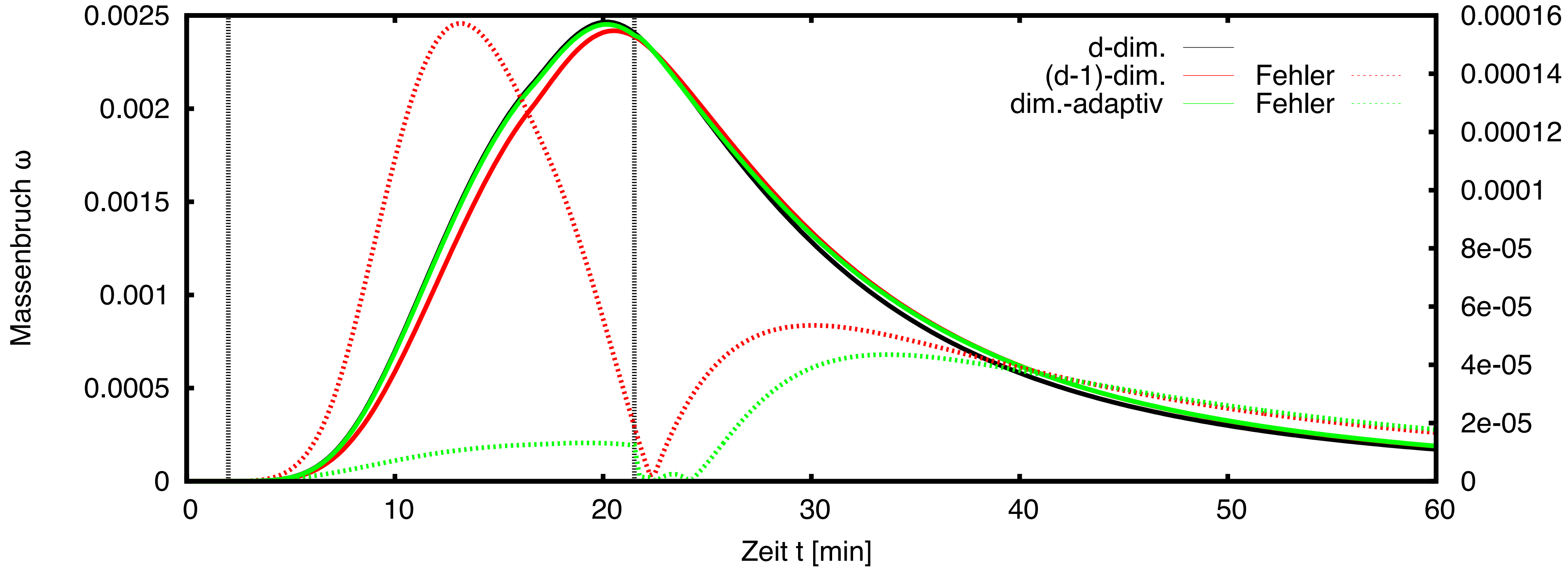
Dimensional Adaptivi

$\epsilon = 0.006$





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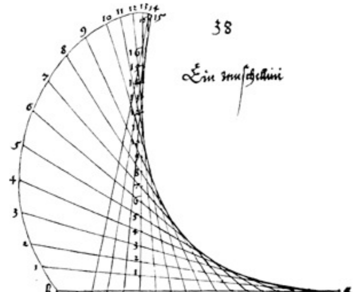
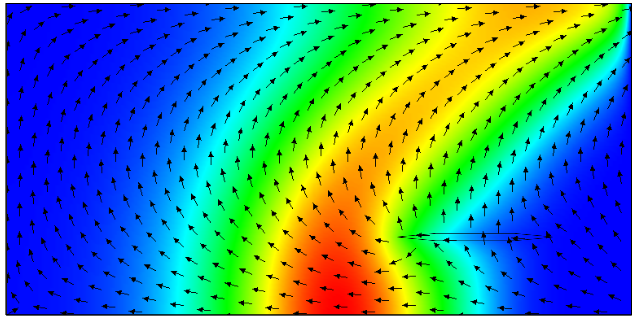
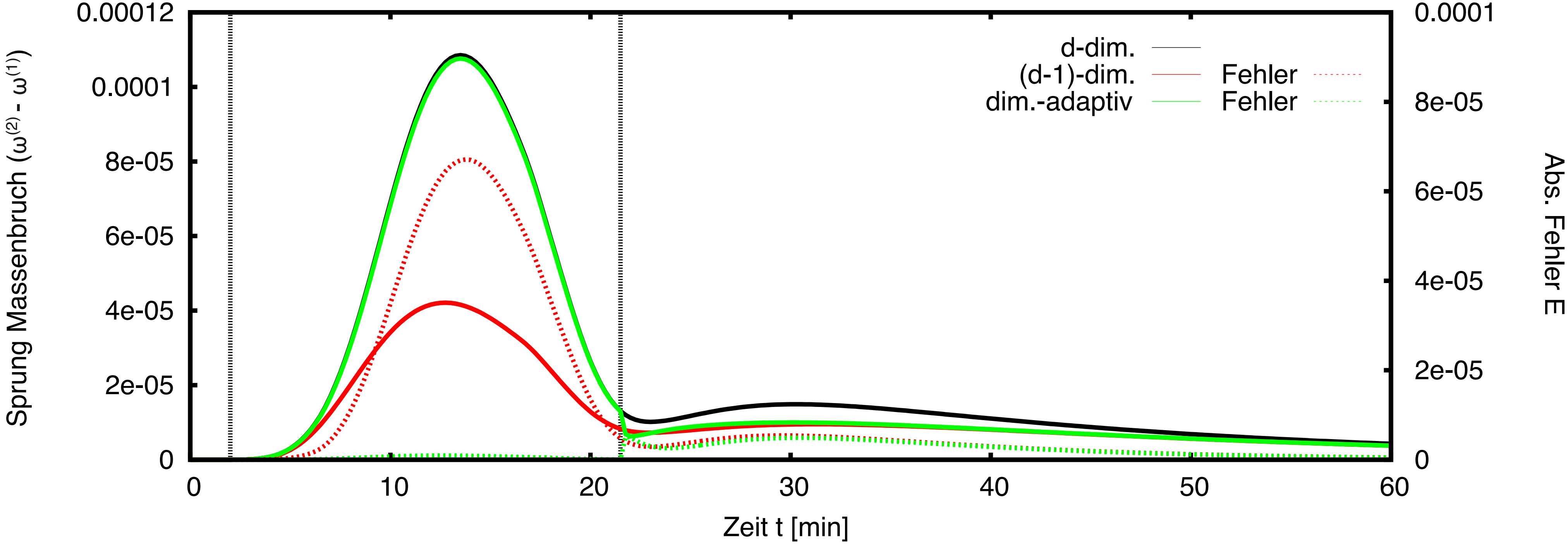


Dimensional Adaptivi



$\epsilon = 0.024$



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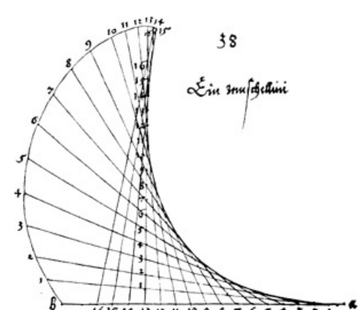
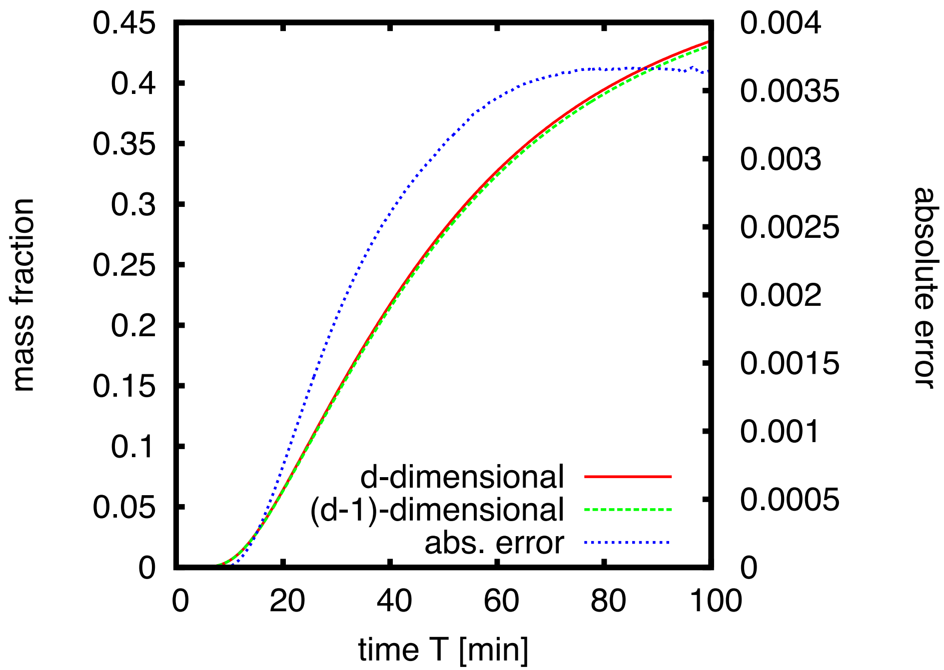
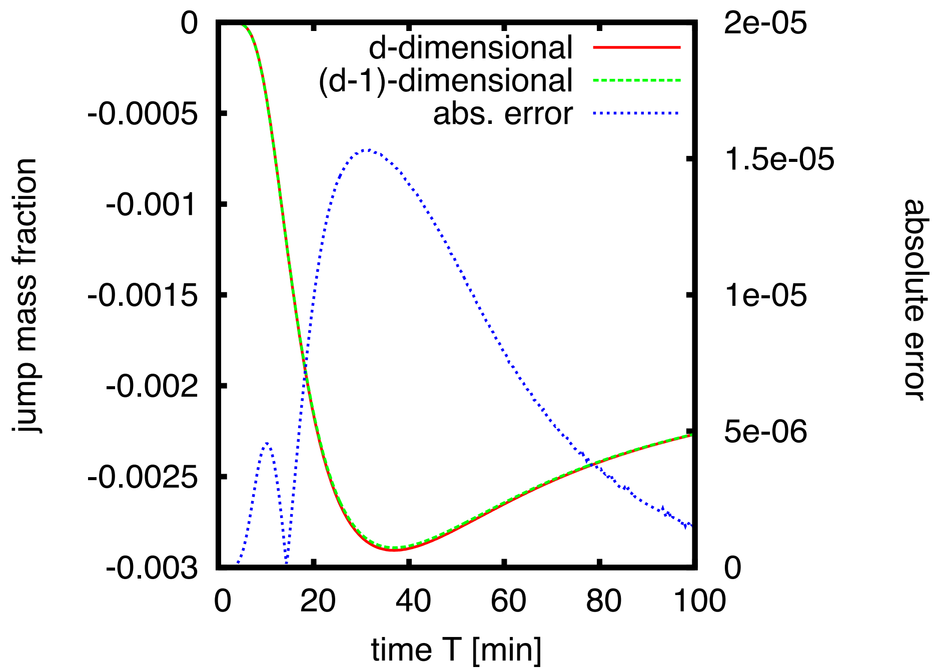


Comparison in 3d

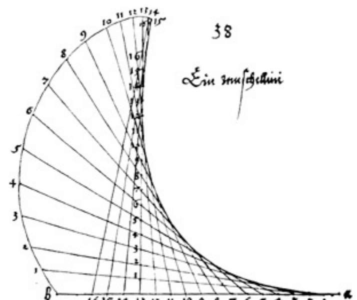
$\epsilon = 0.003$



c



$c_l - c_u$



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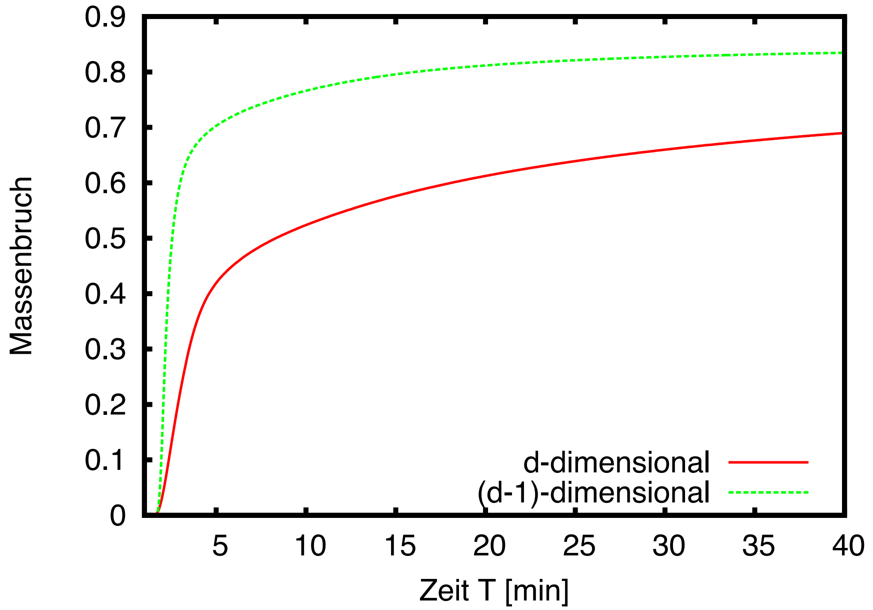
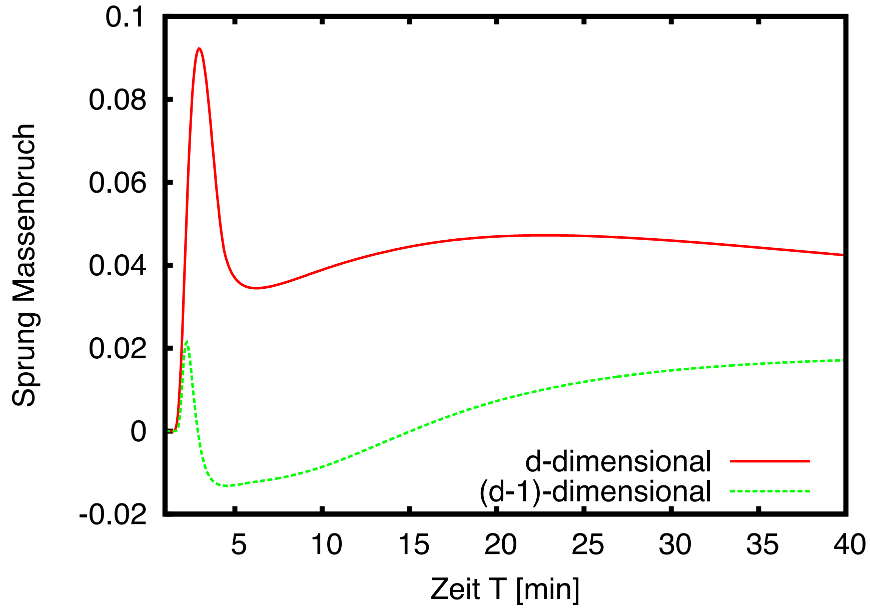
Comparison in 3d

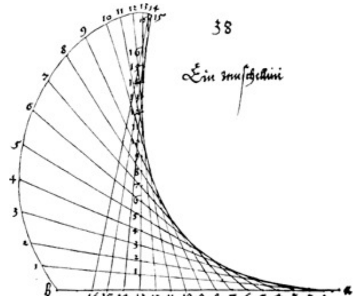
$\epsilon = 0.024$



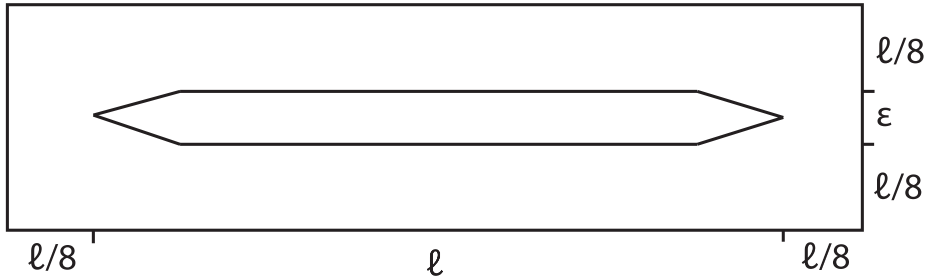
c



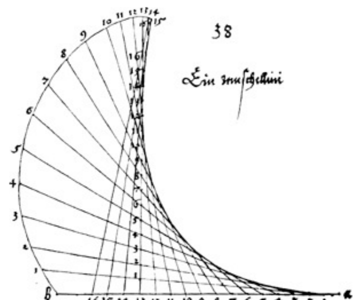
$c_l - c_u$



Test Example



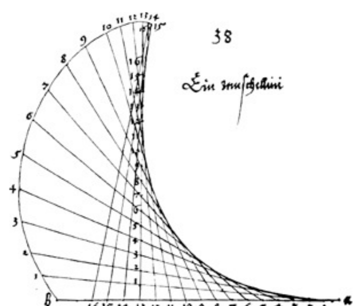
- Variation of
  - Thickness and length of fracture
  - Angle with gravity
  - Parameters (Conductivity,...)
  - Boundary conditions



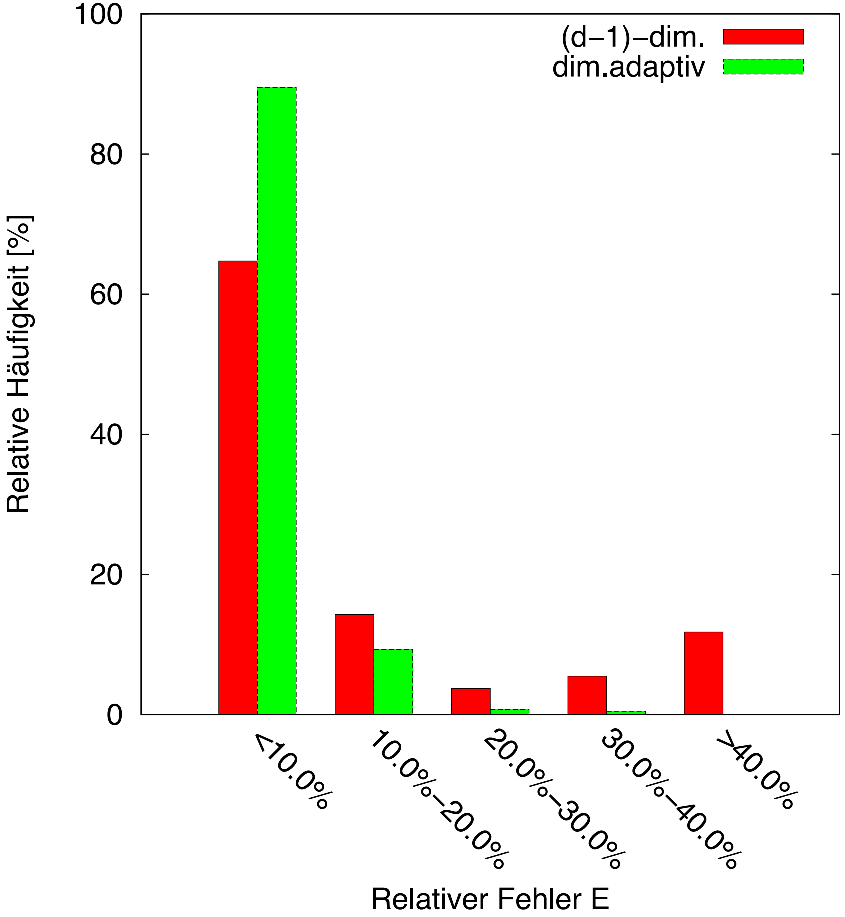
Test Example

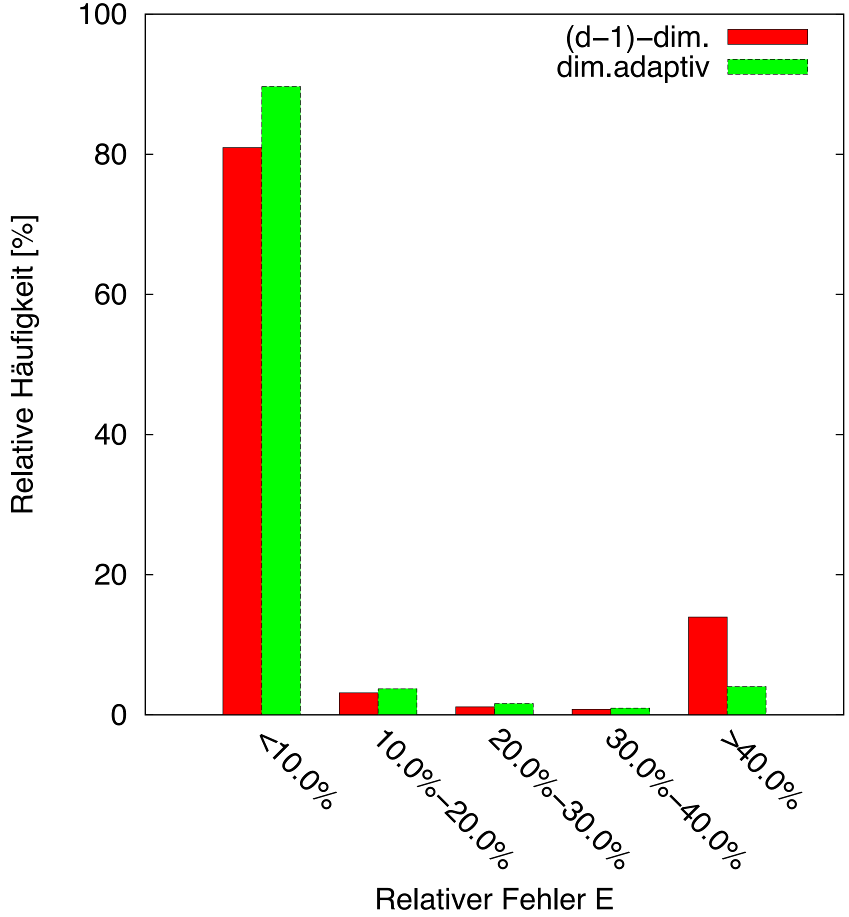
- 3 simulation runs for each configuration:
  - d-dimensional
  - (d-1)-dimensional
  - dimensional-adaptive

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



Test Example: Results





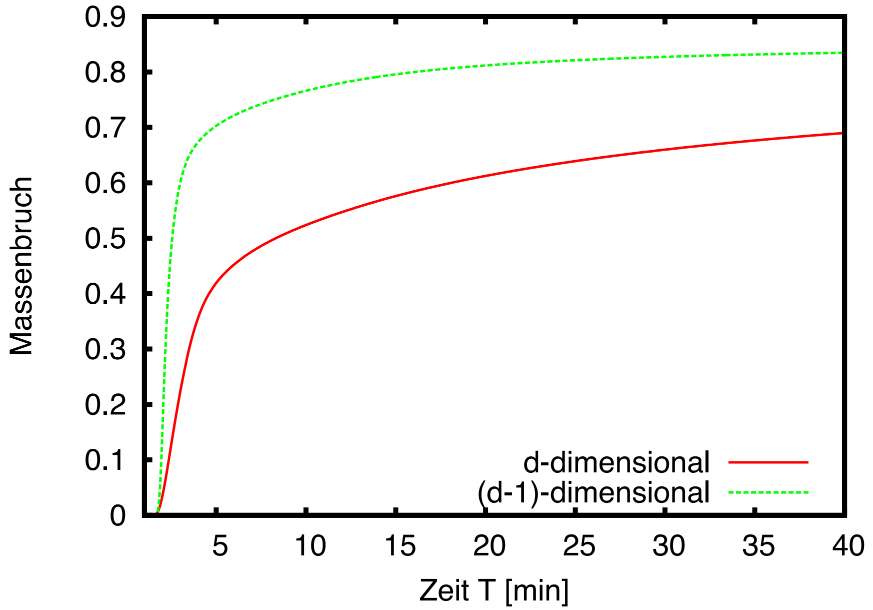
Test Example: Results

		$E_{\text{rel}}(\hat{\omega}_f)$ [%]		$E_{\text{rel}}(\omega_m^{(2)} - \omega_m^{(1)})$ [%]	
		$(d-1)$-dim.	dim.-adaptiv	$(d-1)$-dim.	dim.-adaptiv
Maximum	$\max_{\{i=1,\ldots,N\}} E_i$	87	31	> 100	76
Mean value	$\bar{E} = \frac{1}{N}\sum_{i=1}^{N} E_i$	12	2	24	4
Mean dev.	$\frac{1}{N}\sum_{i=1}^{N} \lvert E_i - \bar{E}\rvert$	14	3	40	7
0.75-Quantil	$F^{-1}(0.75)$	16	1	0	0
0.9-Quantil	$F^{-1}(0.9)$	34	5	28	3

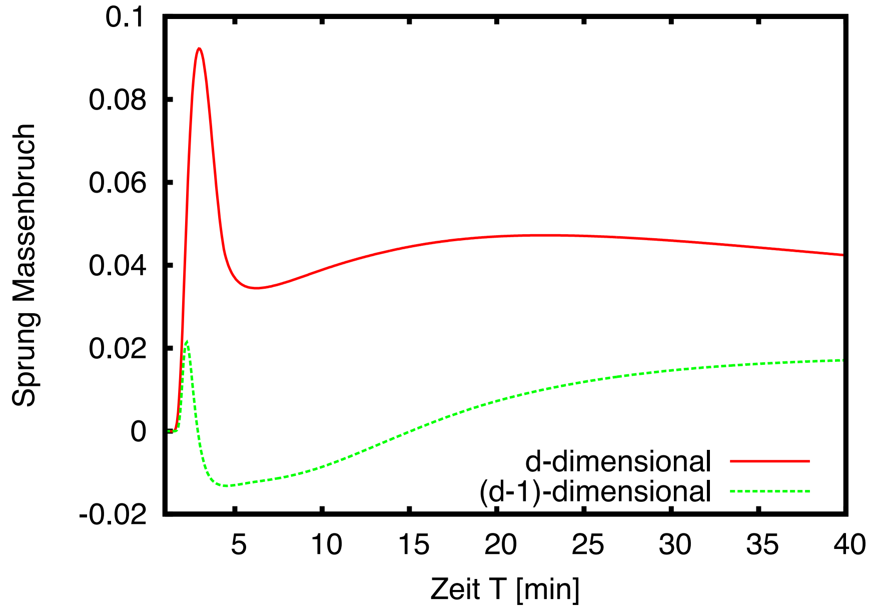
Statistics of N = 1261 test problems

Comparison in 3d

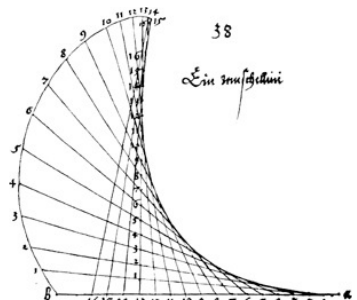
$\epsilon = 0.024$



c



$c_l - c_u$



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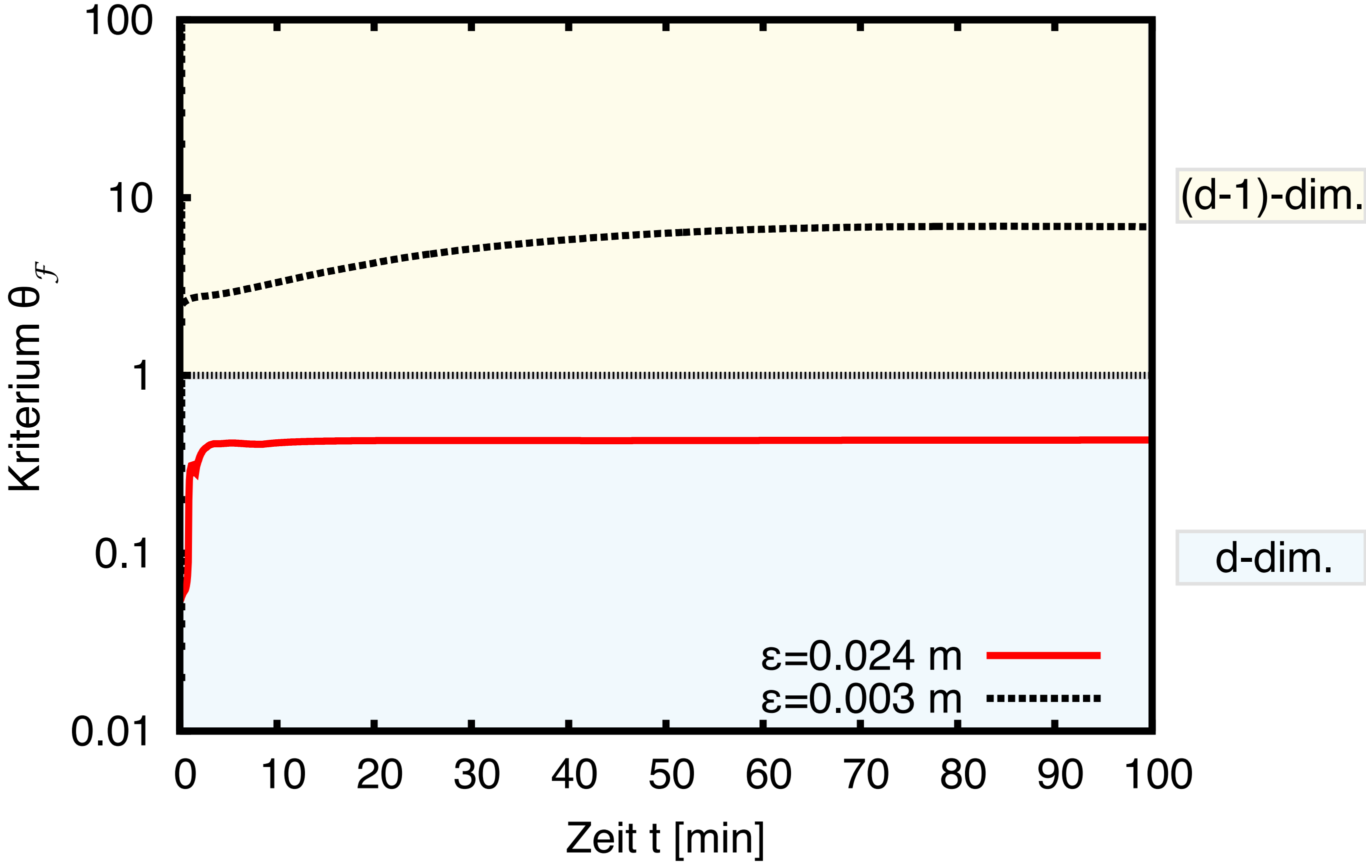
Results Criterion



Selected Publications

A. Grillo, D. Logashenko, S. Stichel, G. Wittum: Simulation of Density-Driven Flow in Fractured Porous Media. *Advances in Water Resources*, 2010

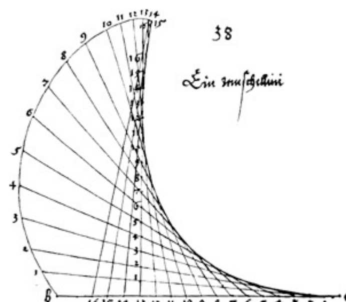
Alfio Grillo, Michael Lampe, Gabriel Wittum: Three-dimensional simulation of the thermohaline-driven buoyancy of a brine parcel. *Comput Vis Sci*, 2010

A. Grillo, M. Lampe, D. Logashenko, S. Stichel, and G. Wittum: Simulation of salinity- and thermohaline-driven flow in fractured por media. *J Por Med*, 2011

Grillo, A., Reiter, S., Logaschenko, D., Stichel, S., Wittum, G.: Models and simulations of variable-density flow in fractured porous media. *IJCSE*, 2013.

Grillo, A., Logashenko, D., Stichel, S., Wittum, G. (2014). Forchheimer's correction in modelling flow and transport in fractured porous media. *Computing and Visualization in Science*, 15(4), 169- 190

Reiter, S., Logashenko, D., Grillo, A., Wittum, G. (2014). Preparation of grids for simulations of groundwater flow in fractured porous media. *Computing and Visualization in Science*, 15(4), 209- 225



Transdermal Drug Delivery

D. Feuchter, M. Heisig, A. Nägel, S. Reiter,
A. Vogel, G. Wittum, R. Wittum
together with
S. Hansen, G. Lee,
C-M. Lehr, R. Lieckfeldt, U. Schäfer

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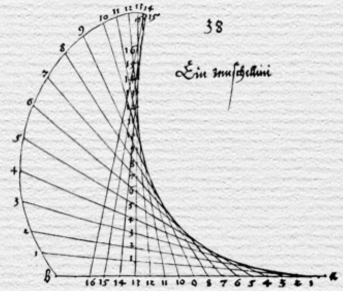
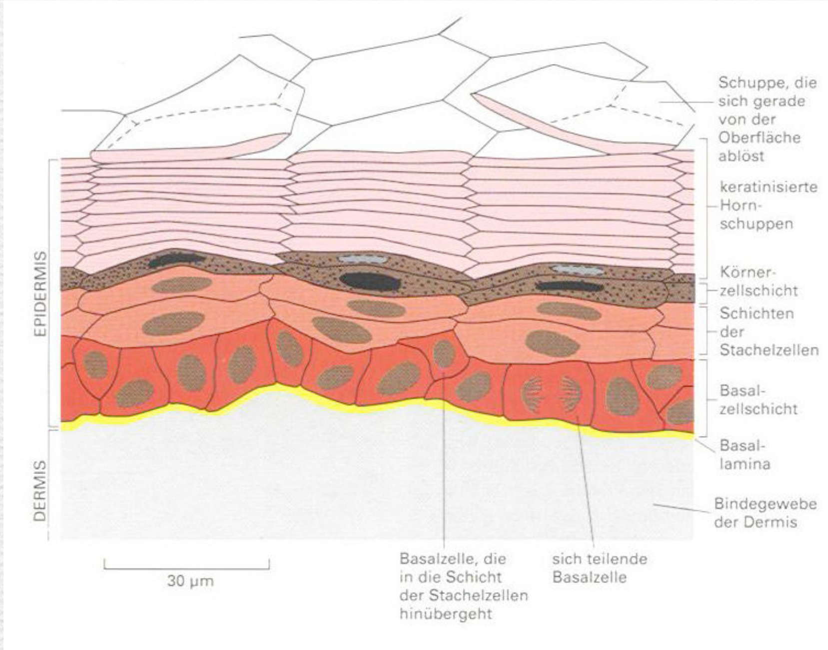
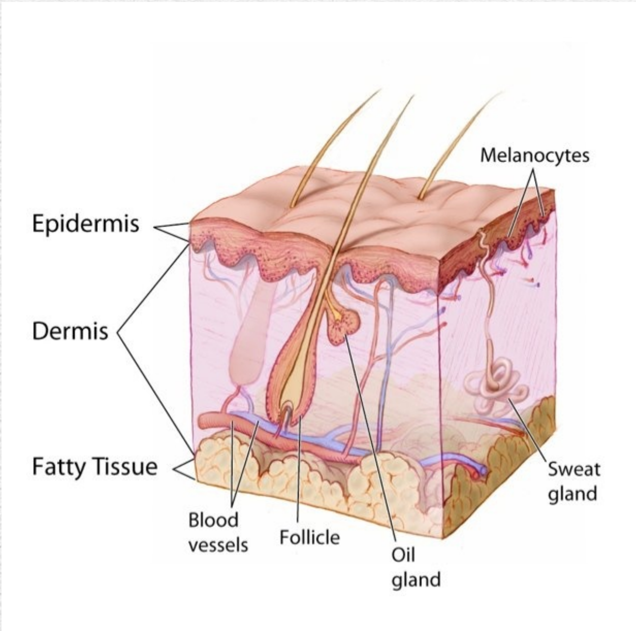


Skin Anatomy



Primary Barrier:
Stratum Corneum (SC)



Goals:

- Characterize Barrier (Permeability, Lag Time)
- Prediction of behavior in an exposure scenario

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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

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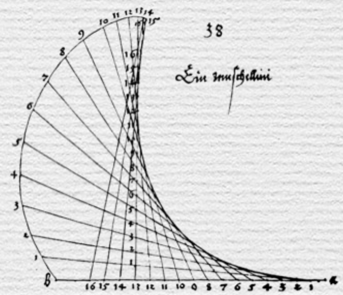
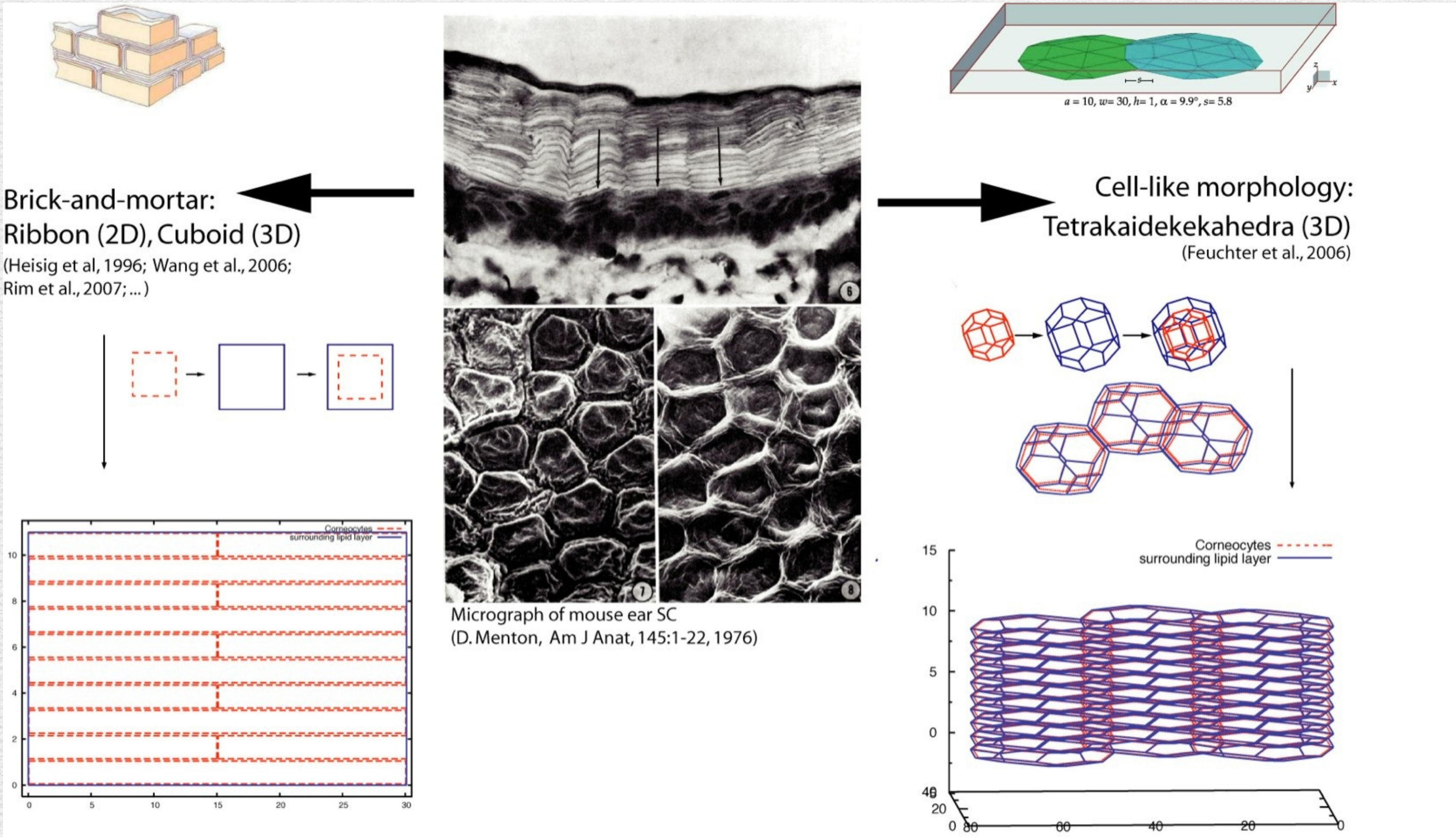


Detailed SC Models



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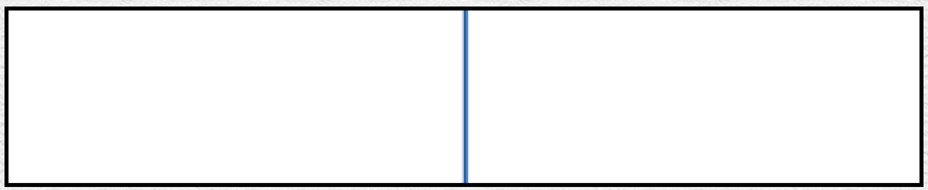
Grid Problem

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



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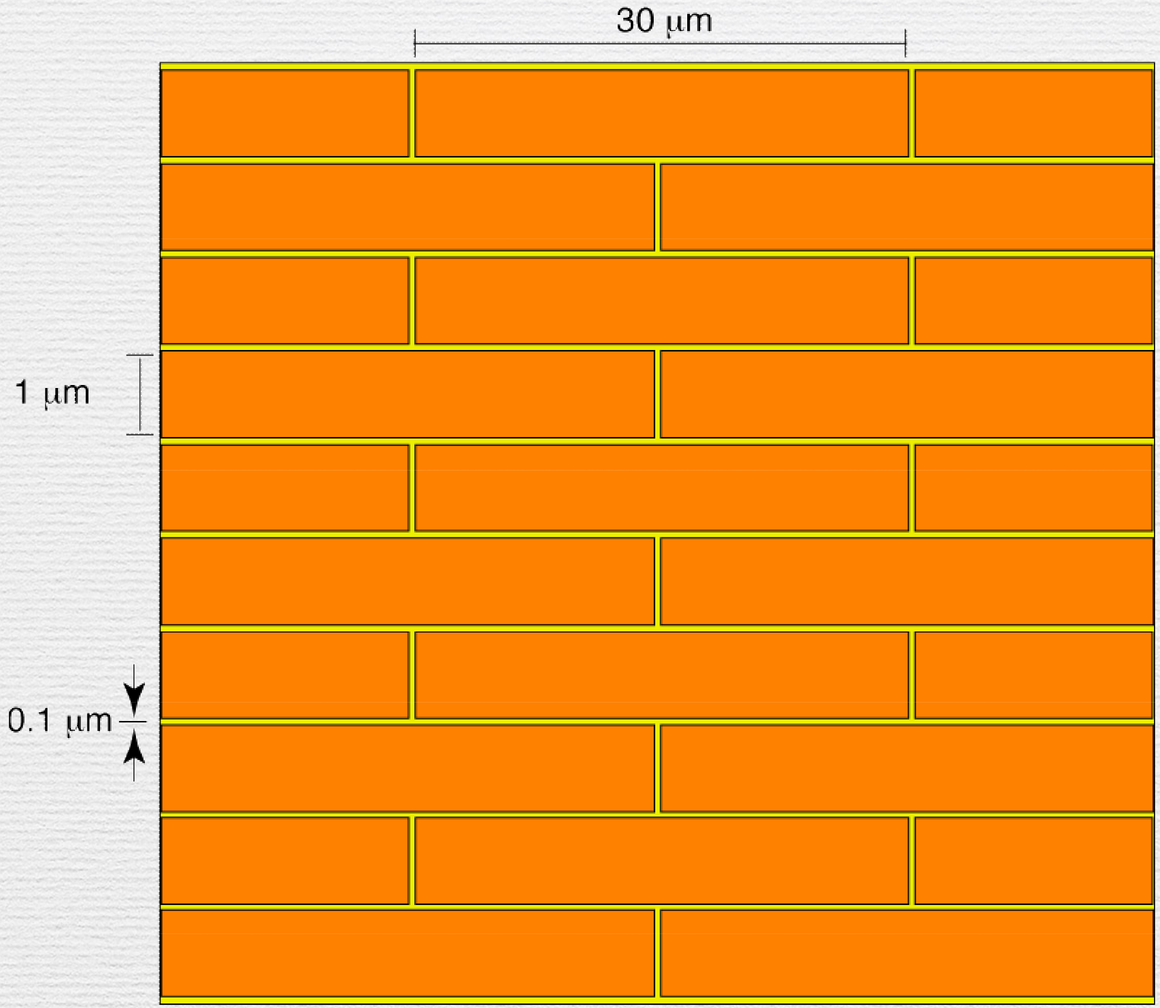
2d Brick and Mortar



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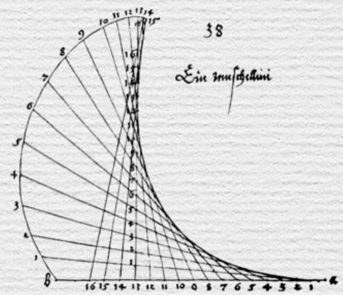
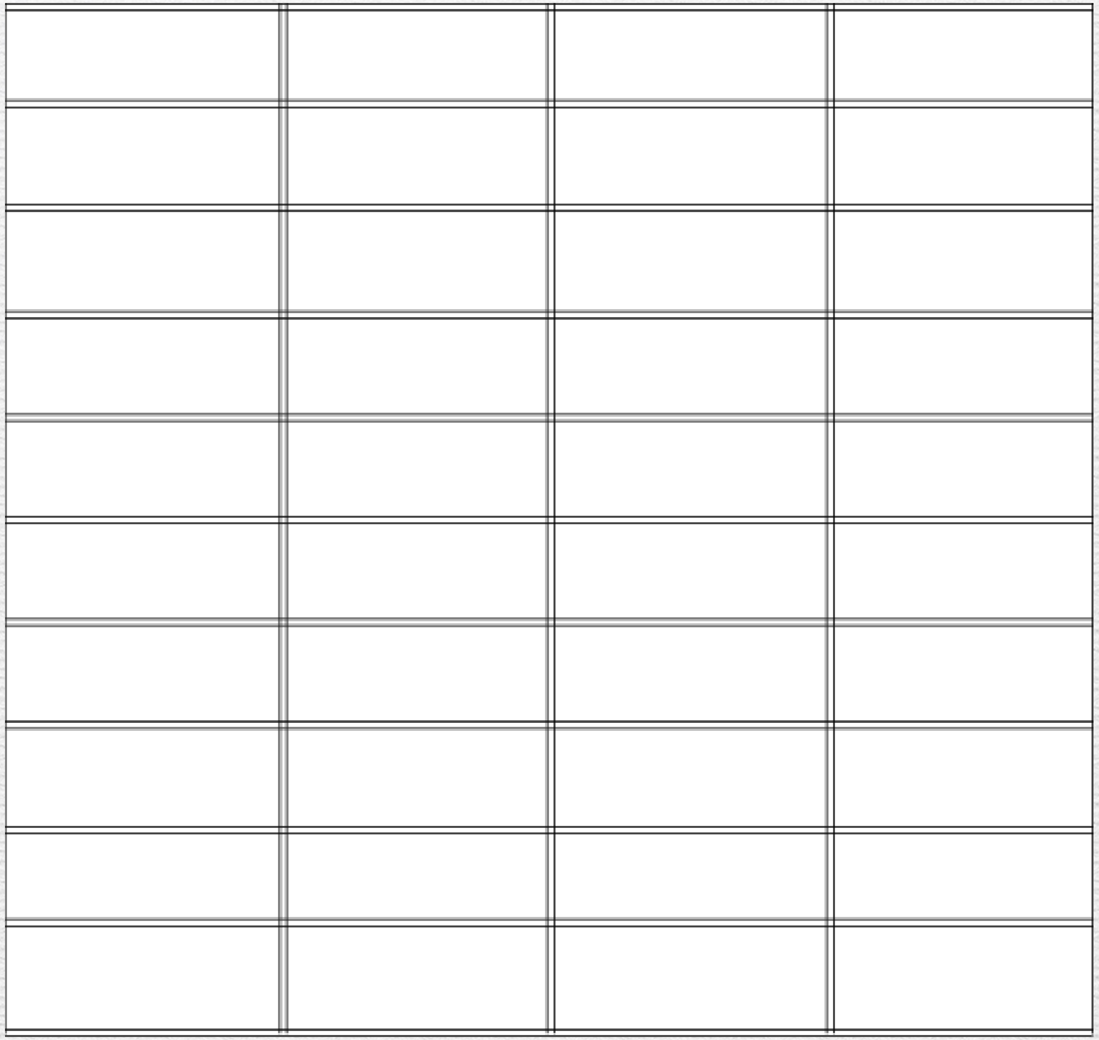


Base Grid

Gridlines follow jumps of coefficients



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Grid Problem

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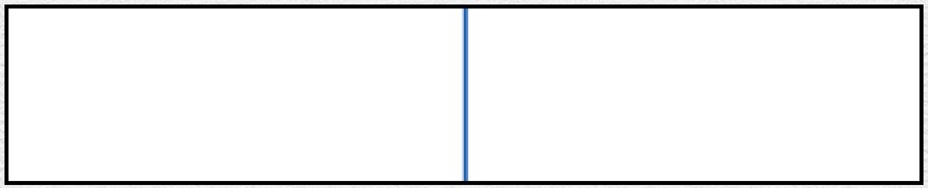

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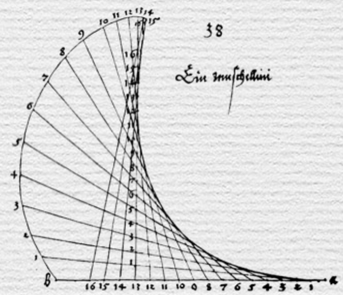
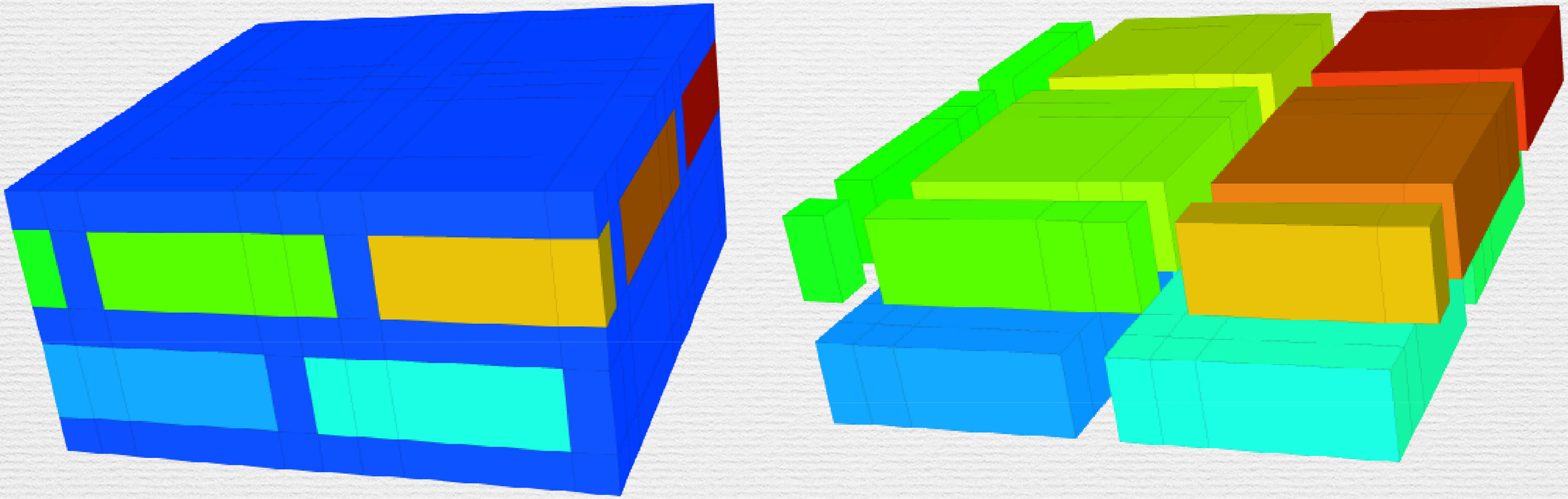
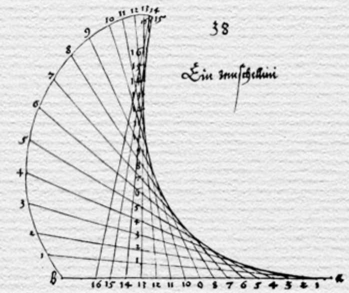


Geometry Models

- 3d Cuboid Model



Cuboid modeller (C. Wagner, 2007)



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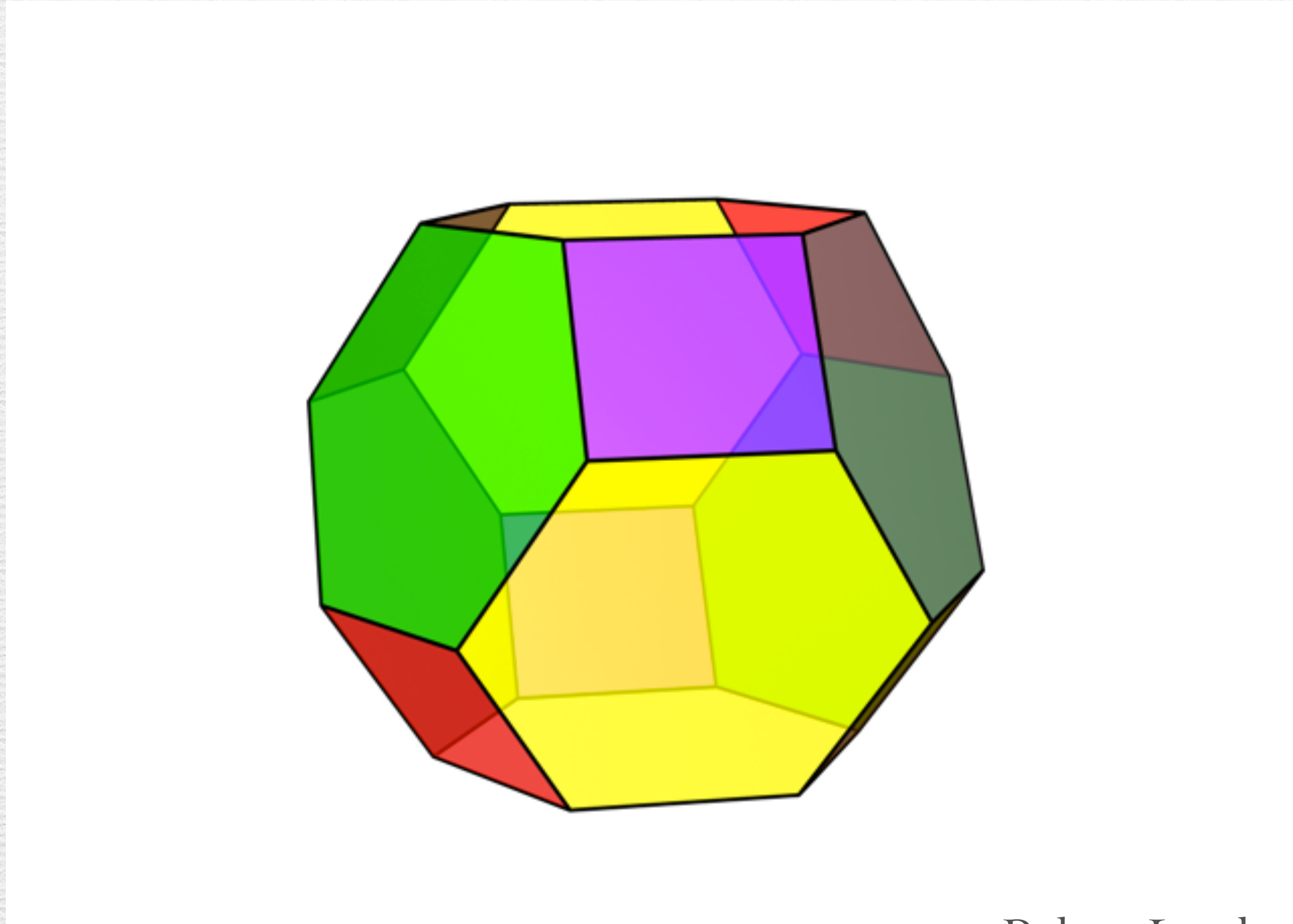
Tetrakaidekahedron (TKD)



Babett Lemke

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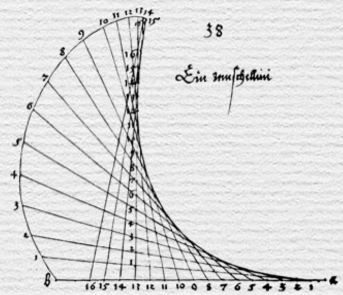
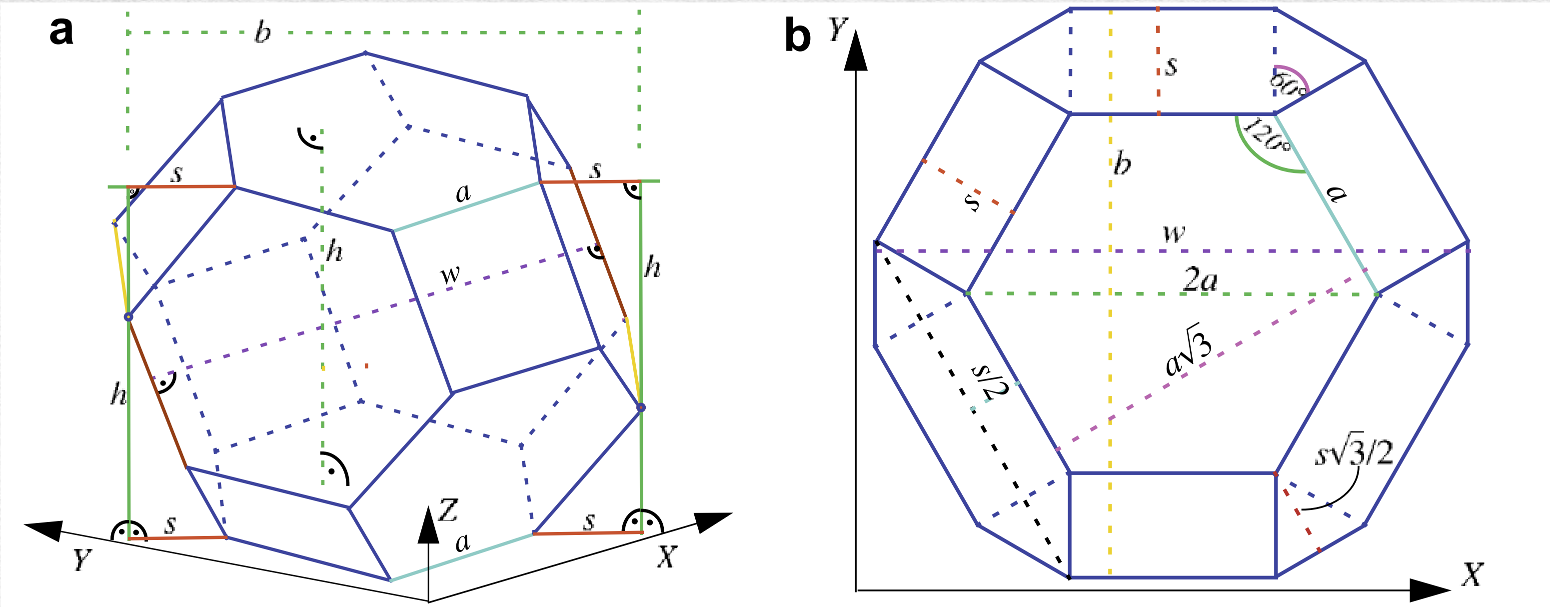
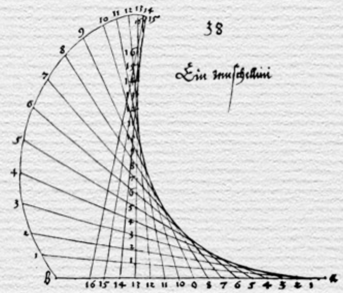


Geometry Models

- 3d Tetrakaidekahedra Model





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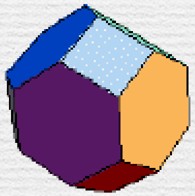
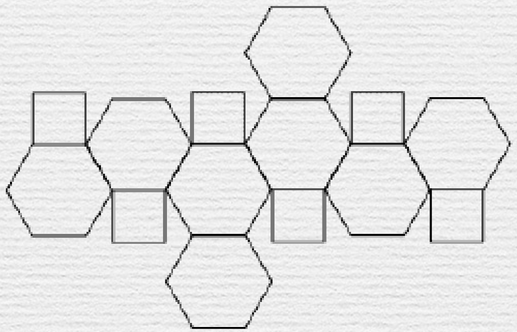
Tetrakaidekahedra Model

- Basic Element:
  - Tetrakaidekahedron (14 faces)





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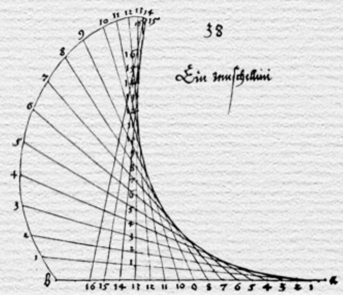
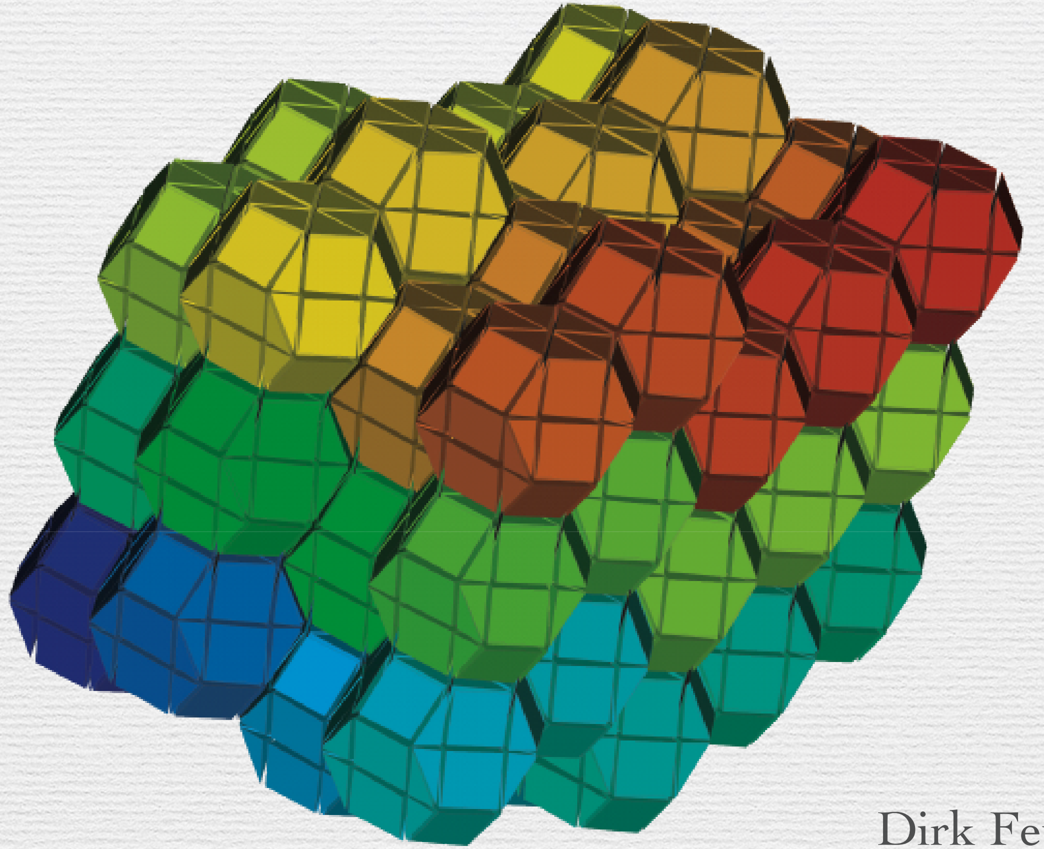


Cluster of TKDs

- 3d Tetrakaidekahedra Model



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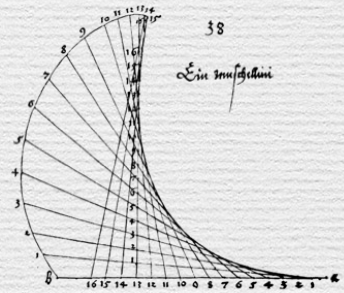

Tetrakaidekahedra Model

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

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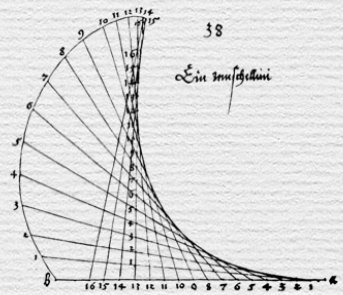

TKD for cells in tissue

- 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

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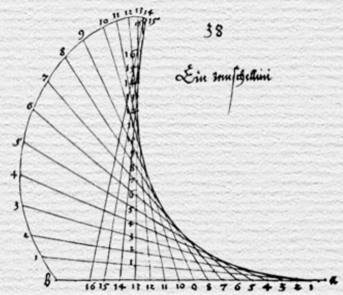
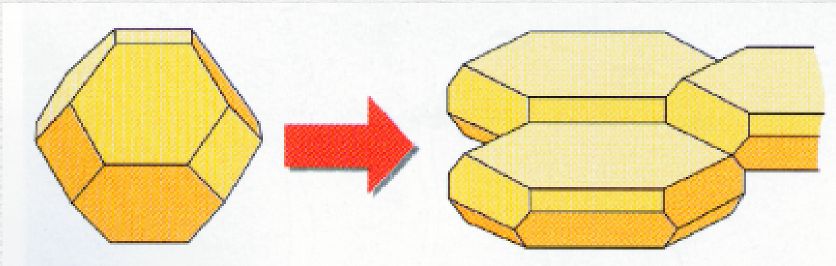


Tetrakaidekahedra Model

- Flattening of Corneocytes



Dirk Feuchter

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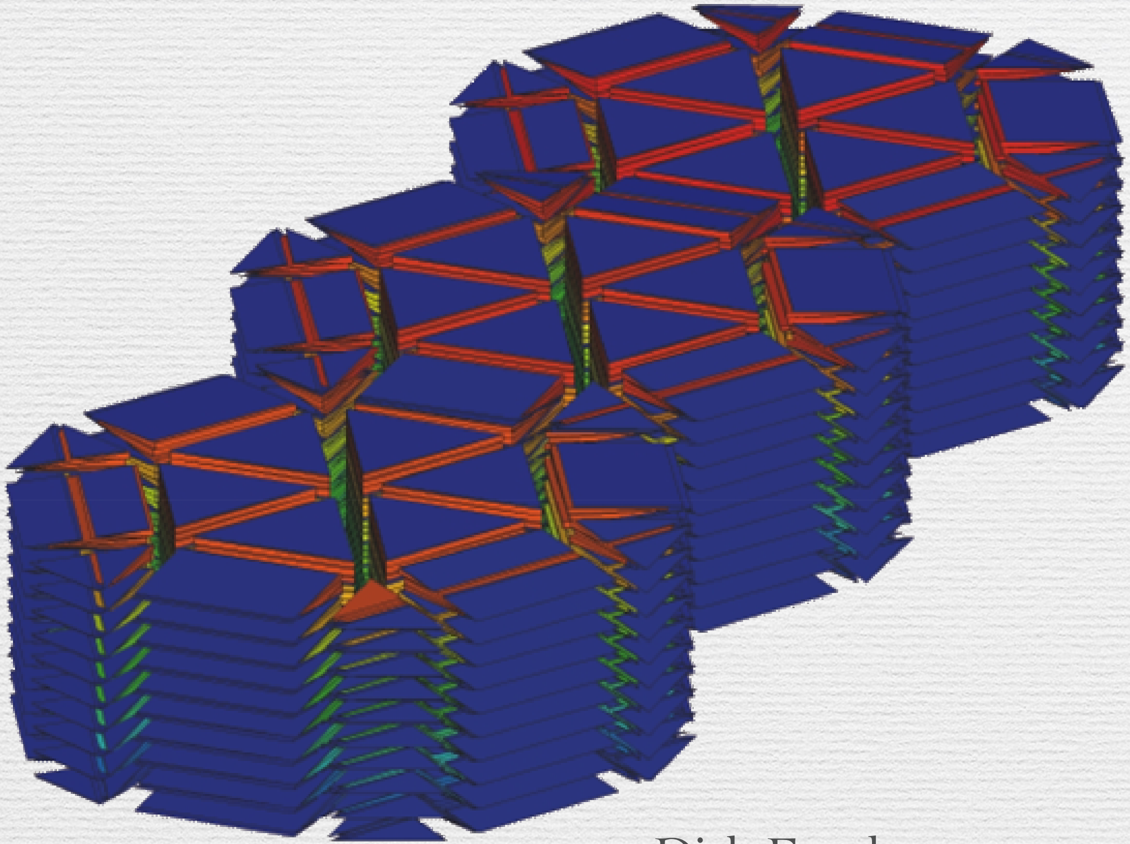
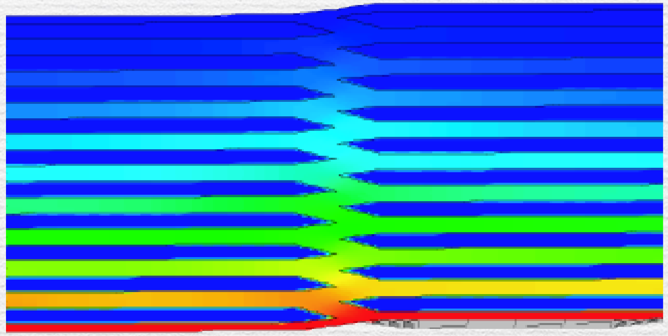
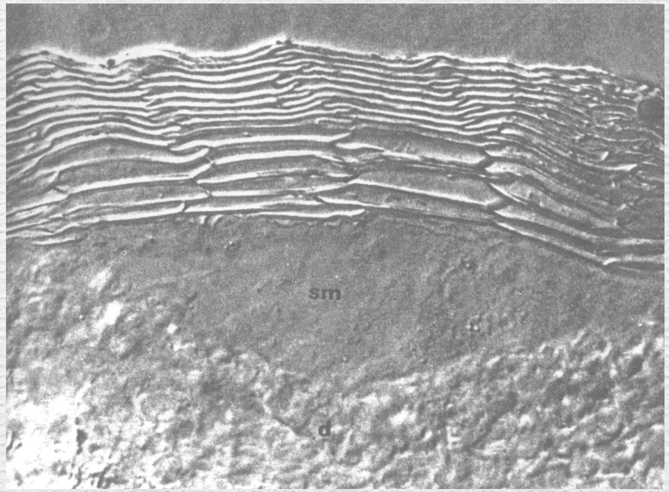
Tetrakaidekahedra Model



Dirk Feuchter





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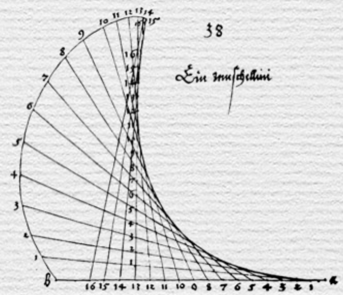

Process Model: Diffusion

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

$$\text{with } \mathbf{D}(x) = \begin{cases} \mathbf{D}_{Lip}(x) & \text{for } x \in \text{ Lipid .} \\ \mathbf{D}_{Cor}(x) & \text{for } x \in \text{ Corneocyte .} \end{cases}$$

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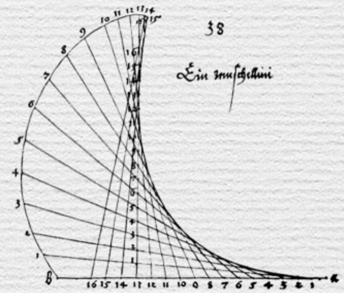

Process Model: Diffusion

Boundary and initial conditions

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

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

Transmission conditions on internal interfaces

$$\mathbf{D}_{Lip} \nabla c_{Lip}(x,t) \cdot \overrightarrow{n} = \mathbf{D}_{Cor} \nabla c_{Cor}(x,t) \cdot \overrightarrow{n}$$

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

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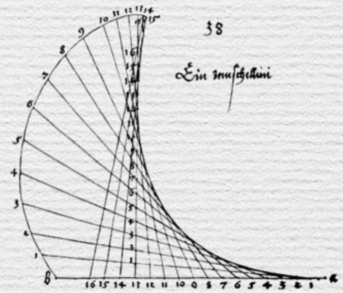
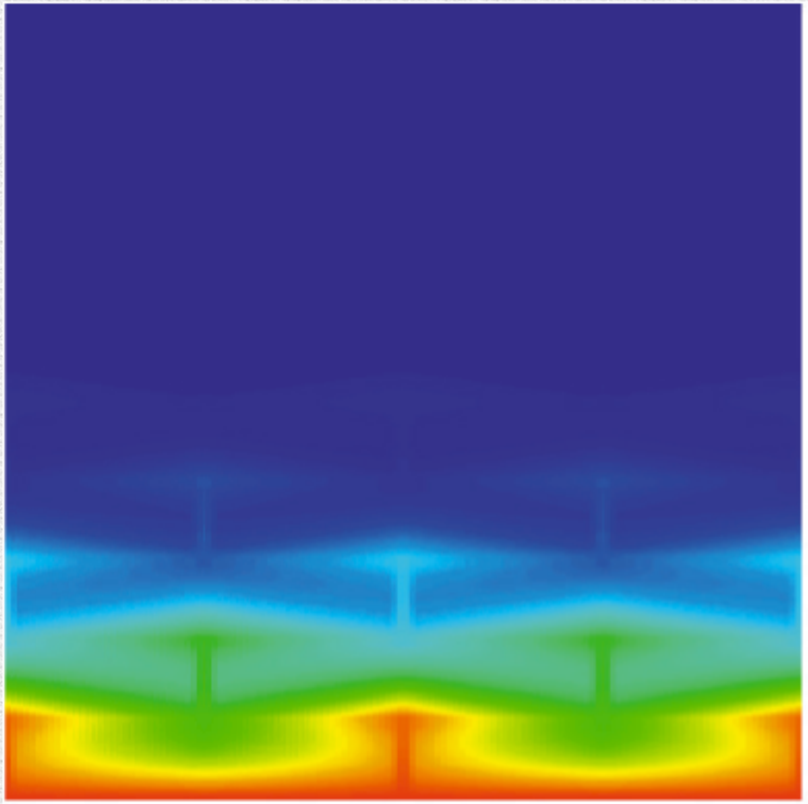
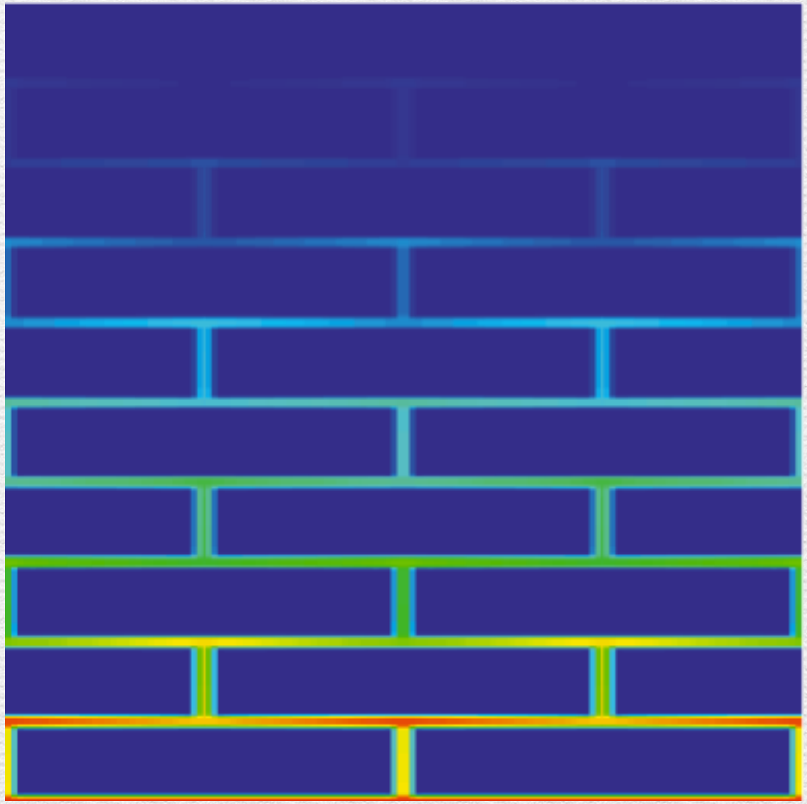


Simulation Results $T = T_\infty / 3$



$\varepsilon = 10^{-4}$



$\varepsilon = 10^{-6}$

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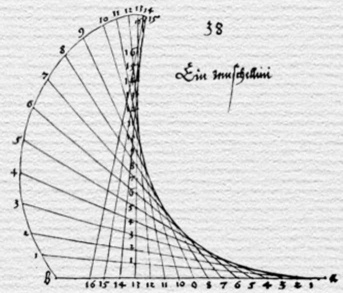
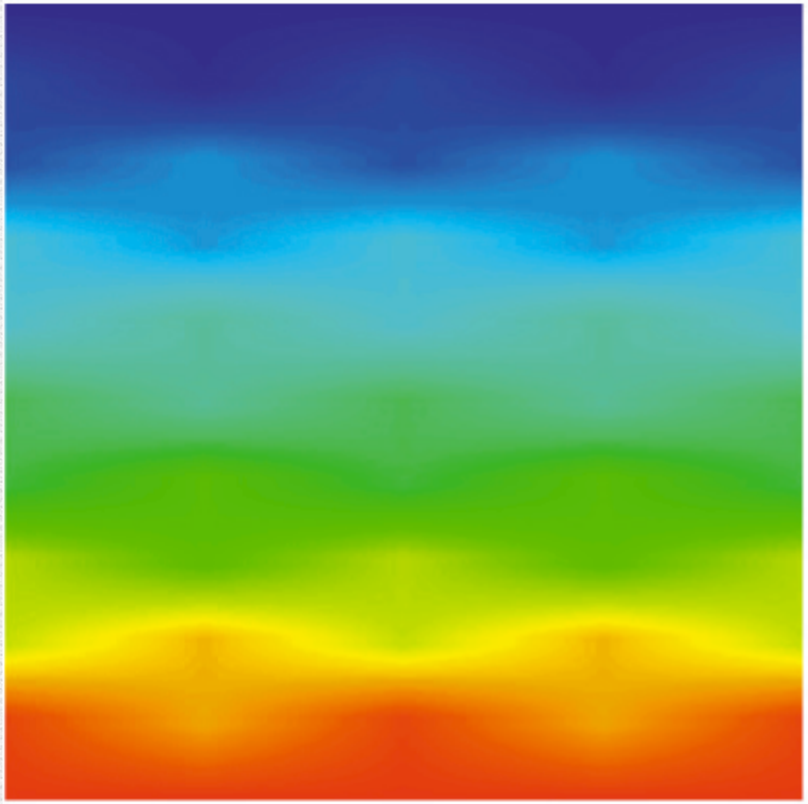
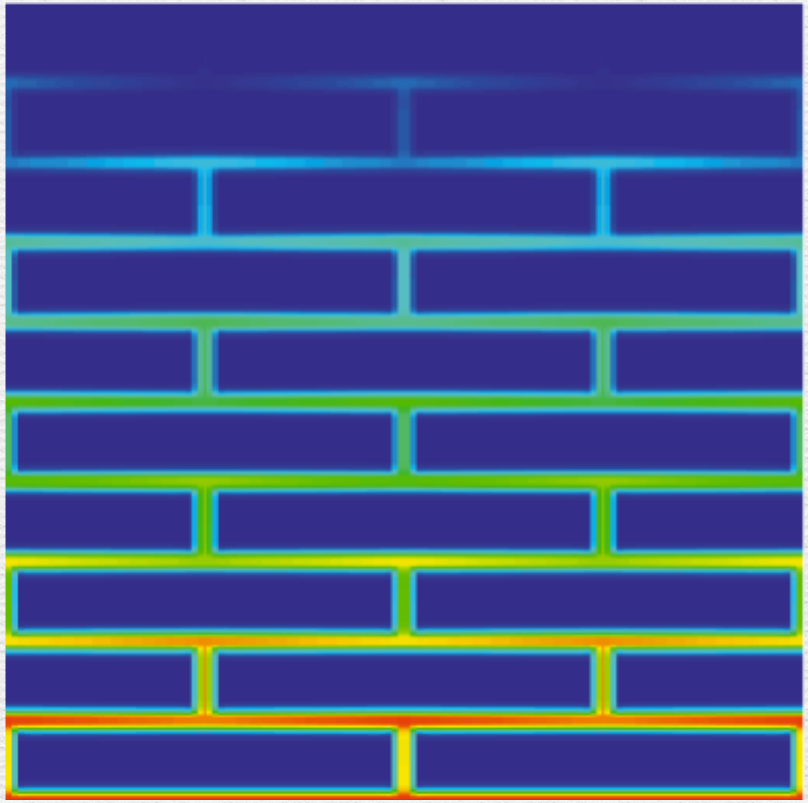


Simulation Results $T=2T_\infty/3$



$\varepsilon = 10^{-4}$



$\varepsilon = 10^{-6}$

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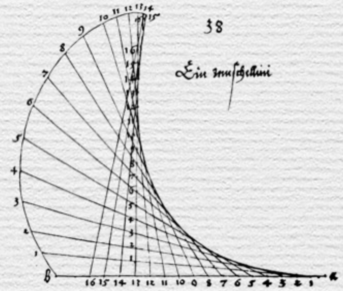
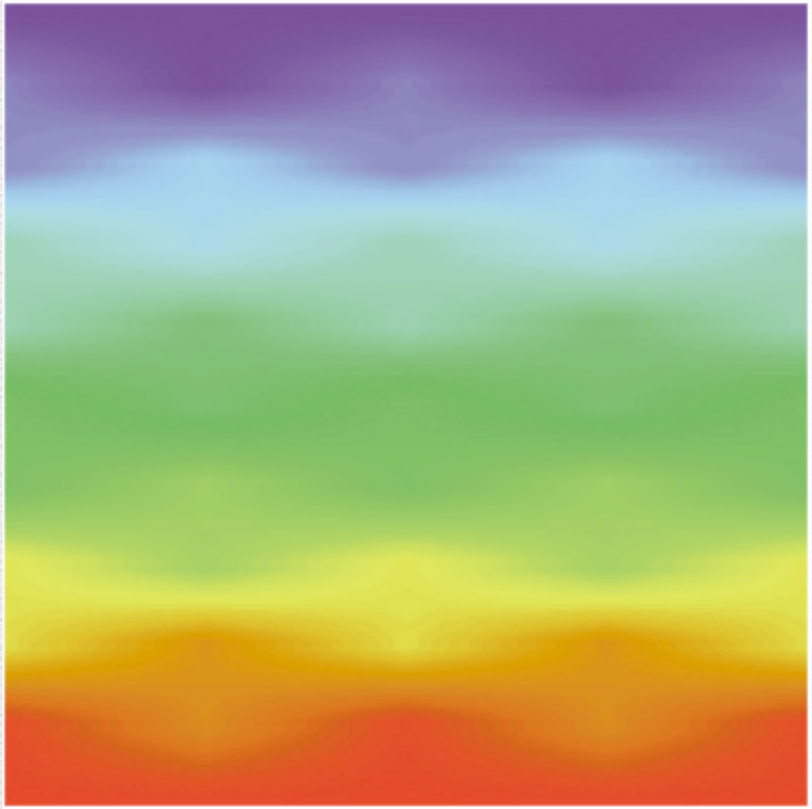
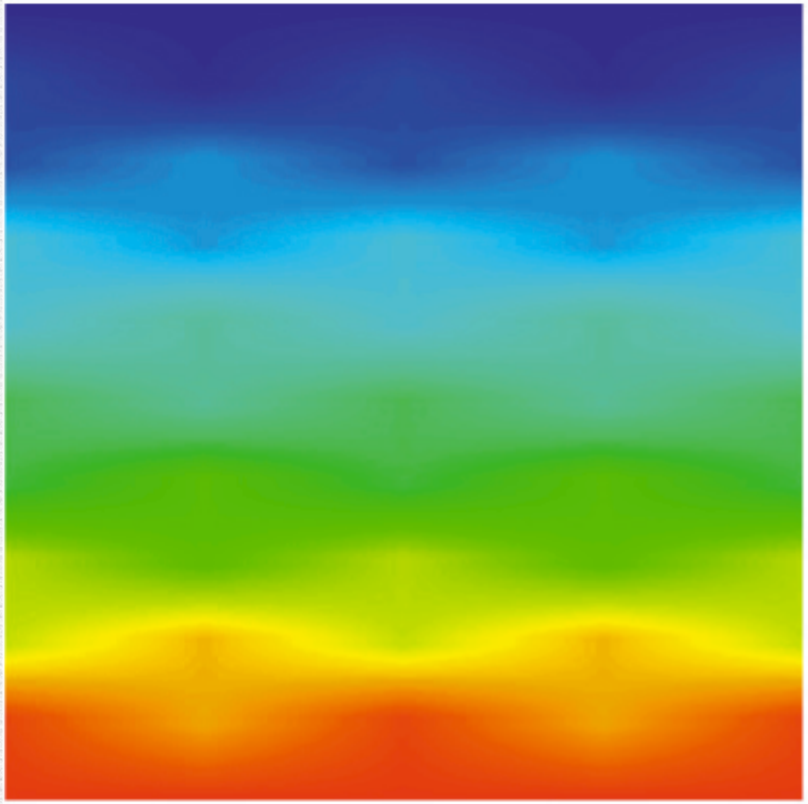


Simulation Results T=T∞



$\varepsilon = 10^{-4}$



$\varepsilon = 10^{-6}$

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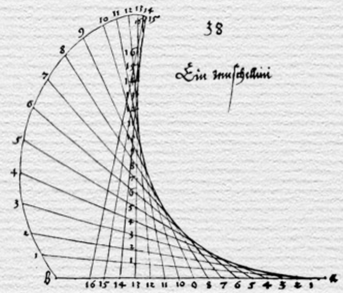

Characterization

- Flux across upper boundary

$$F_{\Gamma_0}(t) = \int_{T_0} D \frac{du}{dt} d\sigma = f_\infty + \sum_j \alpha_j e^{-\lambda_j t}$$

- Mass transported across upper boundary

$$M_{\Gamma_0}(T) = \int_0^T F_{\Gamma_0}(t) dt = f_\infty T + m_0 + \sum_j \beta_j e^{-\lambda_j t} .$$

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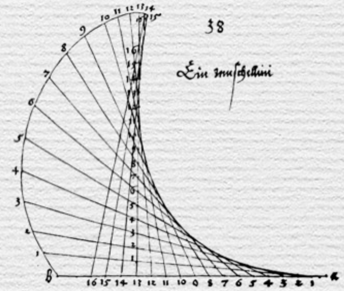
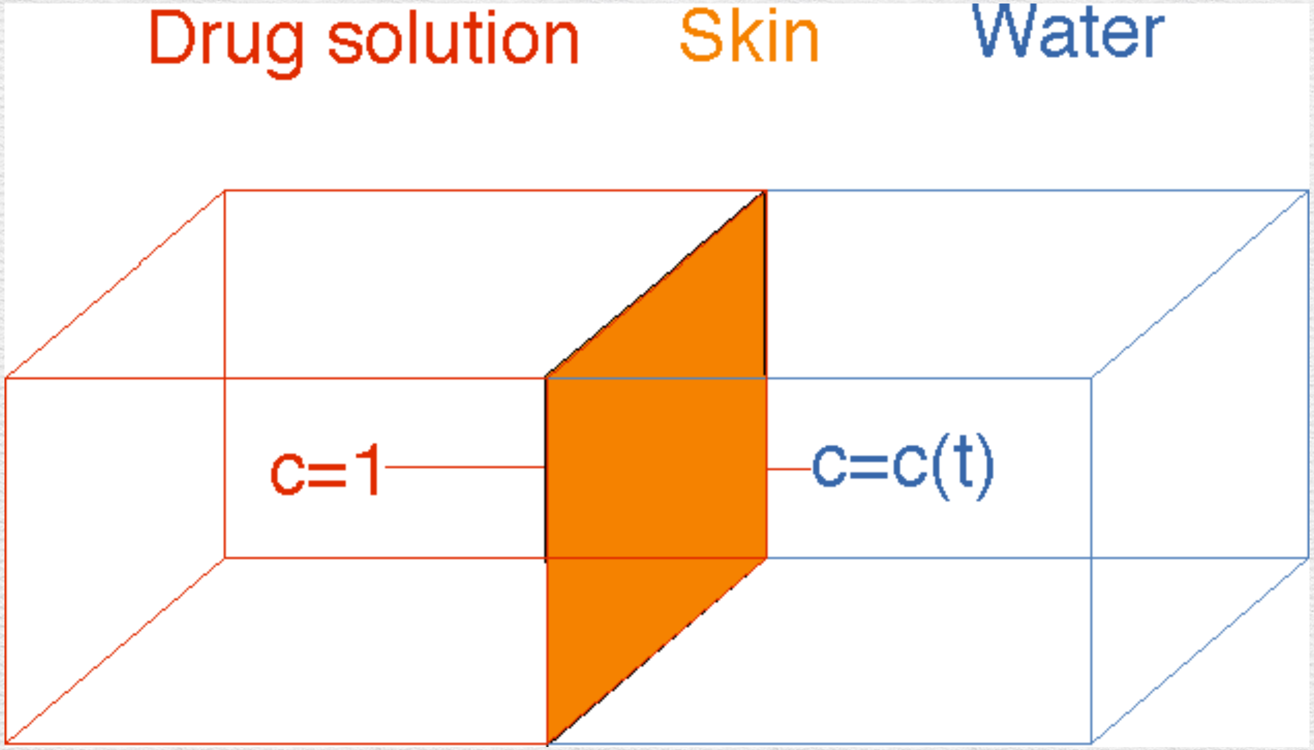
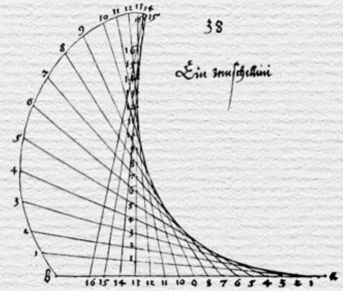


Experiment (schematic)





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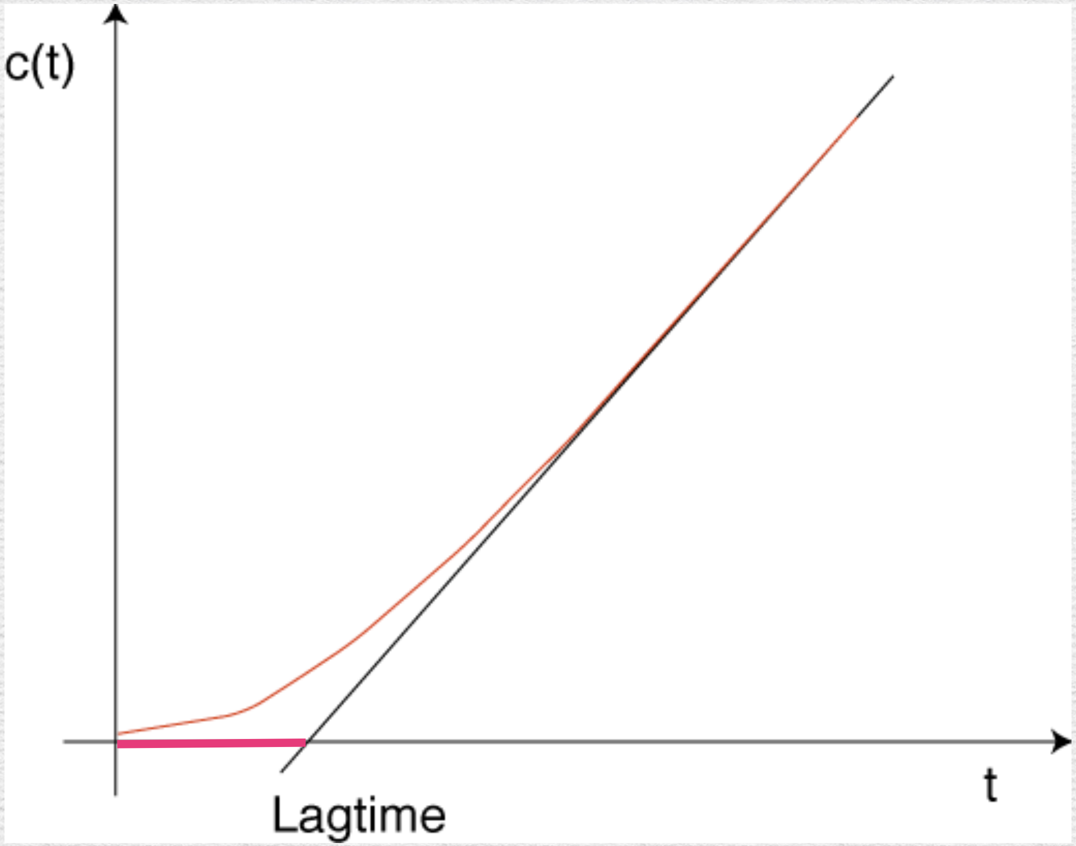
Characterization Lag Time



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Analytical Solutions

1. $\varepsilon = 1$ (homogenuous membrane): $T_{lag} = 20$ sec

2. $\varepsilon = 0$ (impermeable corneocytes): $T_{lag} \approx 1$ h

$$T_{lag,\infty} = \frac{L^2}{6D}$$

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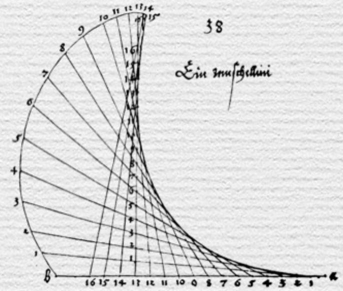
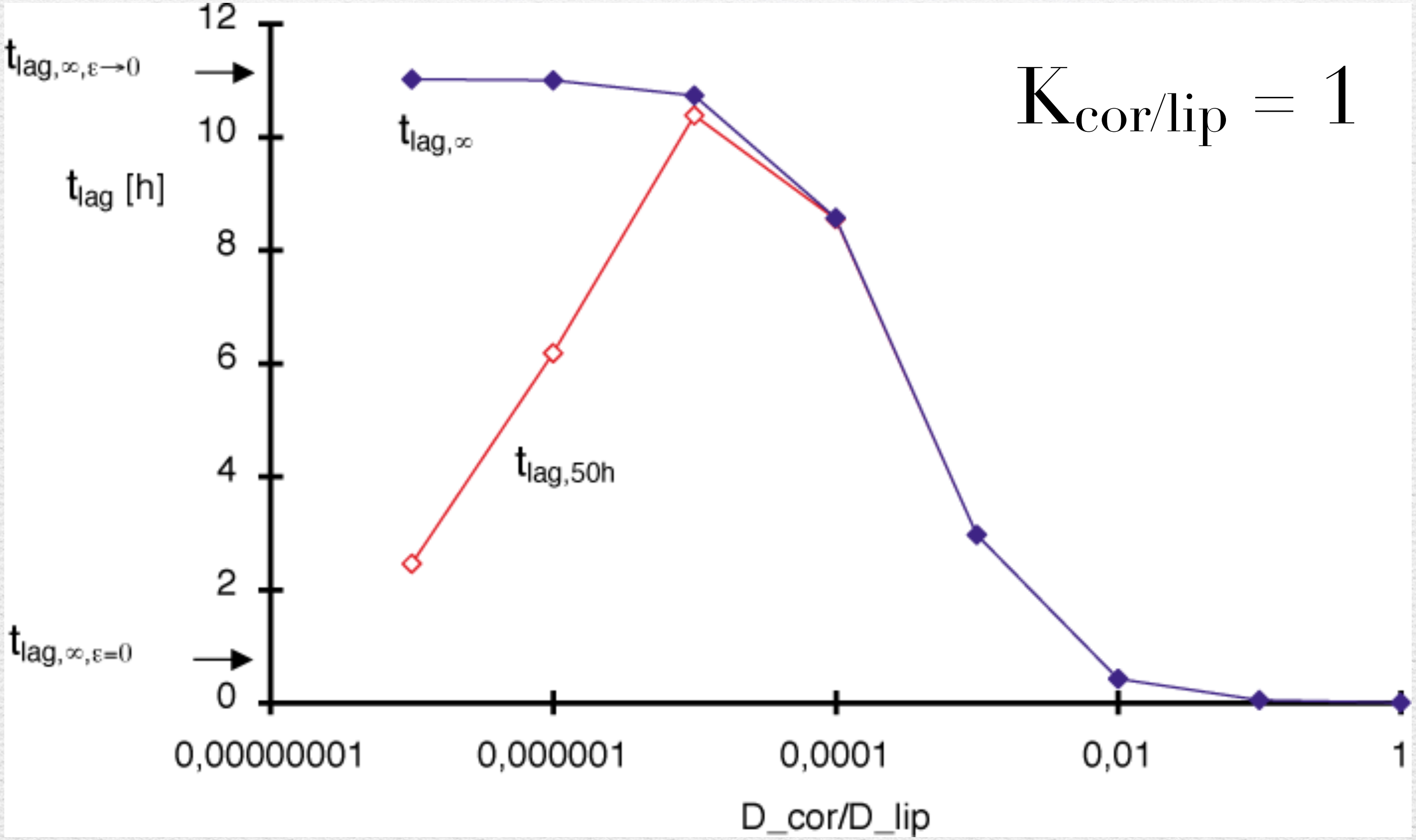


Computed Lag Times



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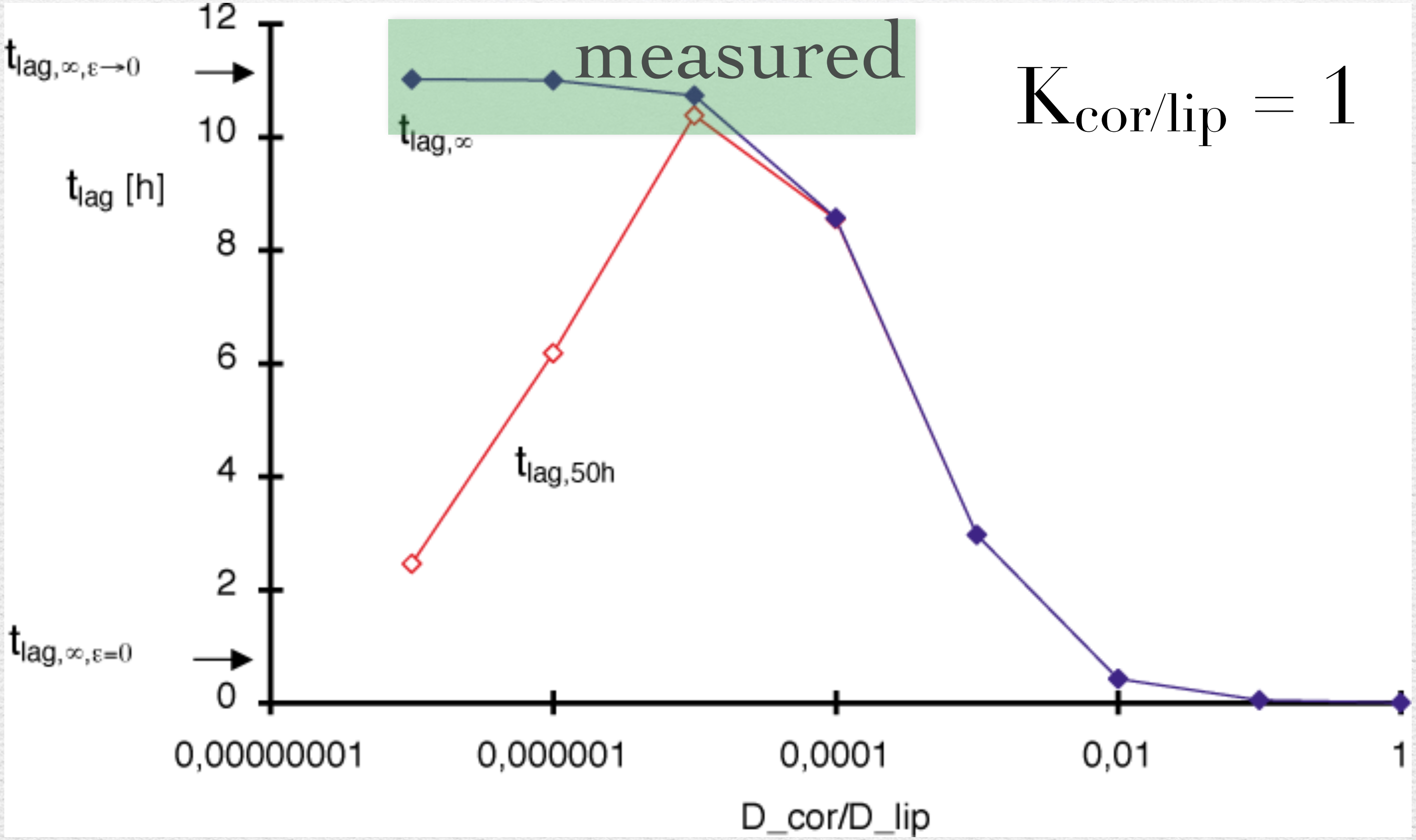
Computed Lag Times



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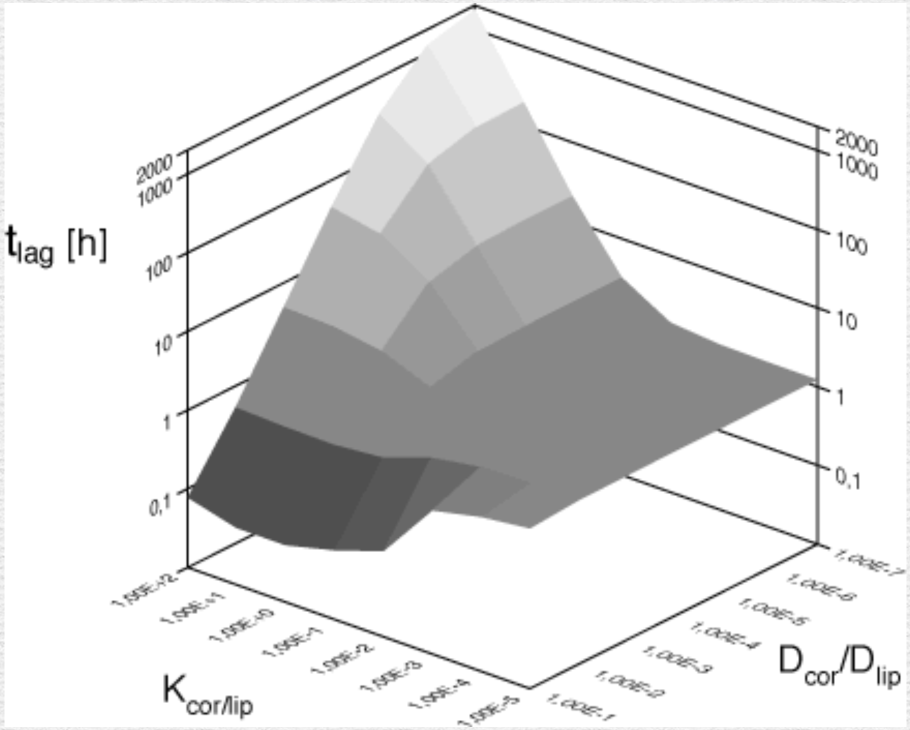
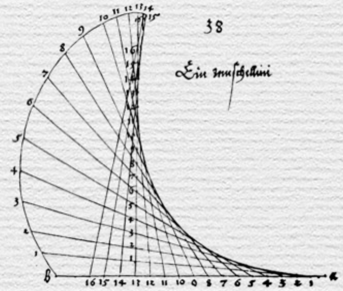
T_{lag} vs. ε and $K_{cor/lip}$





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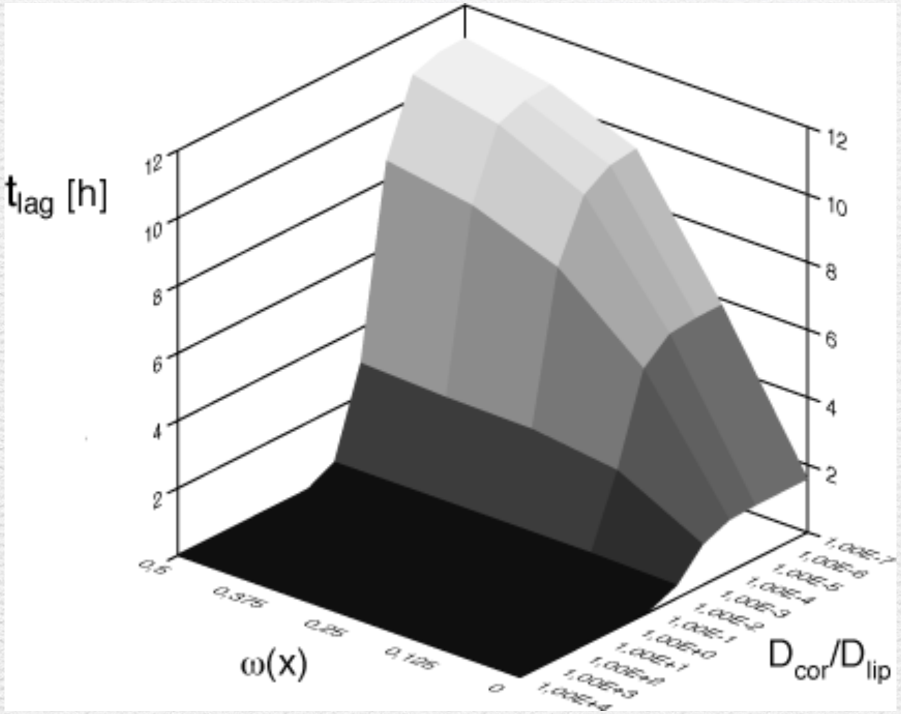
T_{lag} vs. ε and ω



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Simulation: 2D Brick Model

- Lieckfeldt, R., Lee, G, Heisig, M., Wittum, G.: Diffusant concentration profiles within cornecytes and lipid phase of stratum corneum. *Proceed. Internat. Symp. Control. Rel. Bioact. Mater.*, 20 (1993)
- **Intra cellular pathways matter**
- Nearly optimum barrier design,
- Robust w.r.t. insensitivity against shift and corneocyte permeability.

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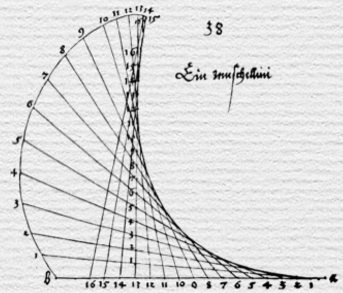

Simulation: 2D Brick Model

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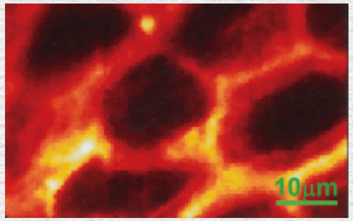
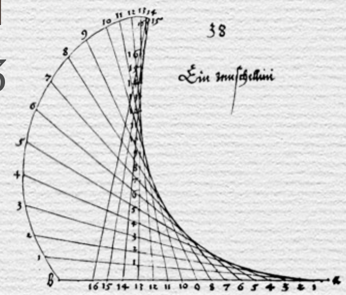
- Intra cellular pathways matter
- Nearly optimum barrier design,
- Robust w.r.t. insensitivity against shift and corneocyte permeability.
- **Experimentally confirmed in 2003!**



Langer et al 2003



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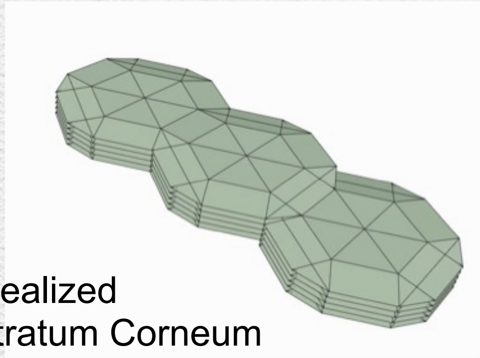
Tetrakaidekahedra based model

A. Nägel



Idealized
Stratum Corneum

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

Transport equation
(w/ diffusion and partition coefficients)

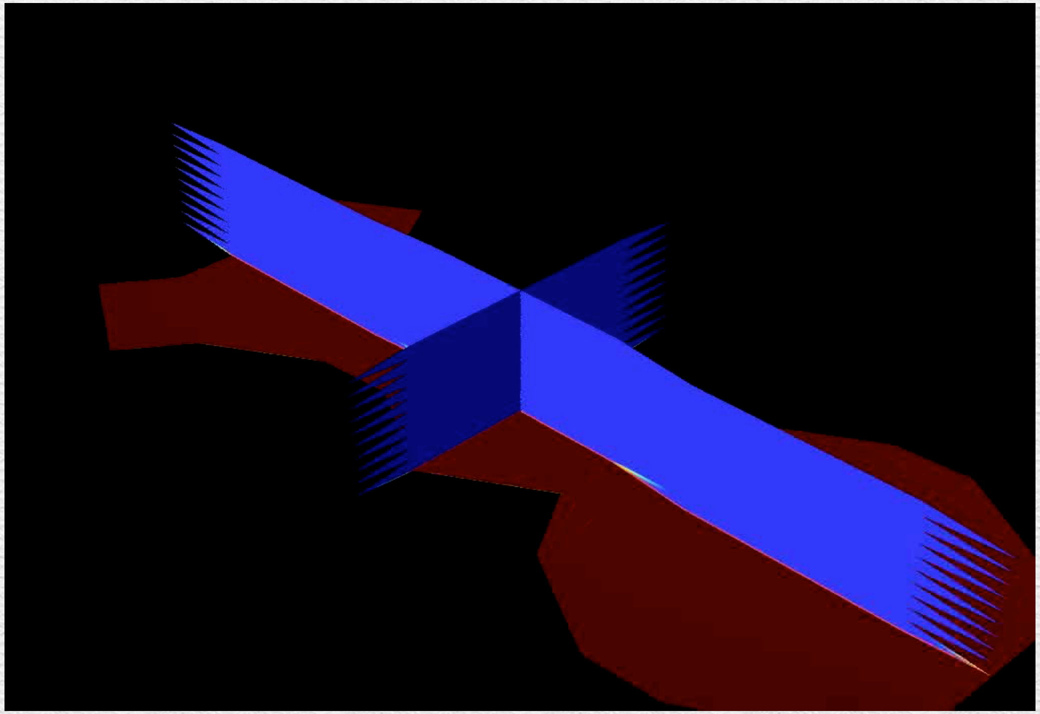
Morphology

&

Process

=

Effect



Corneocyte sponge effect

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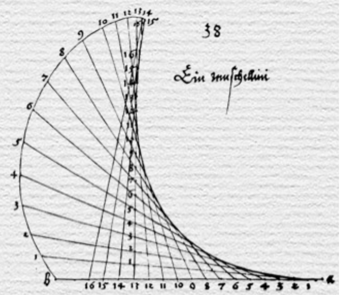
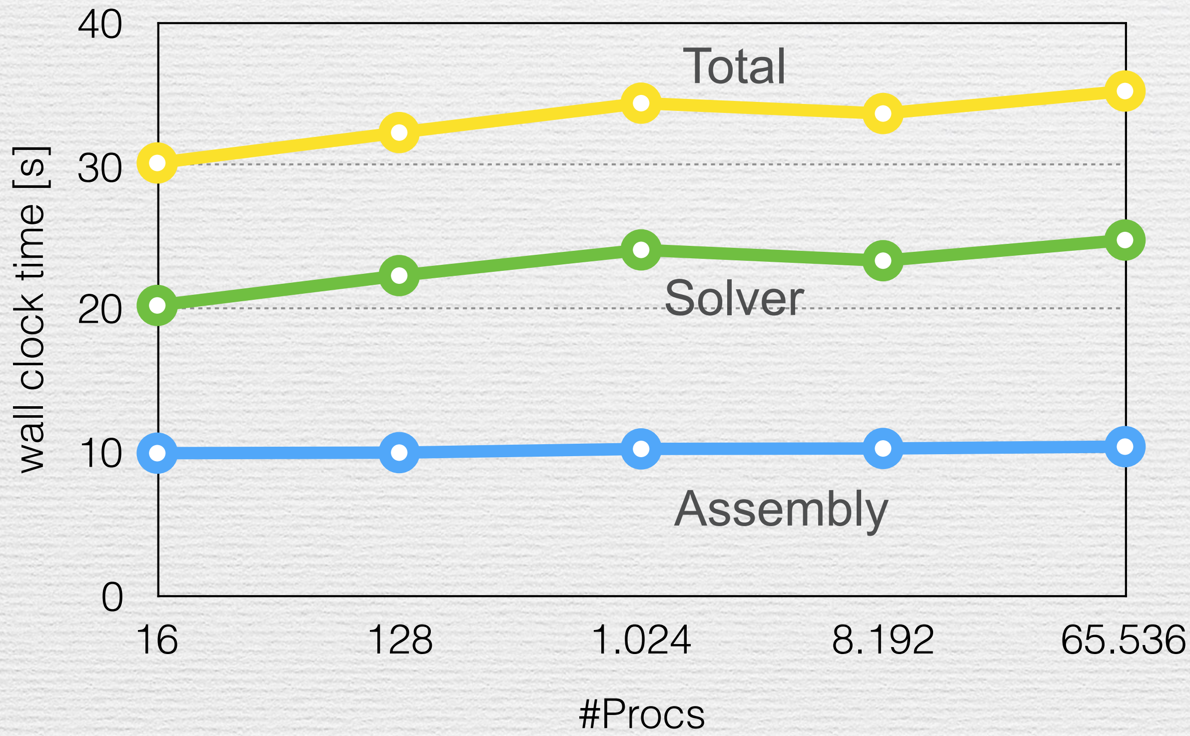
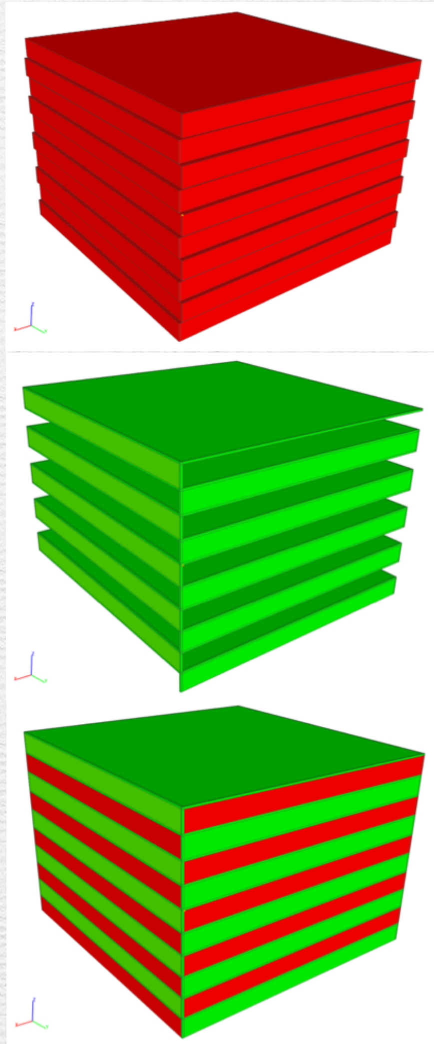
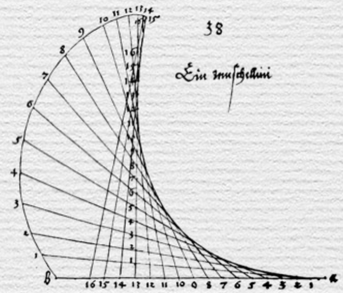


Weak Scaling UG4

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







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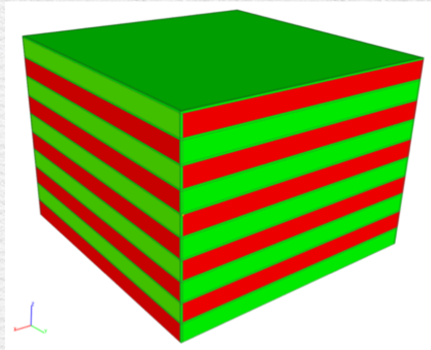
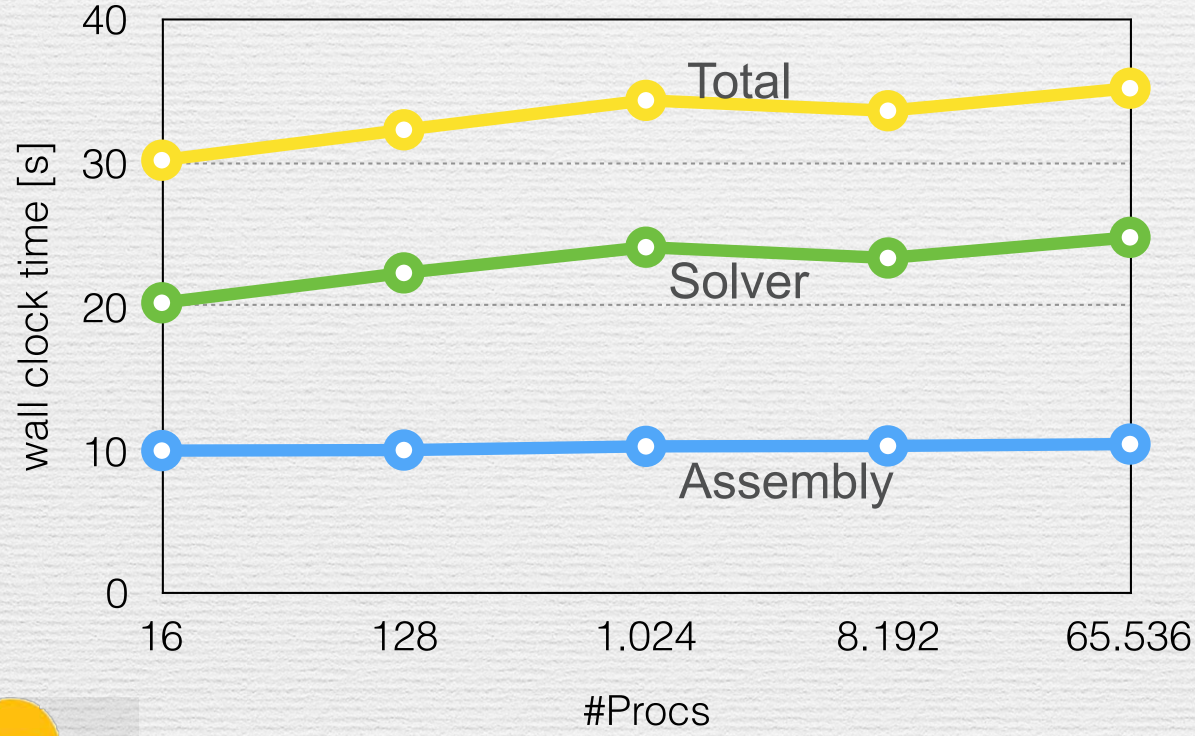
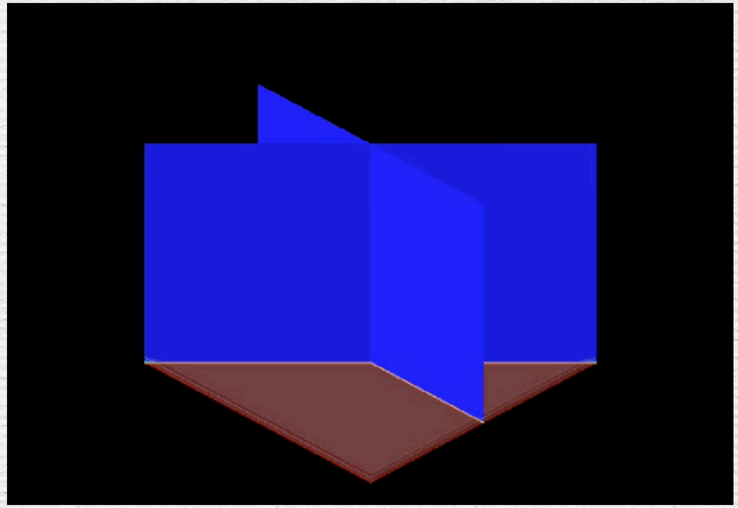
Weak Scaling UG4

A. Nägel



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





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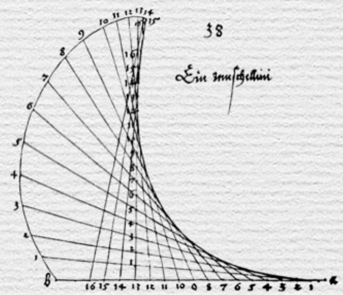
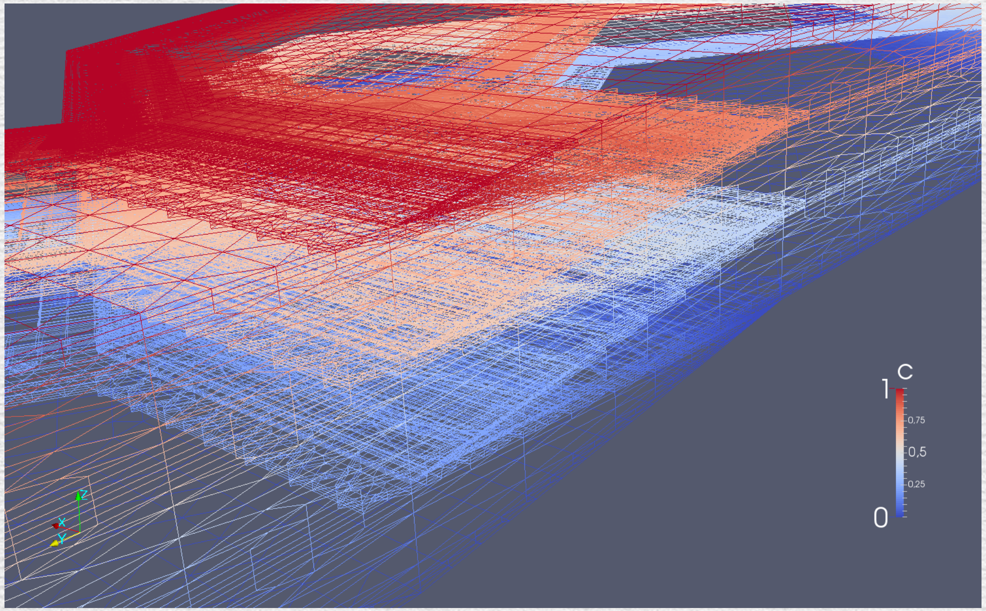
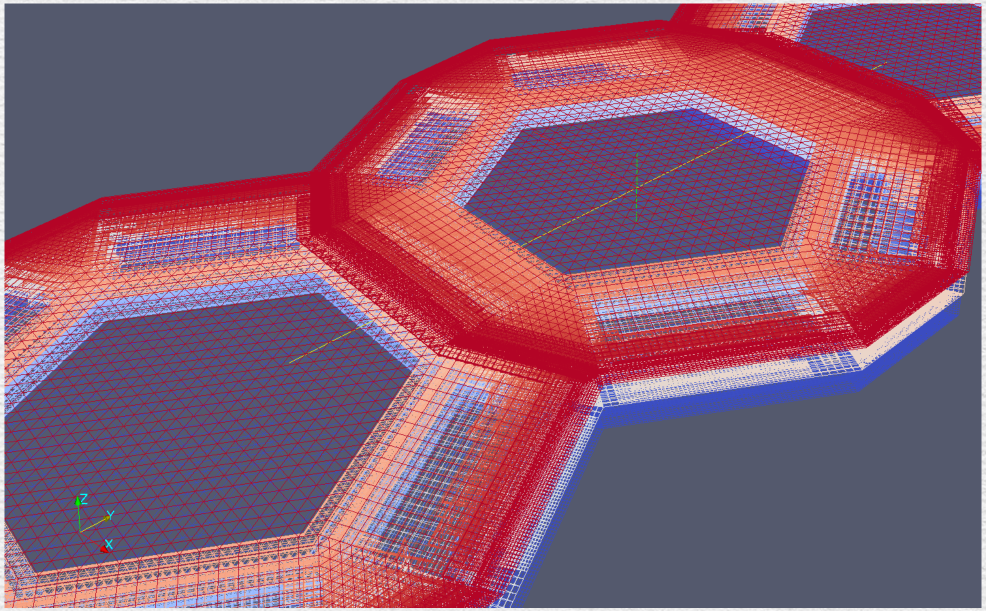


Skin Problem: TKD

Sebastian Reiter

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





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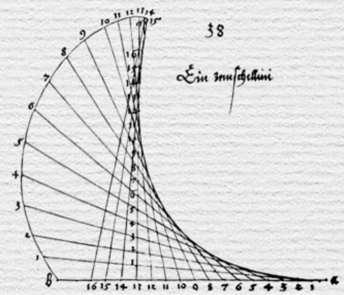
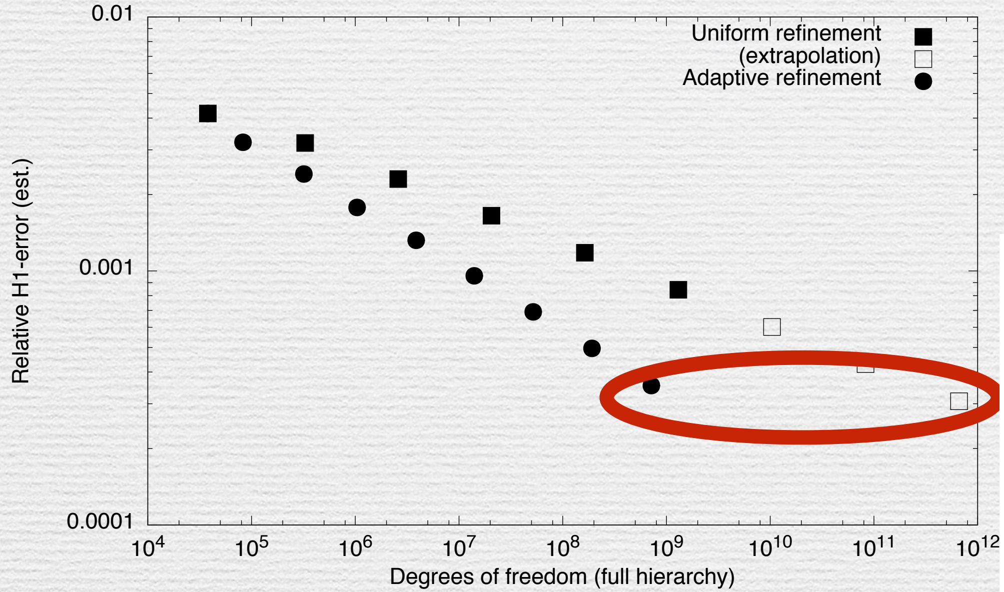


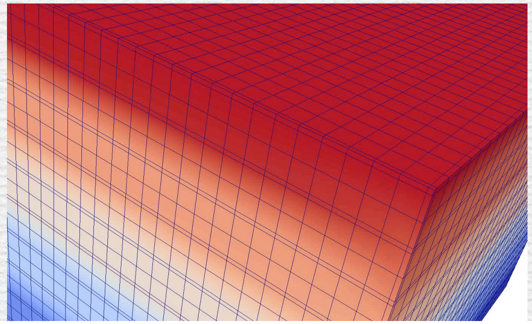
Parallel Adaptivity

A. Nägel, S. Reiter, A. Vogel

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

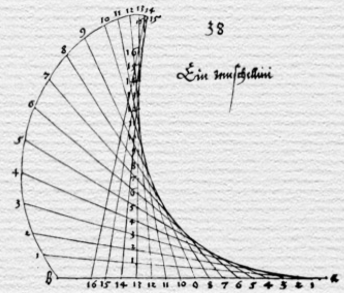
- Base solver UG4: Parallel adaptive mg
  - acceleration by 512 by adaptivity





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

- Importance of adaptivity increases with problem size!



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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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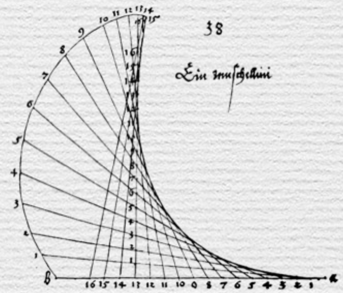
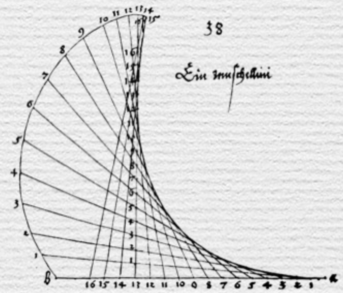


Thank you!



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