Finite Elements — Motivation Lecture

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October 18, 2021

Outline

Contents

Lecture

- Lecturer: Peter Bastian
  Office: INF 205, room 1/401
  email: `peter.bastian@iwr.uni-heidelberg.de`
- Lecture: Mi + Fr 9-11 SR C
  Exercise: Tue 14-16 SR 11
- Lecture homepage:
  `https://conan.iwr.uni-heidelberg.de/teaching/finiteelements_ws2021/`
- Lecture notes available from the homepage
- Moodle page `https://moodle.uni-heidelberg.de/course/view.php?id=10404`
  inscription should be possible without key
- Lecture will be recorded (writing and audio) and put on moodle

Excercises

- Excercises Tue 14-16 in SR 11 organized by Michal Tóth
  Office: INF 205, room 01.224
  email: `michal.toth@iwr.uni-heidelberg.de`
- Registration to excercises via MÜSLI system:
  `https://muesli.mathi.uni-heidelberg.de/lecture/view/1420`
- There will be theoretical and practical excercises
- Practical excercises are important! They will be based on the software DUNE: `www.dune-project.org`
  You will need some UNIX environment (Linux/MacOS)
- Scheme:
  - Exercises can be done in groups of 2. . . 3
  - Exercise given out / handed in Monday evening
  - Discussion of submitted exercises on Tuesday
  - You self-grade your exercise: how many points is it worth?
  - Random selection of presenting groups (a group may be selected even if no member is present!)
- Exercises start Tue, October 26

Exam

- Written exam (Klausur) at the end of the semester
- Date: February 18, 2022
- Requirements:

If I had free wishes

- Be interactive! Ask questions!
- There are no dumb questions!
- Do not miss the practical excercises. Polish your C++ knowledge!

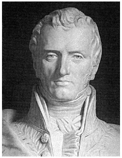
Contents

Equations of Mathematical Physics

- Calculus was invented for (partial) differential equations!
- E.g. to express conservation of mass, momentum and energy in quantitative form
- Famous examples are:
  - Poisson (electrostatics, gravity) 1800
  - Euler (inviscid flow) 1757
  - Navier-Stokes (viscous flow) 1822/1845
  - Maxwell (electrodynamics) 1864
  - Einstein (general relativity 1915
- Solutions in practical situtation only with modern (super) computers!

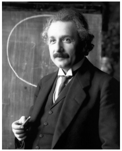

Poisson


Euler


Navier


Stokes


Maxwell


Einstein

Modelling with Partial Differential Equations

- This is a numerics class, but ...
- In order to judge whether a numerically computed solution is reasonable, it is good to have an understanding of the underlying application problem
- In the first part of the lecture we will look at deriving some models
- Let us look at some examples for motivation!

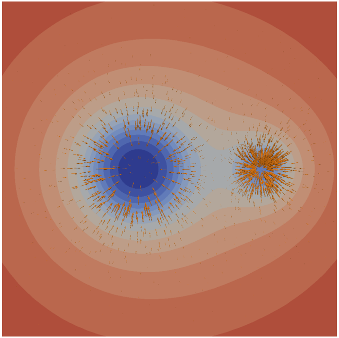
Gravitational Potential (Poisson Equation)

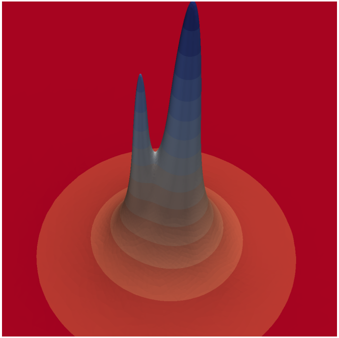
Find function $\Psi(x) : \Omega \to \mathbb{R}$, $\Omega = \mathbb{R}^3$ such that:

$$\partial_{x_1 x_1}\Psi(x) + \partial_{x_2 x_2}\Psi(x) + \partial_{x_3 x_3}\Psi(x) = \nabla \cdot \nabla\Psi(x) = \Delta\Psi(x) = 4\pi G\rho(x)$$

G: gravitational constant, ρ: mass density in kg/m^3

Force acting on small point mass m at point x: $F(x) = -m\nabla\Psi(x)$





Star Formation

Cone nebula from `http://www.spacetelescope.org/images/heic0206c/`

Star Formation: Mathematical Model

Euler equations of gas dynamics:

$$
\begin{aligned}
\partial_t \rho + \nabla \cdot (\rho v) &= 0 && \text{(mass conservation)} \\
\partial_t (\rho v) + \nabla \cdot (\rho v v^T + pI) &= -\rho \nabla \Psi && \text{(momentum conservation)} \\
\partial_t e + \nabla \cdot ((e + p) v) &= -\rho \nabla \Psi \cdot v && \text{(energy conservation)} \\
\Delta \Psi &= 4\pi G \rho && \text{(gravitational potential)}
\end{aligned}
$$

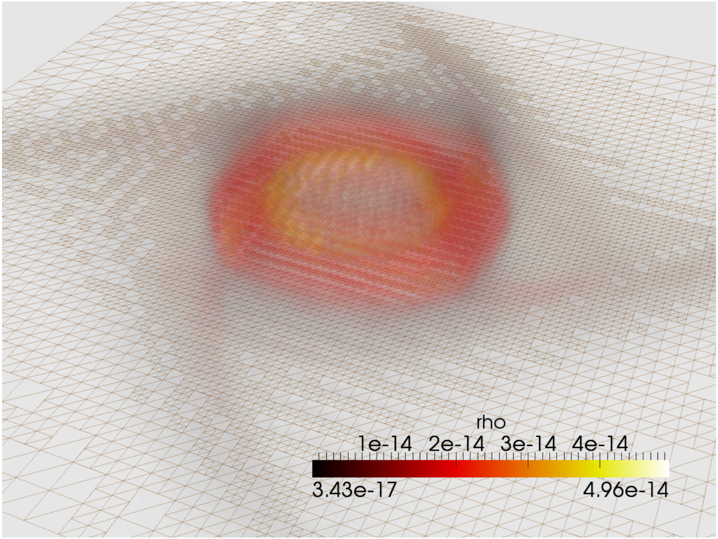
Constitutive relation: $p = (\gamma - 1)(e - \rho \|v\|^2/2)$

Plus the Poisson equation ...

More elaborate model requires radiation transfer, better constitutive relations, friction, ...

Nonlinear system of partial differential equations

Star Formation: Numerical Simulation



(Diploma thesis of Marvin Tegeler, 2011)

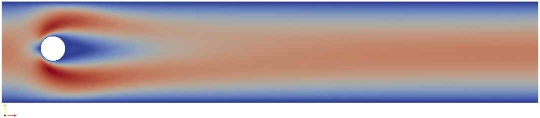
Flow of an Incompressible Fluid

(Incompressible) Navier-Stokes Equations:

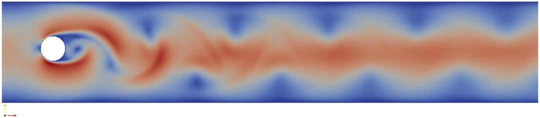
$$
\begin{aligned}
\nabla \cdot v &= 0 \qquad \text{(mass conservation)} \\
\partial_t v + \nabla \cdot (vv^T) - \nu \Delta v + \nabla p &= f \qquad \text{(momentum conservation)}
\end{aligned}
$$

- ρ is independent of pressure
- No compression work, isothermal situation
- Pressure is independent variable
- Existence of solutions is Millenium Prize Problem (in 3d for general data)

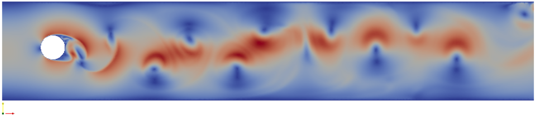
Von Karman Vortex Street



Re 20 (laminar)

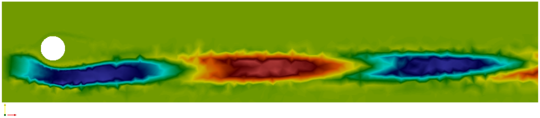


Re 200 (periodic)

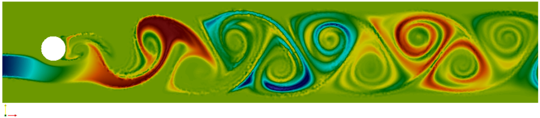


Re 1500 (turbulent)

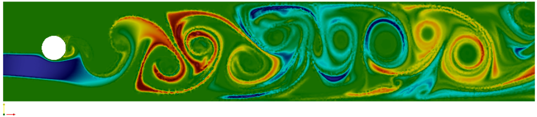
Von Karman Vortex Street



Re 20



Re 200



Re 1500

Surface Flow

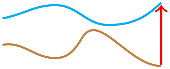
- Starting point: the incompressible Navier-Stokes equations

$$\begin{aligned} \partial_t(\rho v) + \nabla \cdot (\rho v v^T) - \nabla \cdot \sigma(v,p) &= \rho f \\ \nabla \cdot (\rho v) &= 0 \end{aligned}$$

with v velocity, p pressure, ρ (const.) density, σ given by

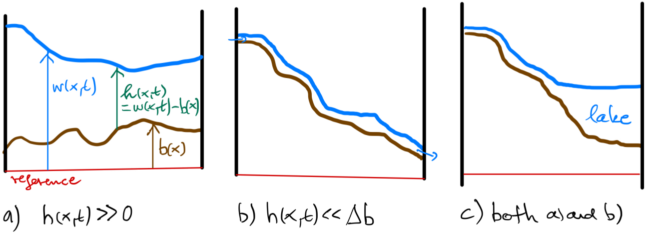
$$\sigma(v,p) = 2\mu\epsilon(v) - pI \quad \text{(stress)}, \qquad \epsilon(v) = \frac{1}{2}(\nabla v + (\nabla v)^T) \quad \text{(strain rate)}$$

- Free surface, no breaking waves $\rightsquigarrow$ time-dependent domain



- Boundary conditions:
  - No-slip boundary condition: $v(x,t) = 0$ (bottom, lateral sides)
  - Navier slip condition $v \cdot n_b = 0, (n_b \times (\sigma(v,p)n_b)) \times n_b + \frac{\beta}{\|n_b\|^3} v = 0$
  - No flow at free surface: $v(x,t) \cdot n_w(x,t) = \frac{\partial w}{\partial t}(x,t)$, $w(x,t)$ surface pos.

Shallow Surface Flow



- Extend of fluid domain much larger in horizontal than in vertical direction
- a) ocean flow, b) and c) land surface flow
- Dimension reduction reduces computational work

Shallow Water Equations

$$\partial_t(\rho h(\hat{x},t)) + \sum_{j=1}^{2} \partial_j(\rho h(\hat{x},t)\bar{v}_j(\hat{x},t)) = 0,$$

$$\partial_t(\rho h\bar{v}_i) + \sum_{j=1}^{2} \partial_j(\rho h\bar{v}_i\bar{v}_j) + \rho g \frac{\partial w}{\partial x_i}(\hat{x},t)h(\hat{x},t)$$
$$- 2\mu\left[(\epsilon(\hat{x}, w(\hat{x},t), t)n_w(\hat{x},t))_i + (\epsilon(\hat{x}, b(\hat{x}), t)n_b(\hat{x}))_i\right] = 0. \quad (i = 1,2)$$

- First-order hyberbolic system for water height h and vertically averaged horizontal velocity $\bar{v}$

$$\bar{v}_i(x_1,x_2,t) = \frac{1}{h(x_1,x_2,t)} \int_{b(x_1,x_2)}^{w(x_1,x_2,t)} v_i(x_1,x_2,x_3,t)\,dx_3 \qquad i = 1,2.$$

- Derived rigorously from Navier-Stokes under very few assumptions:
  - v_3 is very small $\rightsquigarrow$ hydrostatic pressure assumption
  - Velocities do not deviate much from their average $\rightsquigarrow$ $\overline{v_i v_j} \approx \bar{v}_i\bar{v}_j$
  - No internal friction (but surface and bottom friction)

Models Derived from the Shallow Water Equations

- Model friction, e.g. $(\epsilon(\hat{x}, b(\hat{x}), t) n_b(\hat{x}))_i = \alpha \bar{v}_i$ (Navier slip)
- One-dimensional shallow water equations: St. Venant equations
- Diffusive wave approximation

$$\frac{\partial(\rho h)}{\partial t} - \nabla \cdot (c_{dw} \rho h^2(\hat{x}, t) \nabla(h + b)) = 0.$$

  - Momentum equation: keep only gravity and bottom friction
  - Employ Navier slip condition
  - Insert into mass conservation
  - Nonlinear diffusion equation, other nonlinearities are used below
- Kinematic wave approximation

$$\frac{\partial(\rho h)}{\partial t} - \nabla \cdot (c_{kw} \rho h^2(\hat{x}, t) \nabla b(\hat{x})) = 0.$$

  - In addition assume $\partial_i w \approx \partial_i b$ (no lake at rest ...)
  - Nonlinear first-order hyperbolic, similar to Burger's equation

(Shallow) Subsurface Flow

- Flow in fully saturated porous medium (groundwater flow equation):

$$\nabla \cdot v(x,t) = f \quad \text{(mass cons.)}, \quad v(x,t) = -\frac{K(x)}{\mu}\left(\nabla p(x,t) - \rho g\right) \quad \text{(Darcy)}$$

  K permeability, g gravity *vector*

- Can be derived from Stokes equations
- Confined aquifer: elliptic PDE
- Unconfined aquifer
  - With capillary effects: two-phase flow, Richards equation
  - Without capillary effects: Groundwater flow with free surface
- Groundwater flow with free surface and shallow water assumption:

$$\partial_t(\phi u) - \nabla \cdot \left(K \frac{\varrho g}{\mu} h \nabla (h + b) \right) = f$$

  ϕ porosity, b bathymmetry

Coupled Shallow Surface/Subsurface Flow

$$\partial_t w_s - \nabla \cdot \left(\frac{1}{n(x)} \frac{(w_s - b_s(x))^\alpha}{\|\nabla w_s\|^{1-\gamma}} \nabla w_s \right) = f_s(x,t) - q(x, w_s, w_a)$$

$$\phi \partial_t (\min(w_a, b_s) - b_a) - \nabla \cdot (k(x)(w_a - b_a)\nabla w_a) = f_a(x,t) + q(x, w_s, w_a)$$

- Unknown functions: w_s surface water level, w_a groundwater level
- n Manning's number, $0 < \alpha \leq 2$, $0 < \gamma \leq 1$
- $w_a < b_s$: unconfined aquifer, $w_a \geq b_s$: confined aquifer
- Exchange term (infiltration - exfiltration)

$$q(x, w_s, w_a) = L_i \frac{\max(w_s - b_s(x), 0)}{C + \max(w_s - b_s(x), 0)} \max(w_s - w_a, 0) - L_e \max(w_a - w_s, 0)$$

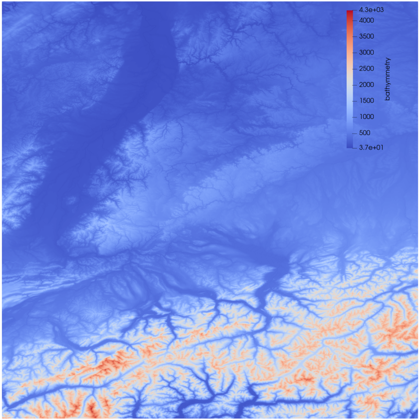
  Instantaneous transfer from surface to groundwater
- Can model rivers, lakes, surface flow, groundwater flow

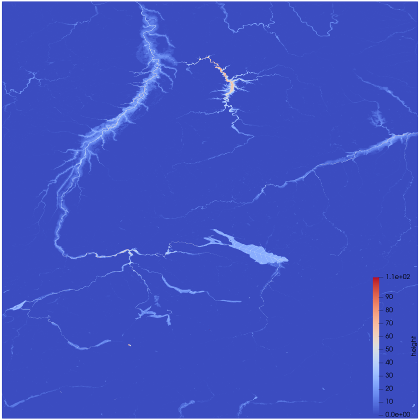
Example: Surface Flow in Baden-Württemberg

Setup:

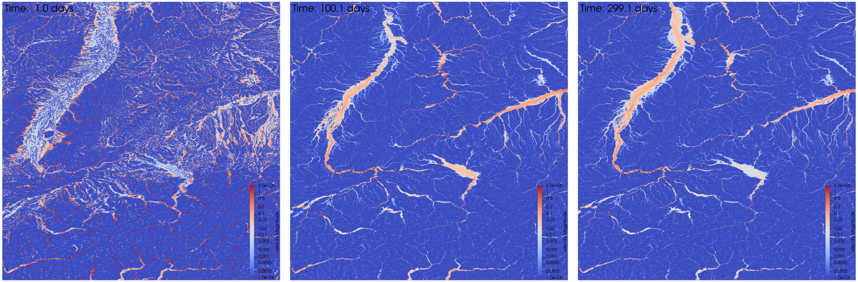
- Only surface flow model with $n = 1$, $\alpha = 1$, $\gamma = 1/2$
- "Hydrologically conditioned" digital elevation model (DEM) from Hydrosheds[1] at $90m$ resolution
- 4800^2 cells
- Constant forcing average rainfall (2 liter per m^2 and day)

[1] https://www.hydrosheds.org/

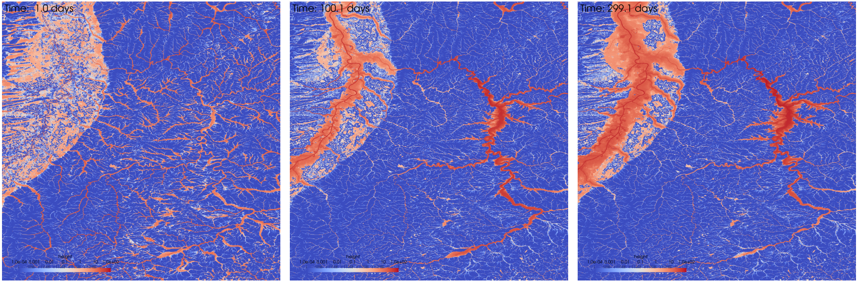




- Left: Hydrologically conditioned DEM from `www.hydrosheds.org`
- Right: Water height after 300 days with initial height $1m$



- Left: flow velocity after 1 day, initial height $1m$
- Middle: flow velocity after 100 days, initial height $1m$
- Right: flow velocity after 300 days, initial height $1m$



- Focus on Neckar river, water height
- $1m$ initial height, 1, 100, 300 days

The Parameter Problem

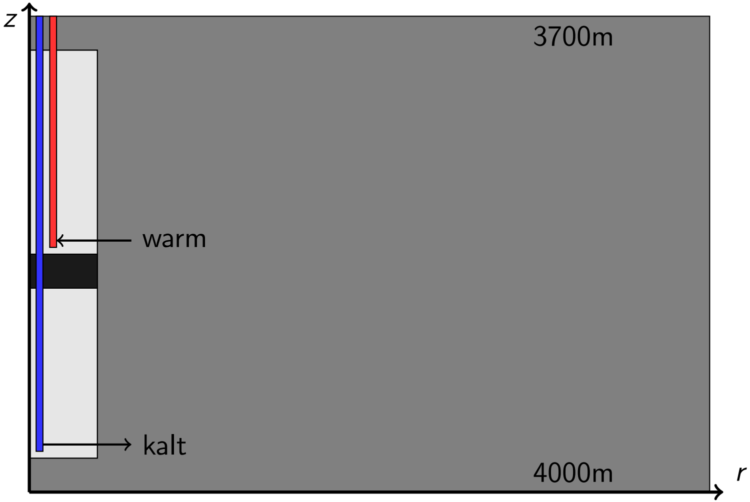
Such high fidelity models need many spatially distributed parameters:

- n, α, γ parameters in surface flow model
  - depend on land cover
- ϕ, K porosity and permeability in groundwater flow
  - difficult, permeability varies by orders of magnitude
- L_i, L_e in exchange terms
  - difficult, interface free flow / porous medium difficult to model
- b_s, b_a bathymmetries
  - b_s needs to be "hydrologically conditioned", b_a much more uncertain
- f_s, f_a precipitation, groundwater pumping
  - precipitation available, but at coarse resolution

Data that can be used for parameter estimation:

- River levels and discharge
- Groundwater levels

Geothermal Power Plant



Geothermal Power Plant: Mathematical Model

Coupled system for water flow and heat transport:

$$\partial_t(\phi\rho_w) + \nabla\cdot\{\rho_w u\} = f \qquad \text{(mass conservation)}$$

$$u = \frac{k}{\mu}(\nabla p - \rho_w g) \qquad \text{(Darcy's law)}$$

$$\partial_t(c_e\rho_e T) + \nabla\cdot q = g \qquad \text{(energy conservation)}$$

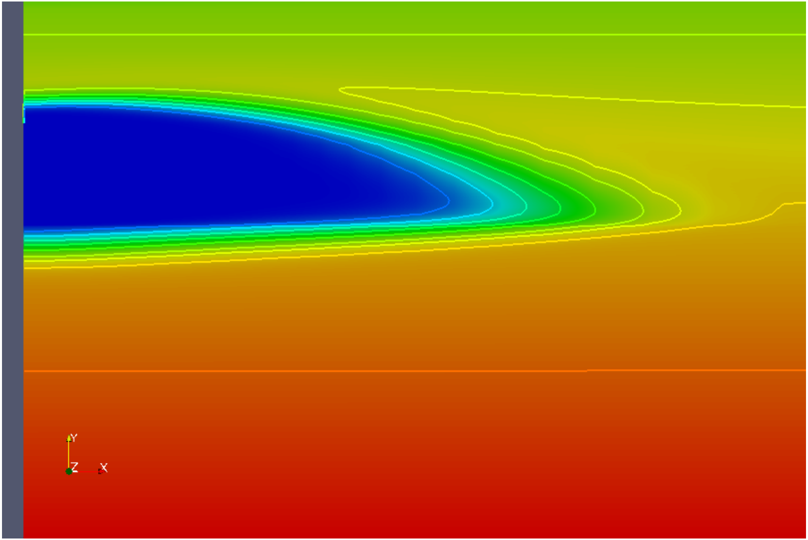
$$q = c_w\rho_w u T - \lambda\nabla T \qquad \text{(heat flux)}$$

Nonlinearity: $\rho_w(T)$, $\rho_e(T)$, $\mu(T)$

Permeability $k(x)$: 10^{-7} in well, 10^{-16} in plug

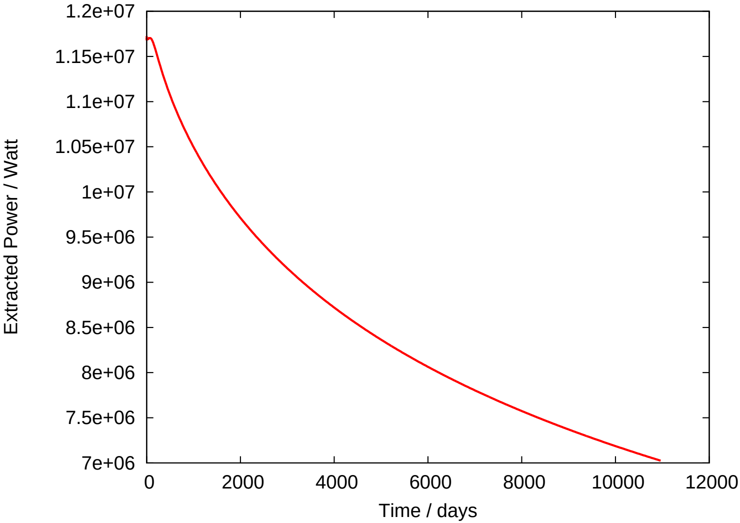
Space and time scales: R=15 km, r_b=14 cm, flow speed 0.3 m/s in well, power extraction: decades

Geothermal Power Plant: Results



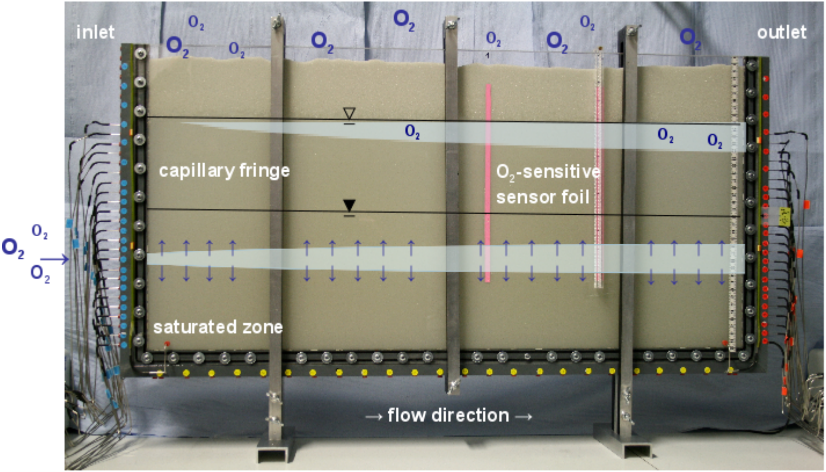
Temperature after 30 years of operation

Geothermal Power Plant: Results



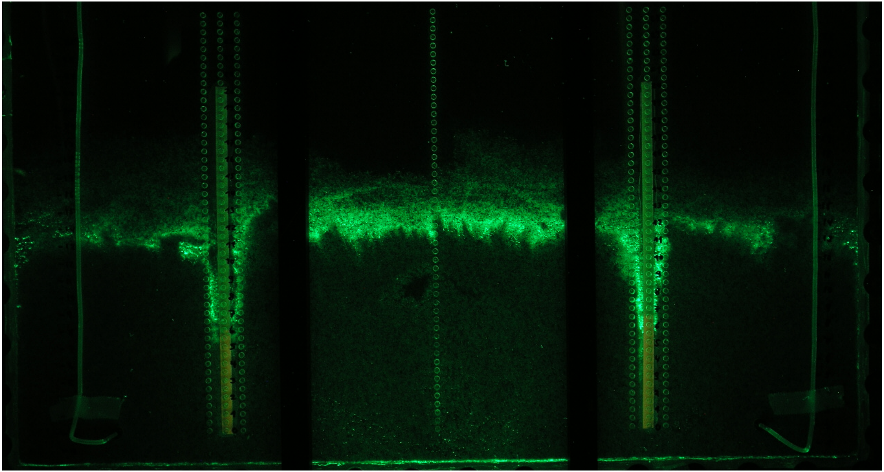
Extracted power over time

Bacterial Growth and Transport in Capillary Fringe



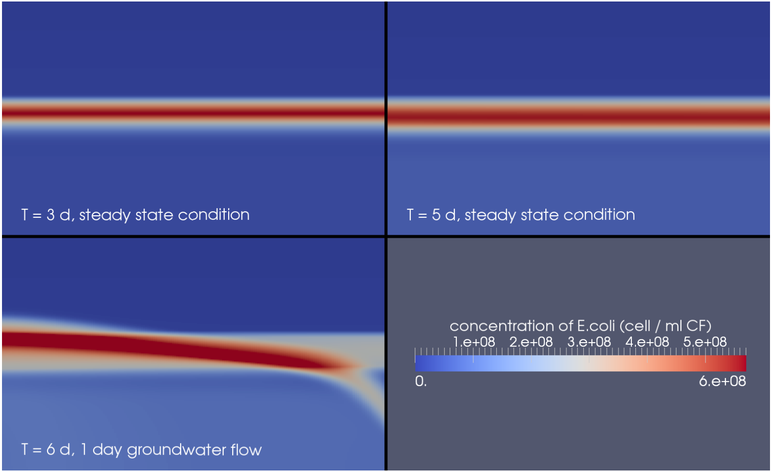
DFG Research Group 831 DyCap, Experiment by C. Haberer, Tübingen

Bacterial Growth and Transport in Capillary Fringe



Experiment by Daniel Jost, KIT, Karlsruhe

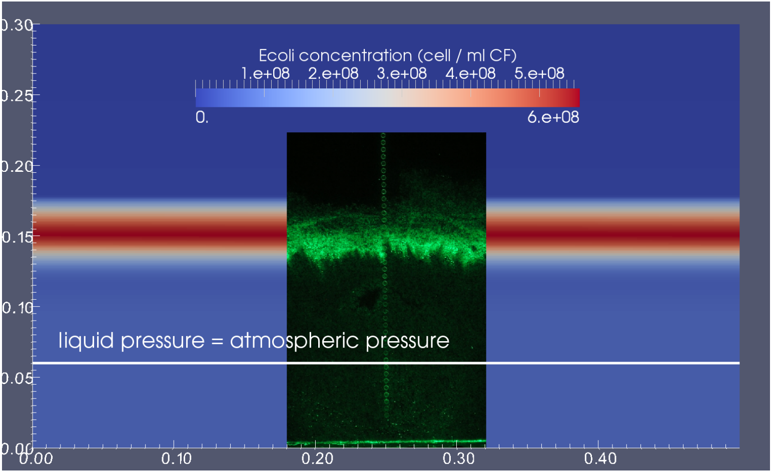
Reactive Multiphase Simulation



Unknowns: pressure, saturation, bacteria concentration, carbon concentration, oxygen concentration

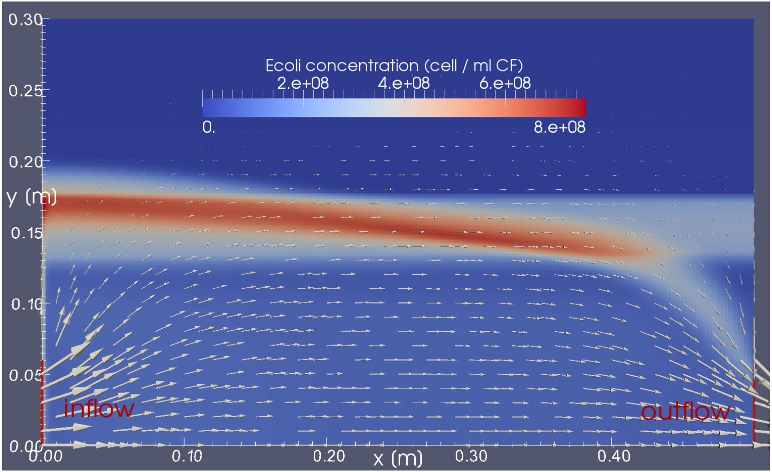
Simulation by Pavel Hron

Reactive Multiphase Simulation



Simulation by Pavel Hron

Reactive Multiphase Simulation



Simulation by Pavel Hron

Propagation of Electromagnetic Waves

(Macroscopic)Maxwell equations:

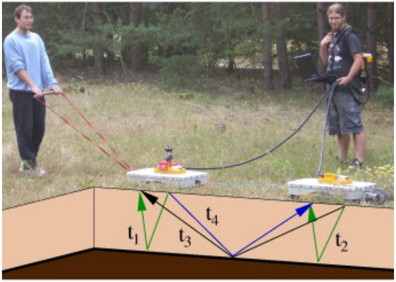
$$
\begin{aligned}
\nabla \times E &= -\partial_t B && \text{(Faraday)} \\
\nabla \times H &= j + \partial_t D && \text{(Ampère)} \\
\nabla \cdot D &= \rho && \text{(Gauß)} \\
\nabla \cdot B &= 0 && \text{(Gauß for magnetic field)}
\end{aligned}
$$

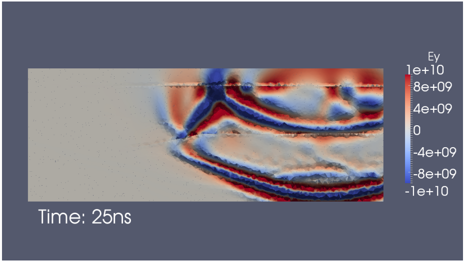
Constitutive relations:

$$
\begin{aligned}
D &= \epsilon_0 E + P && (D\text{: electric displacement field, } P\text{: polarization}) \\
B &= \mu_0 (H + M) && (H\text{: magnetizing field, } M\text{: magnetization})
\end{aligned}
$$

Linear, first-order hyperbolic system

Application: Geo-radar





Soil physics group Heidelberg

Simulation: Jorrit Fahlke

Second Order Model Problems

- Poisson equation: gravity, electrostatics **(elliptic type)**

$$
\begin{aligned}
\Delta u &= f && \text{in } \Omega \\
u &= g && \text{on } \Gamma_D \subseteq \partial\Omega \\
\nabla u \cdot \nu &= j && \text{on } \Gamma_N =\subseteq \partial\Omega \setminus \Gamma_D
\end{aligned}
$$

- Heat equation **(parabolic type)**

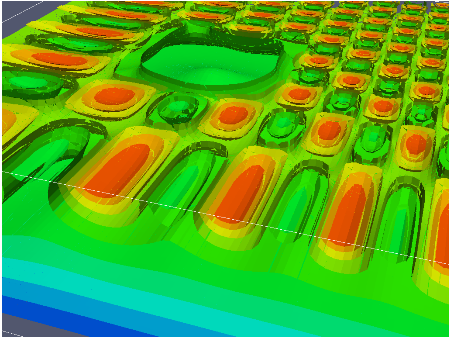
$$
\begin{aligned}
\partial_t u - \Delta\nabla u &= f && \text{in } \Omega \times \Sigma,\ \Sigma = (t_0, t_0 + T) \\
u &= u_0 && \text{at } t = t_0 \\
u &= g && \text{on } \partial\Omega
\end{aligned}
$$

- Wave equation (sound propagation) **(hyperbolic type)**

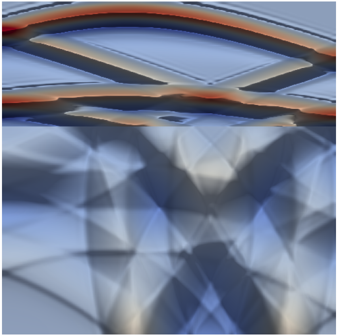
$$
\partial_{tt} u - \Delta u = 0 \quad \text{in } \Omega
$$

Second Order Model Problems

Solutions have different behavior



(parabolic)



(hyperbolic)

Contents

What is a Solution to a PDE?

Strong form: Consider the model problem

$$-\Delta u + u = f \quad \text{in } \Omega, \qquad \nabla u \cdot \nu = 0 \quad \text{on } \partial\Omega$$

Assume u is a solution and v is an arbitrary (smooth) function, then

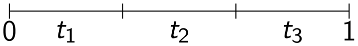
$$\begin{aligned}
& & \int_\Omega (-\Delta u + u) v \, dx &= \int_\Omega fv \, dx \\
\Leftrightarrow & & -\int_\Omega (\nabla \cdot \nabla u) v \, dx + \int_\Omega uv \, dx &= \int_\Omega fv \, dx \\
\Leftrightarrow & & \int_\Omega \nabla u \cdot \nabla v \, dx - \int_{\partial\Omega} (\nabla u \cdot \nu) v \, dx + \int_\Omega uv \, dx &= \int_\Omega fv \, dx \\
\Leftrightarrow & & \int_\Omega \nabla u \cdot \nabla v + uv \, dx &= \int_\Omega fv \, dx \\
\Leftrightarrow & & a(u, v) &= l(v)
\end{aligned}$$

Weak form: Find $u \in H^1(\Omega)$ s. t. $a(u, v) = l(v)$ for all $v \in H^1(\Omega)$.

The Finite Element (FE) Method

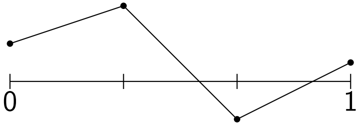
Idea: Construct finite-dimensional subspace $U \subset H^1(\Omega)$

Partition domain Ω into "elements" t_i:



$$\Omega = (0,1),\ T_h = \{t_1, t_2, t_3\}$$

Construct function from piecewise polynomials, e.g. linears:



$$U_h = \{u \in C^0(\Omega) \ : \ u|_{t_i} \text{ is linear } \}$$

Insert in weak form: $U_h = \text{span}\{\phi_1, \ldots, \phi_N\}$, $u_h = \sum_{j=1}^N x_j \phi_j$, then

$$u_h \in U_h \ : \ a(u_h, \phi_i) = l(\phi_i), \quad i = 1, \ldots, N \qquad \Leftrightarrow \qquad \boxed{\mathrm{Ax} = \mathrm{b}}$$

Contents

Challenges for PDE Software

- **Many different PDE applications**
  - Multi-physics
  - Multi-scale
  - Inverse modeling: parameter estimation, optimal control
- **Many different numerical solution methods, e.g. FE/FV**
  - No single method to solve all equations!
  - Different mesh types: mesh generation, mesh refinement
  - Higher-order approximations (polynomial degree)
  - Error control and adaptive mesh/degree refinement
  - Iterative solution of (non-)linear algebraic equations
- **High-performance Computing**
  - Single core performance: Often bandwidth limited
  - Parallelization through domain decomposition
  - Robustness w.r.t. to mesh size, model parameters, processors
  - Dynamic load balancing in case of adaptive refinement

DUNE Software Framework

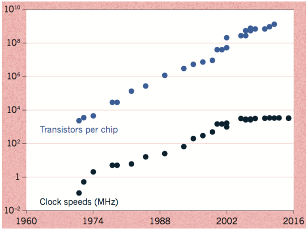
Distributed and **U**nified **N**umerics **E**nvironment

Domain specific abstractions for the numerical solution of PDEs with grid based methods.

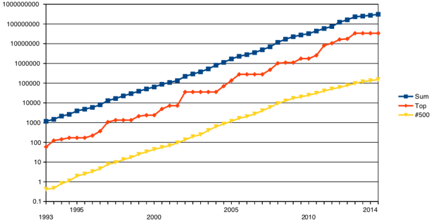
Goals:

- Flexibility: Meshes, discretizations, adaptivity, solvers.
- Efficiency: Pay only for functionality you need.
- Parallelization.
- Reuse of existing code.
- Enable team work through standardized interfaces.

Trends in Computer Architecture



Moore's law
Nature, 530 (2016), pp. 144-147



Supercomputer performance (GFLOPs/s)
https://commons.wikimedia.org/w/index.php?curid=33540287

- Power wall
  - Power consumption is limiting factor for exascale computing
  - Clock rate stagnates but Moore's law is still valid
- Memory wall
  - Bandwidth not sufficient to sustain peak performance
- ILP wall
  - Revival of vectorization in form of SIMD instructions

Efficient Algorithms are Key

- Solution of large sparse algebraic systems $F(z) = 0$
- Consider linear case $Ax = b$, $A \in \mathbb{R}^{N \times N}$:
  - Non-sparse Gauß elimination: $O(N^3)$
  - Sparse Gauß elimination: $O\left(N^{\frac{3(d-1)}{d}}\right)$
  - Multigrid: $O(N)$

N	Gauß elimination $\frac{2}{3}N^3$	multigrid $1000N$
1000	0,66 s	0,001 s
10000	660 s	0,01 s
100000	7,6 days	0,1 s
10^6	21 years	1 s
10^7	21.000 years	10 s

Run-time @ 1 GFLOPs/s

AMG Weak Scaling Results

- AAMG in DUNE is Ph. D. work of **Markus Blatt**
- BlueGene/P at Jülich Supercomputing Center
- $P \cdot 80^3$ degrees of freedom (5120^3 finest mesh), CCFV
- Poisson problem, 10^{-8} reduction
- AMG used as preconditioner in BiCGStab (2 V-Cycles!)

procs	1/h	lev.	TB	TS	It	TIt	TT
1	80	5	19.86	31.91	8	3.989	51.77
8	160	6	27.7	46.4	10	4.64	74.2
64	320	7	74.1	49.3	10	4.93	123
512	640	8	76.91	60.2	12	5.017	137.1
4096	1280	10	81.31	64.45	13	4.958	145.8
32768	2560	11	92.75	65.55	13	5.042	158.3
262144	5120	12	188.5	67.66	13	5.205	256.2

Note: Lecture on Friday, October 22 will be given by Michal Tóth!