Finite Elements
(Numerical Solution of Partial Differential Equations)

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Outline

Contents

Lecture

- Lecturer: Peter Bastian
  Office: INF 205, room 1/401
  email: `peter.bastian@iwr.uni-heidelberg.de`
- Di+Do 14-16 SR B
  Exercise: Mi 16-18 Pool 3rd Floor
- Lecture homepage:
  `https://conan.iwr.uni-heidelberg.de/teaching/finiteelements_ws2017/`
- Lecture notes available from the homepage
- Taking notes is not needed

Excercises

- Excercises (Mi 16-18 computer pool room #2 on 3rd floor) organized by Linus Seelinger
  Office: INF 205, room 01.218
  email: `linus.seelinger@iwr.uni-heidelberg.de`
- Linus Seelinger is on a research stay until Nov 6
  until then Marian Piatkowski `marian.piatkowski@iwr.uni-heidelberg.de` takes over
- Registration to excercises via MÜSLI system:
  `https://muesli.mathi.uni-heidelberg.de/lecture/view/802`
- There will be theoretical and practical excercises
- Practical excercises are important! They are based on the software DUNE:
  `www.dune-project.org`
- Acceptance to final exam (oral or written):
  - Present **two** excercise solutions
  - Selection by chance (with one refusal)
  - Probably a little project
- Exercises start Wed, October 25

If I had Wishes

- Be interactive! Ask questions!
- There are no dumb questions!
- Do not miss the practical excercises. Polish your C++ knowledge ...
- We are always looking for students to help improving/extending our software ...

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

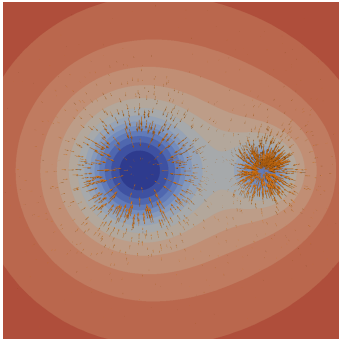
Gravitational Potential (Poisson Equation)

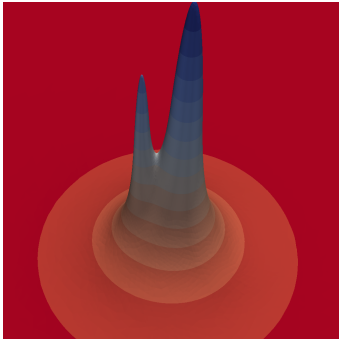
Find function $\Psi(x) : \Omega \to \mathbb{R}$, $\Omega = \mathbb{R}^3$ such that:

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

G: gravitational constant, ρ: mass density in $\mathrm{kg/m^3}$

Force acting on 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:

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

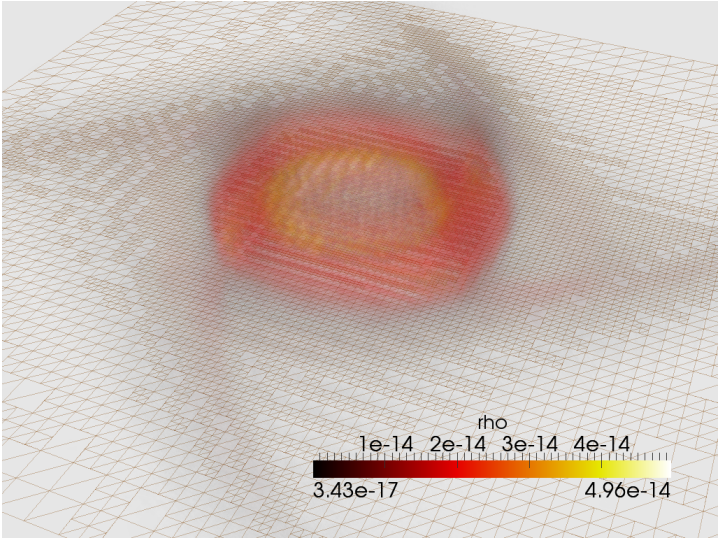
Constitutive relation: $p = (\gamma - 1)(e - \rho \|v\|^2/2)$

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

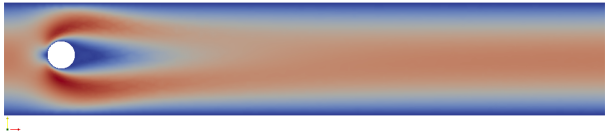
(Incompressible) Navier-Stokes Equations:

$$\nabla \cdot v = 0 \qquad \text{(mass conservation)}$$

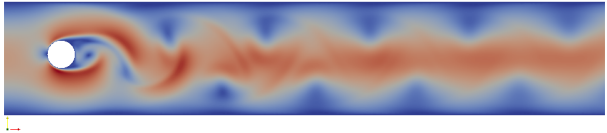
$$\partial_t v + \nabla \cdot (vv^T) - \nu \Delta v + \nabla p = f \qquad \text{(momentum conservation)}$$

- 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)

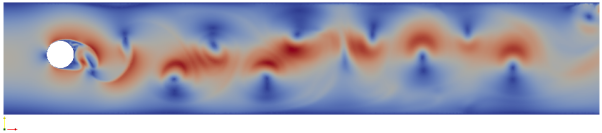
Von Karman Vortex Street



Re 20 (laminar)

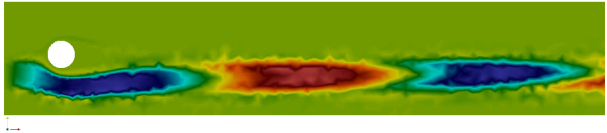


Re 200 (periodic)

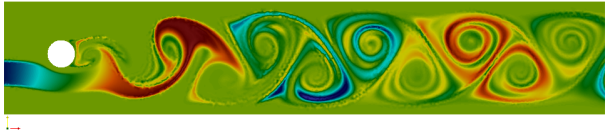


Re 1500 (turbulent)

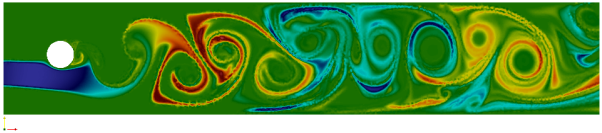
Von Karman Vortex Street



Re 20



Re 200



Re 1500

Propagation of Electromagnetic Waves

(Macroscopic)Maxwell equations:

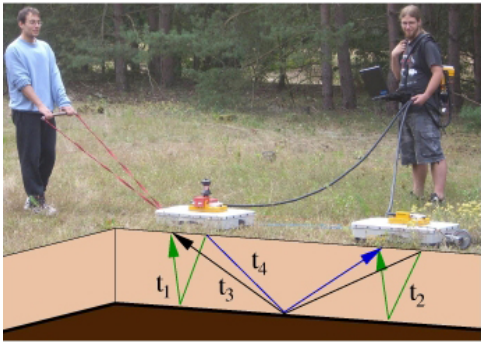
$$\nabla \times E = -\partial_t B \qquad \text{(Faraday)}$$
$$\nabla \times H = j + \partial_t D \qquad \text{(Ampère)}$$
$$\nabla \cdot D = \rho \qquad \text{(Gauß)}$$
$$\nabla \cdot B = 0 \qquad \text{(Gauß for magnetic field)}$$

Constitutive relations:

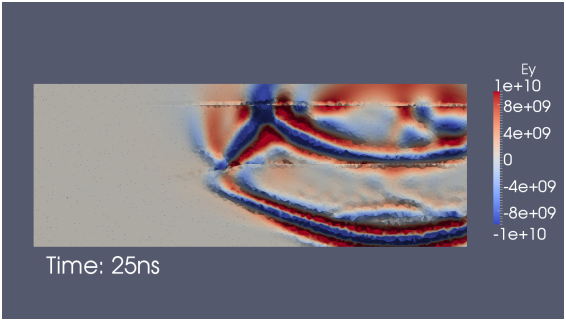
$$D = \epsilon_0 E + P \qquad (D\text{: electric displacement field, } P\text{: polarization})$$
$$B = \mu_0 (H + M) \qquad (H\text{: magnetizing field, } M\text{: magnetization})$$

Linear, first-order hyperbolic system

Application: Geo-radar

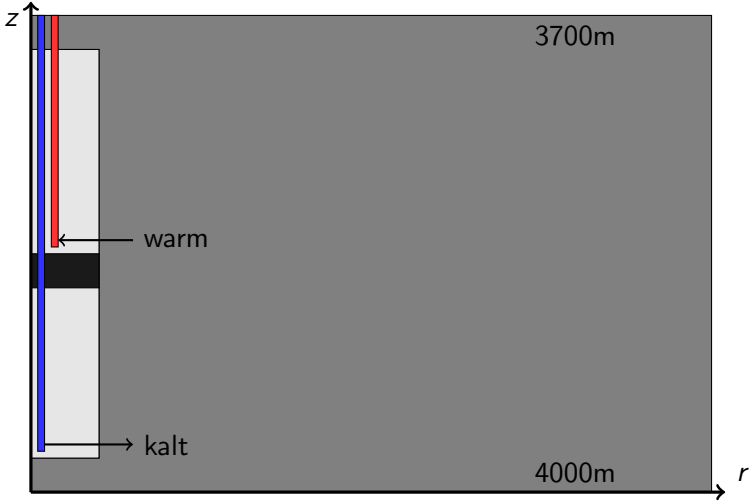


Soil physics group Heidelberg



Simulation: Jorrit Fahlke

Geothermal Power Plant



Geothermal Power Plant: Mathematical Model

Coupled system for water flow and heat transport:

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

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

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

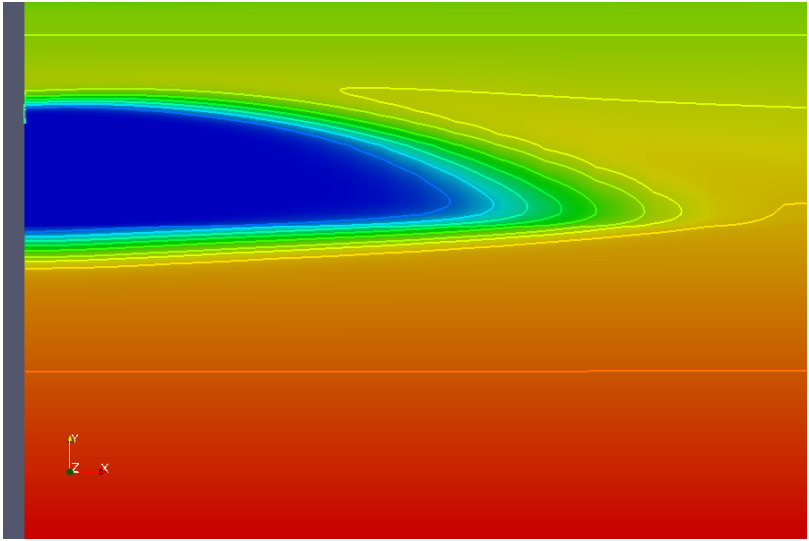
$$q = c_w\rho_w u T - \lambda\nabla T \qquad \text{(heat flux)}$$

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

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

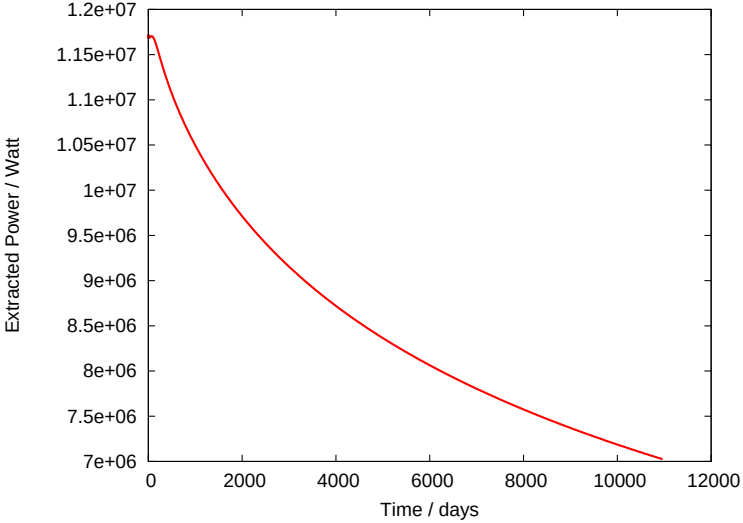
Space and time scales: R=15 km, r_b=14 cm, flow speed 0.3 m/s in well, power extraction: decades

Geothermal Power Plant: Results



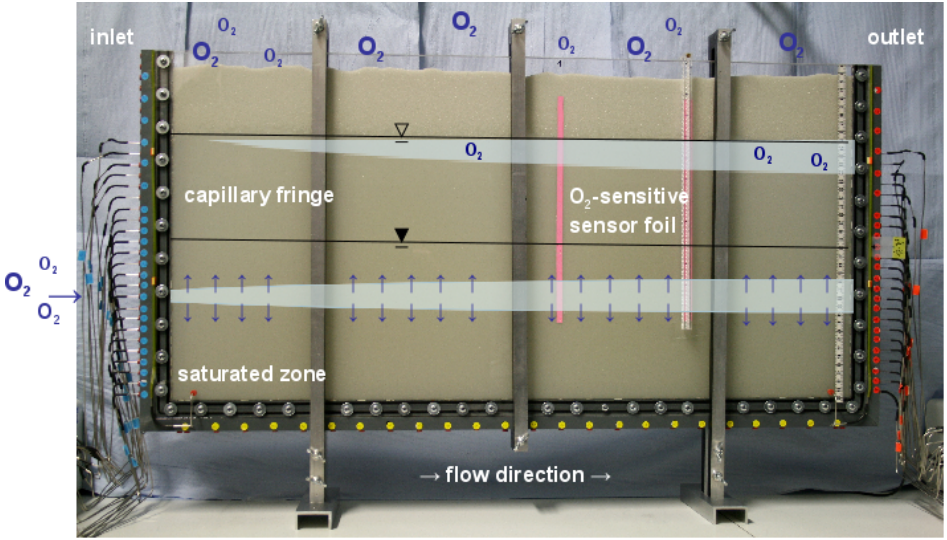
Temperature after 30 years of operation

Geothermal Power Plant: Results



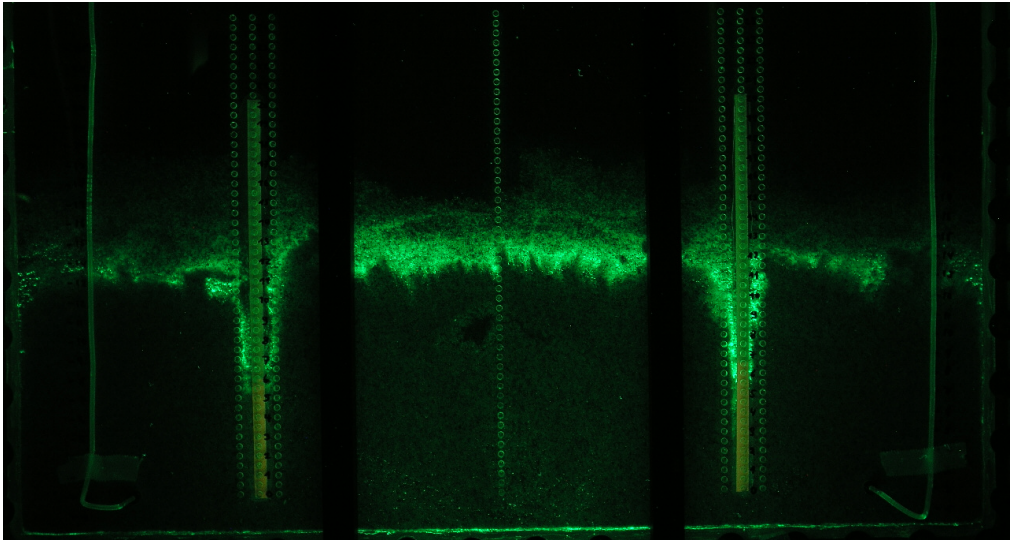
Extracted power over time

Bacterial Growth and Transport in Capillary Fringe



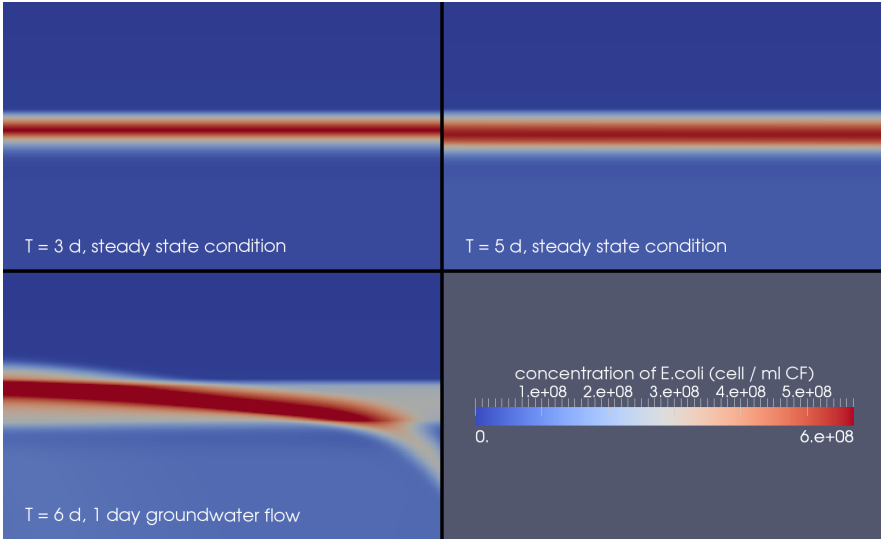
DFG Research Group 831 DyCap, Experiment by C. Haberer, Tübingen

Bacterial Growth and Transport in Capillary Fringe



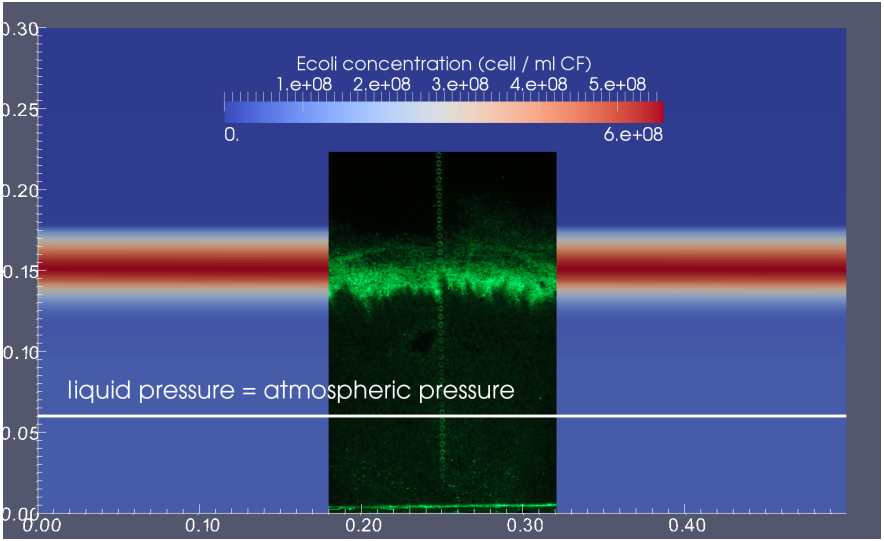
Experiment by Daniel Jost, KIT, Karlsruhe

Reactive Multiphase Simulation



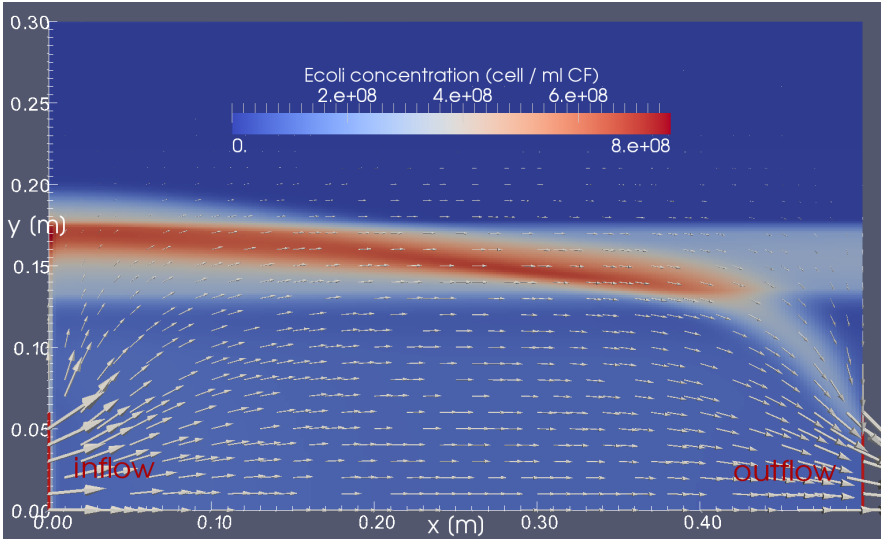
Unknowns: pressure, saturation, bacteria concentration, carbon concentration, oxygen concentration

Reactive Multiphase Simulation



Simulation by Pavel Hron

Reactive Multiphase Simulation



Simulation by Pavel Hron

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)**

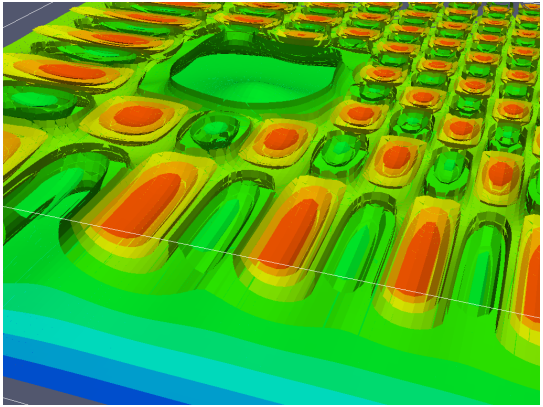
$$\begin{aligned} \partial_t u - \Delta \nabla u &= f && \text{in } \Omega \times \Sigma,\ \Sigma = (t_0, t_0 + T) \\ u &= u_0 && \text{at } t = t_0 \\ u &= g && \text{on } \partial\Omega \end{aligned}$$

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

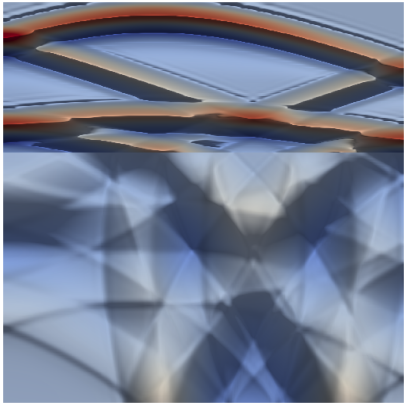
$$\partial_{tt} u - \Delta u = 0 \quad \text{in } \Omega$$

Second Order Model Problems

Solutions have different behavior



(parabolic)



(hyperbolic)

Contents

What is a Solution to a PDE?

Strong form: Consider the model problem

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

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

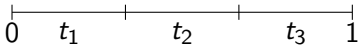
$$\begin{aligned}
& & \int_\Omega (-\Delta u + u) v \, dx &= \int_\Omega f v \, dx \\
&\Leftrightarrow & -\int_\Omega (\nabla \cdot \nabla u) v \, dx + \int_\Omega u v \, dx &= \int_\Omega f v \, dx \\
&\Leftrightarrow & \int_\Omega \nabla u \cdot \nabla v \, dx - \int_{\partial\Omega} (\nabla u \cdot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

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

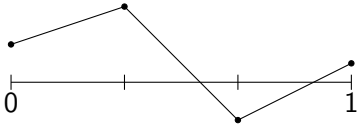
Idea: Construct finite-dimensional subspace $U \subset H^1(\Omega)$

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

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

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

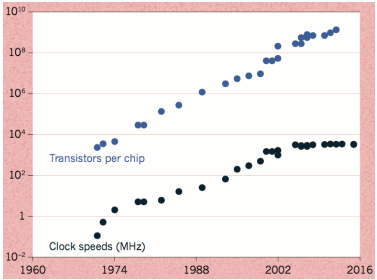
Distributed and **U**nified **N**umerics **E**nvironment

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

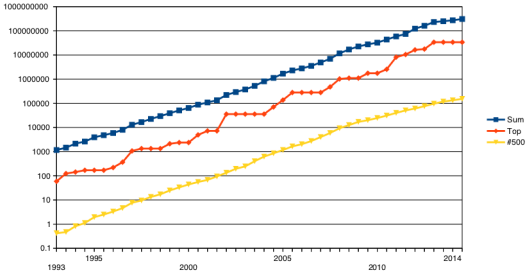
Goals:

- 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