Numerik 2 Motivation

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Outline

Contents

Lecture

- Lecturer: Peter Bastian
  Office: INF 368, room 420
  email: peter.bastian@iwr.uni-heidelberg.de
- Room and time (note change of room on Wednesday):
  Wed 11-13 (INF 329, SR26), Fr 9-11 (INF 350 / OMZ R U014)
  Enter Otto Meyerhoff Center (building 350) from the east side!
- Lecture homepage:
  http://conan.iwr.uni-heidelberg.de/teaching/numerik2_ss2014/
- Lecture notes available from the homepage
- I will extend the lecture notes during the course (>chapter 10)

Excercises

- Excercises designed by Pavel Hron (and myself)
  Office: INF 368, room 422
  email: pavel.hron@iwr.uni-heidelberg.de
- Student tutor: René Hess
- Excercises are managed via the MUESLI system:
  https://www.mathi.uni-heidelberg.de/muesli/lecture/view/326
  Please register if you have not yet done so!
- Time to be determined via doodle:
  http://doodle.com/me6s99nufwaeinbd#table
  Currently available: Mo 14-16, Wed 14-16 (preferred)
- There will be theoretical and practical excercises
- Practical excercises use the software DUNE:
  www.dune-project.org

Contents

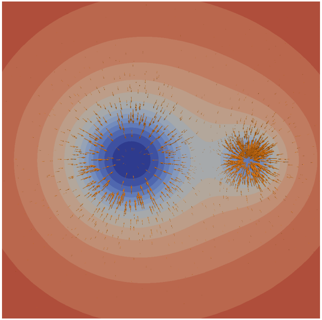
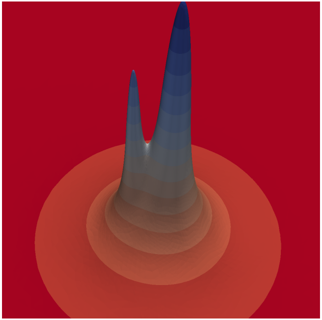
Gravitational Potential

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 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 plus gravity:

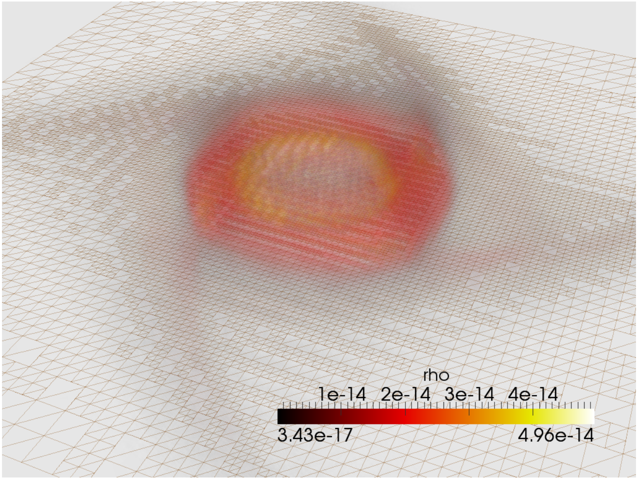
$$
\begin{aligned}
\partial_t \rho + \nabla \cdot (\rho v) &= 0 && \text{(mass conservation)} \\
\partial_t(\rho v) + \nabla \cdot (\rho v v^T + pI) &= -\rho \nabla \Psi && \text{(momentum conservation)} \\
\partial_t e + \nabla \cdot ((e+p)v) &= -\rho \nabla \Psi \cdot v && \text{(energy conservation)}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

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

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).

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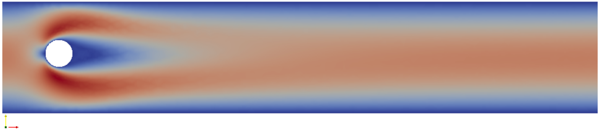
Flow of an Incompressible Fluid

(Incompressible) Navier-Stokes Equations:

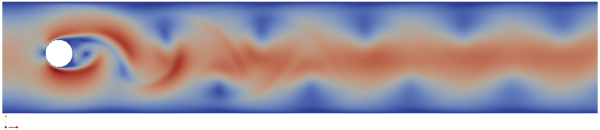
$$\begin{aligned} \nabla \cdot v &= 0 \quad \text{(mass conservation)} \\ \partial_t v + \nabla \cdot (vv^T) - \nu \Delta v + \nabla p &= f \quad \text{(momentum conservation)} \end{aligned}$$

- ρ is independent of pressure
- No compression work, isothermal situation
- Pressure is independent variable
- Existence of solutions is Millenium Prize Problem

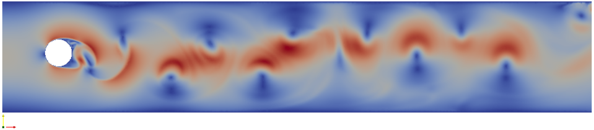
Von Karman Vortex Street



Re 20 (laminar)

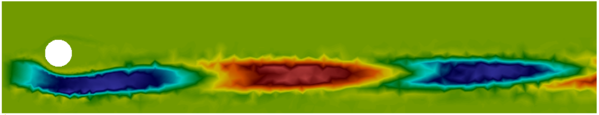


Re 200 (periodic)

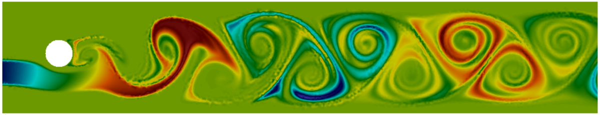


Re 1500 (turbulent)

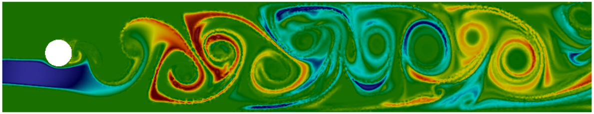
Von Karman Vortex Street



Re 20



Re 200



Re 1500

Propagation of Electromagnetic Waves

(Macroscopic)Maxwell equations:

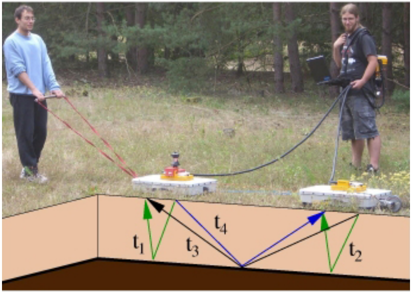
$$\nabla \times E = -\partial_t B \qquad \text{(Faraday)}$$
$$\nabla \times H = j + \partial_t D \qquad \text{(Ampère)}$$
$$\nabla \cdot D = \rho \qquad \text{(Gauß)}$$
$$\nabla \cdot B = 0 \qquad \text{(Gauß for magnetic field)}$$

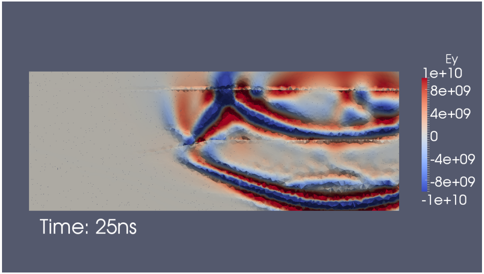
Constitutive relations:

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

Linear, first-order hyperbolic system

Application: Geo-radar

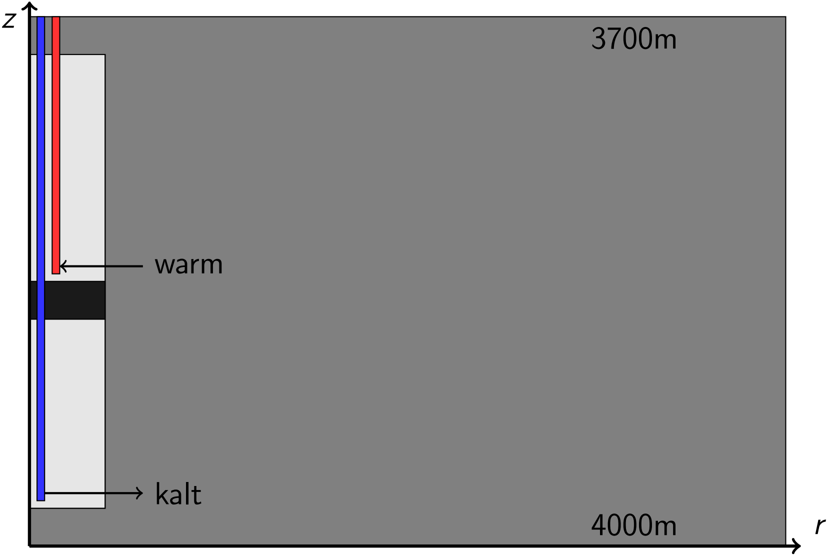




Soil physics group Heidelberg

Simulation: Jorrit Fahlke

Geothermal Power Plant



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Geothermal Power Plant: Mathematical Model

Coupled system for water flow and heat transport:

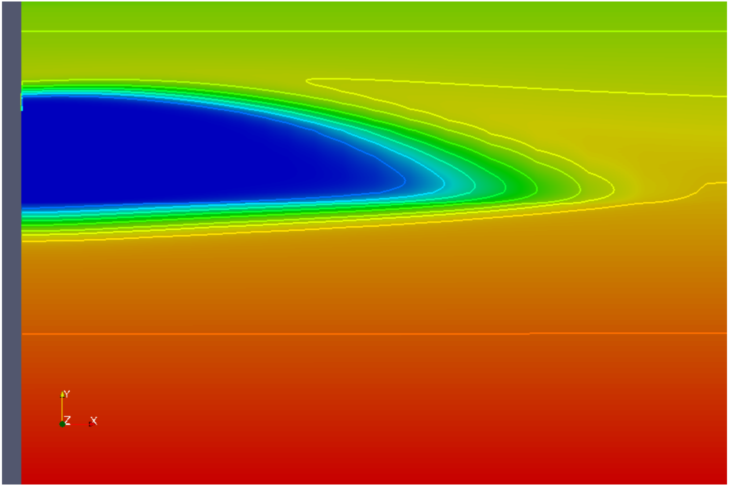
$$
\begin{aligned}
\partial_t(\phi\rho_w) + \nabla\cdot\{\rho_w u\} &= f && \text{(mass conservation)}\\
u &= \frac{k}{\mu}(\nabla p - \rho_w g) && \text{(Darcy's law)}\\
\partial_t(c_e\rho_e T) + \nabla\cdot q &= g && \text{(energy conservation)}\\
q &= c_w\rho_w u T - \lambda\nabla T && \text{(heat flux)}
\end{aligned}
$$

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

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

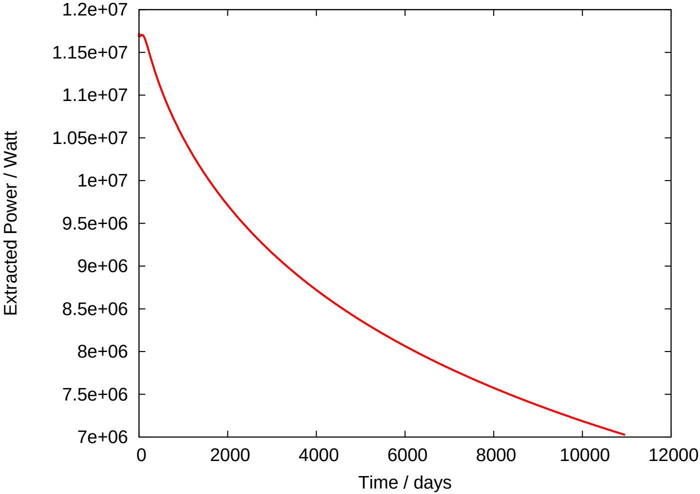
Space and time scales: R=15 km, r_b=14 cm, flow speed 0.3 m/s in well, power extraction: decades

Geothermal Power Plant: Results



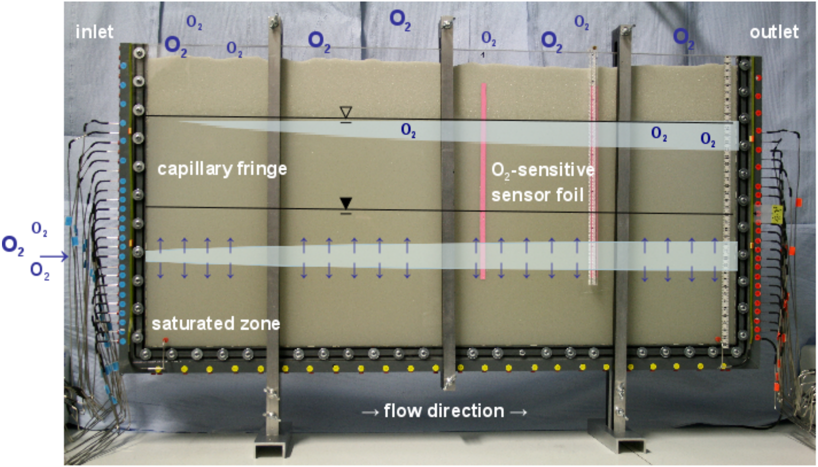
Temperature after 30 years of operation

Geothermal Power Plant: Results



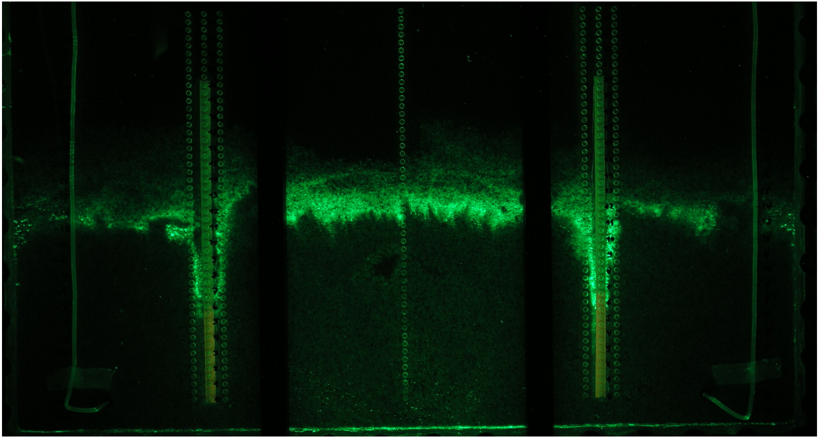
Extracted power over time

Bacterial Growth and Transport in Capillary Fringe



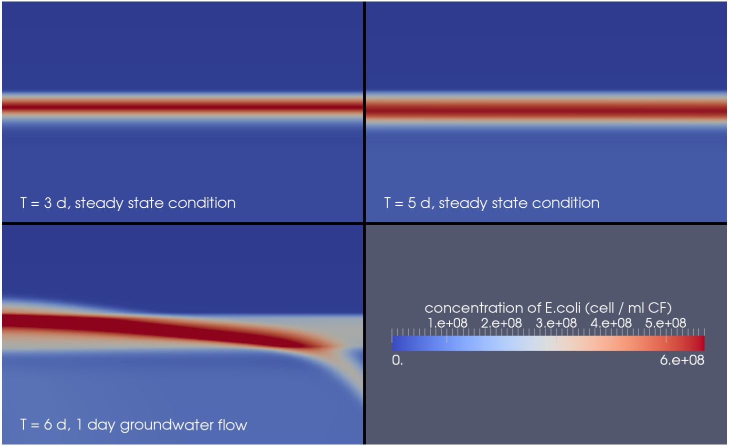
DFG Research Group 831 DyCap, Experiment by C. Haberer, Tübingen

Bacterial Growth and Transport in Capillary Fringe



Experiment by Daniel Jost, KIT, Karlsruhe

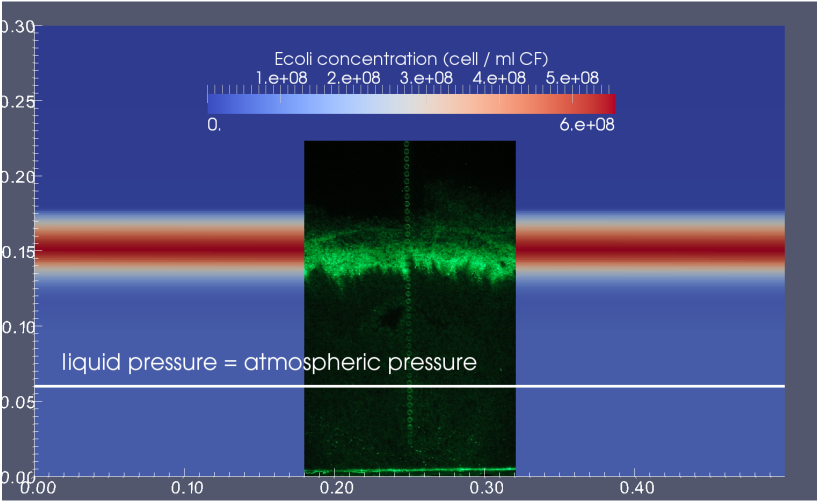
Reactive Multiphase Simulation



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

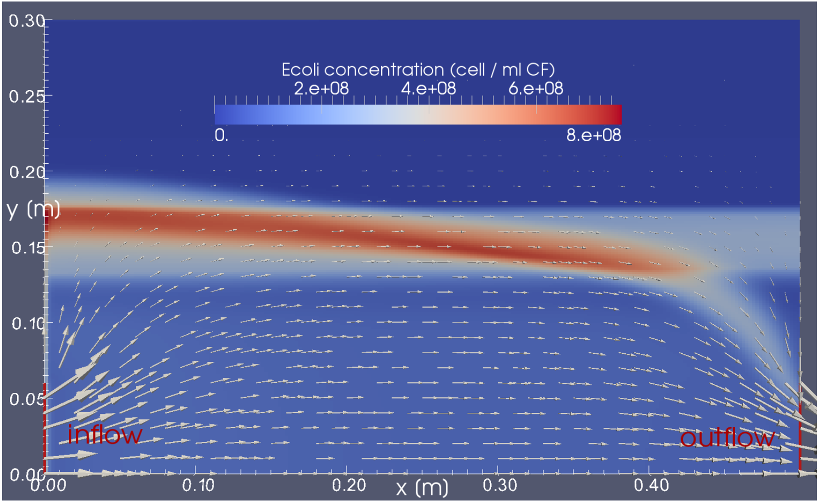
Simulation by Pavel Hron

Reactive Multiphase Simulation



Simulation by Pavel Hron

Reactive Multiphase Simulation



Simulation by Pavel Hron

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)**

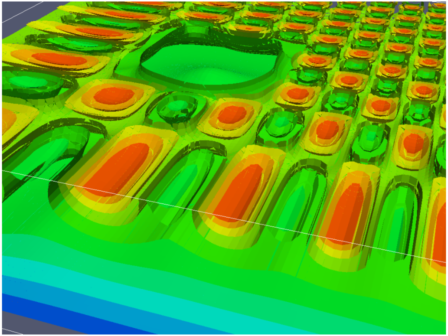
$$\begin{aligned} \partial_t u - \Delta\nabla u &= f && \text{in } \Omega \times \Sigma,\ \Sigma = (t_0, t_0 + T) \\ u &= u_0 && \text{at } t = t_0 \\ u &= g && \text{on } \partial\Omega \end{aligned}$$

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

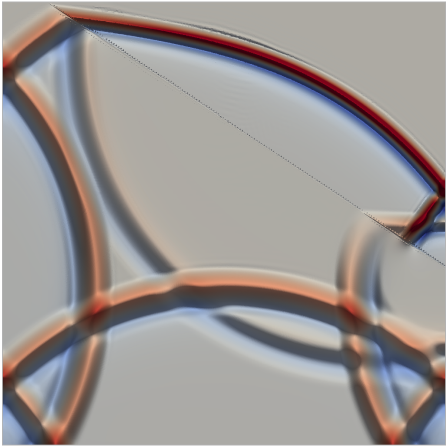
$$\partial_{tt} u - \Delta u = 0 \quad \text{in } \Omega$$

Second Order Model Problems

Solutions have different behavior



(parabolic)



(hyperbolic)

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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

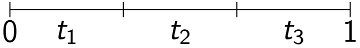
$$\begin{aligned}
& \int_\Omega (-\Delta u + u) v \, dx = \int_\Omega fv \, dx \\
\Leftrightarrow \quad & -\int_\Omega (\nabla \cdot \nabla u) v \, dx + \int_\Omega uv \, dx = \int_\Omega fv \, dx \\
\Leftrightarrow \quad & \int_\Omega \nabla u \cdot \nabla v \, dx - \int_{\partial\Omega} (\nabla u \cdot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

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

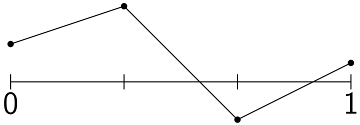
Idea: Construct finite-dimensional subspace $U \subset H^1(\Omega)$

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

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

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.

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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