Finite Elements
(Numerical Solution of Partial Differential Equations)

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Outline

Organizational Stuff

Partial Differential Equations are Ubiquitous

Preview: The Finite Element Method

DUNE
Contents

Organizational Stuff
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
e-mail: 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
— Be interactive! Ask questions!

— There are no dumb questions!

— Do not miss the practical exercises. Polish your C++ knowledge . . .

— We are always looking for students to help improving/extending our software . . .
Partial Differential Equations are Ubiquitous
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 situation only with modern (super) computers!
Gravitational Potential (Poisson Equation)

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

$$\partial_{x_1x_1} \Psi(x) + \partial_{x_2x_2} \Psi(x) + \partial_{x_3x_3} \Psi(x) = \nabla \cdot \nabla \Psi(x) = \Delta \Psi(x) = 4\pi G \rho(x)$$

$G$: gravitational constant, $\rho$: 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:

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0$$  \hspace{1cm} (mass conservation)

$$\partial_t (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}^T + p \mathbf{I}) = -\rho \nabla \Psi$$ \hspace{1cm} (momentum conservation)

$$\partial_t \mathbf{e} + \nabla \cdot ((\mathbf{e} + p) \mathbf{v}) = -\rho \nabla \Psi \cdot \mathbf{v}$$ \hspace{1cm} (energy conservation)

$$\Delta \Psi = 4\pi G \rho$$ \hspace{1cm} (gravitational potential)

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

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:

\[ \nabla \cdot \mathbf{v} = 0 \]  
\( \text{(mass conservation)} \)

\[ \partial_t \mathbf{v} + \nabla \cdot (\mathbf{v} \mathbf{v}^T) - \nu \Delta \mathbf{v} + \nabla p = f \]  
\( \text{(momentum conservation)} \)

- \( \rho \) 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:

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

Constitutive relations:

\[ D = \varepsilon_0 E + P \quad \text{\(D\): electric displacement field, \(P\): polarization)} \]
\[ B = \mu_0 (H + M) \quad \text{\(H\): magnetizing field, \(M\): magnetization} \]

Linear, first-order hyperbolic system
Application: Geo-radar

Soil physics group Heidelberg

Simulation: Jorrit Fahlke
Geothermal Power Plant

[Diagram of a geothermal power plant with depth indicated by 'z' and radial distance by 'r'. The depth ranges from 3700m to 4000m, with 'warm' and 'kalt' (cold) regions.]
Geothermal Power Plant: Mathematical Model

Coupled system for water flow and heat transport:

\[
\partial_t (\phi \rho_w) + \nabla \cdot \{ \rho_w u \} = f \quad \text{ (mass conservation)}
\]

\[
u = \frac{k}{\mu}(\nabla p - \rho_w g) \quad \text{ (Darcy’s law)}
\]

\[
\partial_t (c_e \rho_e T) + \nabla \cdot q = g \quad \text{ (energy conservation)}
\]

\[
q = c_w \rho_w u T - \lambda \nabla T \quad \text{ (heat flux)}
\]

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

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

Space and time scales: \( R=15 \text{ km}, r_b=14 \text{ cm}, \) 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

Unkowns: 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**)

  \[ \Delta u = f \quad \text{in } \Omega \]
  \[ u = g \quad \text{on } \Gamma_D \subseteq \partial \Omega \]
  \[ \nabla u \cdot \nu = j \quad \text{on } \Gamma_N = \subseteq \partial \Omega \setminus \Gamma_D \]

- Heat equation (**parabolic type**)

  \[ \partial_t u - \Delta \nabla u = f \quad \text{in } \Omega \times \Sigma, \Sigma = (t_0, t_0 + T) \]
  \[ u = u_0 \quad \text{at } t = t_0 \]
  \[ u = g \quad \text{on } \partial \Omega \]

- 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

Preview: The Finite Element Method
What is a Solution to a PDE?

**Strong form:** Consider the model problem

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

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

\[
\int_{\Omega} (-\Delta u + u)v \, dx = \int_{\Omega} fv \, dx \\
\iff -\int_{\Omega} (\nabla \cdot \nabla u)v \, dx + \int_{\Omega} uv \, dx = \int_{\Omega} fv \, dx \\
\iff \int_{\Omega} \nabla u \cdot \nabla v \, dx - \int_{\partial \Omega} (\nabla u \cdot \nu)v \, dx + \int_{\Omega} uv \, dx = \int_{\Omega} fv \, dx \\
\iff \int_{\Omega} \nabla u \cdot \nabla v + uv \, dx = \int_{\Omega} fv \, dx \\
\iff a(u, v) = l(v)
\]

**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 $\Omega$ into “elements” $t_i$:

$$\begin{align*}
0 & \quad t_1 & \quad t_2 & \quad t_3 & \quad 1 \\
\end{align*}$$

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

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

$$u_h \in U_h : a(u_h, \phi_i) = l(\phi_i), \quad i = 1, \ldots, N \quad \Leftrightarrow \quad Ax = b$$
Contents

DUNE
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 Unified Numerics Environment

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

- **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

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

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

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Run-time @ 1 GFLOPs/s
AAMG 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!)

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