Numerics II

Informationen

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Freie Universität Berlin

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Information

Lecture
Dr. Robert Gruhlke `r.gruhlke@fu-berlin.de`

Tutorial:
André-Alexander Zepernick `a.zepernick@fu-berlin.de`

Sekretariat:
Sandra Lindstädt, Arnimallee 6, Raum 141
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Dates (see Whiteboard)

Lecture:
Mo **12:00-14:00**, Wed **12:00-14:00** in A3/Hs 001 Hörsaal (Arnimallee 3-5) 31 sessions

Tutorial:
Wed **10:00-12:00**, Fr **08:00-10:00** in A6/SR 025/026 Seminarraum (Arnimallee 6)
Start: 17.10.2025

Info: Internet

Whiteboard for current information and materials:
Skript, Slides, Excercise sheets and announcements.

- Registration for tutorial classes via Whiteboard
- First Exercise: **15.10.2025** online.
- Return:
  - Exercises: Whiteboard (prefered in LaTeX).
  - **Overleaf.com** provides a platform for shared working on LaTex documents !
- **Groups of 3** to solve them
- programming language: **Python 3**.

Info: Finalizing the module

Final exam will be made **oral**. Dates will be announced via Whiteboard.

Active Participation:

- At least 50% of the points.

Topics

I Numeric of Ordinary differential equations

"*Modeling continuous dynamics in computation*"

- Neural ODEs for generative modeling — training continuous-time neural networks for image generation (e.g. create your favorite cat images).
- Simulating epidemic models (SIR) or chemical kinetics where system behavior evolves continuously.
- Foundation for extensions to stochastic differential equations:
  - Motion of particles in physics or finance models driven by stochastic differential equations.

Topics

II Differential Algebraic Equations (Basic Ideas)

"*When physical contraints meet dynamics*"

- Simulation of electric circuits (Kirchhoff laws + device dynamics). $\rightarrow$ Used in SPICE simulators for chips and hardware.
- Multibody mechanics: robotic arms, vehicle suspensions — constraints like joints or rods lead naturally to DAEs.
- Power grids and chemical processes: balancing algebraic constraints and differential evolution in real time.

In short: DAEs arise whenever differential laws are coupled with "must-hold" constraints.

III Symplectic methods (Basic ideas)

"*When energy preservation matters*"

- Long-term simulation of planetary motion (e.g. NASA trajectory prediction).
- Molecular dynamics — keeping total energy stable over millions of time steps.
- Quantum and Hamiltonian systems — maintaining invariants like momentum and phase space volume.

These methods are key in physics-based simulations where naive numerical solvers for ordinary differential equations would drift in energy.

IV Iterative solution of linear systems

"*Solving the unsolvable efficiently*"

- Sparse linear systems from discretized PDEs — too large for direct solvers.
- PageRank and large-scale graph problems (Google-scale computations).
- Machine learning: conjugate gradient and stochastic methods inside large optimizers (e.g. training transformers).

Iterative solvers are the workhorses behind every modern simulation and **AI** training pipeline.