TU Berlin Advanced Topics from Scientific Computing Winter Semester 2024/2025

Slide lecture 1

Jürgen Fuhrmann

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- Name: Dr. Jürgen Fuhrmann (no, not Prof.)
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- Course homepage:

https://www.wias-berlin.de/people/fuhrmann/AdSciComp-WS2425/

- Experience/Field of work:
 - Numerical solution of partial differential equations (PDEs)
 - Development, investigation, implementation of finite volume discretizations for nonlinear systems of PDEs
 - Ph.D. on multigrid methods
 - Applications: electrochemistry, semiconductor physics, groundwater...
 - Software development:
 - WIAS code pdelib (http://pdelib.org)
 - Julia PDE solver package VoronoiFVM.jl (http://github.dom/j-fu/VoronoiFVM.jl) + package ecosystem
 - Languages: C, C++, Python, Lua, Fortran, Julia
 - Visualization: OpenGL, VTK, Makie.jl

- Lecture material will be available via https://www.wias-berlin.de/people/fuhrmann/AdSciComp-WS2425/
- All code examples and project assignments will be in Julia, either as notebooks or as Julia files. Things should work on Linux, MacOSX, Windows
- I will develop course projects on various topics in groups of 2-3 students. I will offer standard and advanced topics. The later are connected to my research projects.
- Portfolio exams will be based on course projects

Intended aims and topics of this course

- Introduction to Julia as fresh approach to combine efficient computation with easy composability
- Focus on partial differential equation (PDE) solution
 - Solution of large linear systems of equations
 - Finite element and finite volume methods
 - Mesh generation
 - Nonlinear solvers
 - Automatic differentiation
 - Aspects of parallelization, Visualization
- Elements of Scientific Computing not covered:
 - Stochastic methods
 - Machine learning but see the Course "Julia Programming for ML" by Adrian Hill, https://adrianhill.de/julia-ml-course/

 These will involve the implementation of the numerical solution of a certain problem formulated as partial differentiation or system of PDEs, and a report on the implementation including the description of the methods used. I am currently working in the following fields and look for interested students:

- Electrochemical systems (electrocatalysis experimentation, batteries, fuel cells, biological ion channels)
- Semiconductor devices and solar cells
- · Geothermal flows, reactive flows in porous media
- Control volume finite elements and algebraic flux correction
- Tooling for Scientific computing: mesh generation, visualization

Upon interest I can formulate a course project based on one of these topics which may develop into a master thesis. In particular, my institute offers the possibility for female students to apply for the WIAS female master program.

- Variant A: "Classical": in-person, Wed 16:00-18:00, material uploaded as Pluto notebooks, pdf, html
- Variant B: "Post-Covid": online, material uploaded as Pluto notebooks, pdf, html, lectures recorded with occasional reuse of previous year's video. In-Person consultation Wed 16:00-18.00.