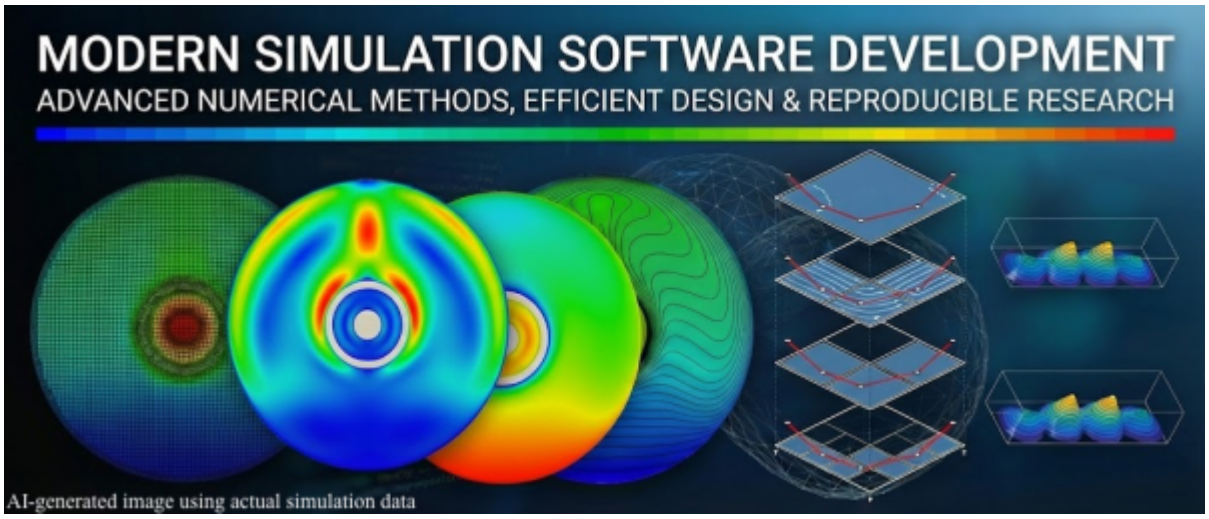
1 Modern Simulation Software Development

Summer 2026 · ACoM · RWTH Aachen University



A course for graduate students (e.g., master program in CES, SiSc, Math, Physics, etc.) on development of modern numerical software for simulation of complex engineering problems.

Lecturers: Dr. Lambert Theisen & Dr. Georgii Oblapenko

ECTS: 5 · **Format:** 2SWS lecture + 1SWS tutorial (tutorials merged to 2SWS slots every other week, 1SWS=45mins/week)

Registration: Opens 11 March 2026 via RWTHOnline (course 11.00153)

Module: *Current Topics in Computational Science and Engineering* (*Aktuelle Themen in Computational Science and Engineering*)

1.1 Goals & Topics

Advanced numerical methods for solving PDEs are presented and discussed, along with aspects of efficient numerical software design, focusing on robustness, accuracy in large-scale simulations, and reproducible research. Students gain insight into how modern simulation software is designed, implemented, and validated for real-world scientific and engineering applications.

Topics include (among others):

- Finite difference methods
- Finite element and discontinuous Galerkin methods
- Iterative solvers
- Particle-based methods
- Introduction to uncertainty quantification

1.2 Lectures

#	Topic	Notes	Slides	Date
1	Introduction	Notes	Slides	15.4.2026
2	Introduction to the Finite Element Method	Notes	Slides	22.4.2026
3	FEM II: nonlinear Poisson, Stokes with heat transport, eigenvalue problems	Notes	Slides · Notebook	29.4.2026
4	FEMI: Time, Preconditioners, PETSc	Notes	Slides	6.5.2026
5	Timestepping methods	Notes	Slides · Notebook	13.5.2026
6	Finite Volume Methods	-	-	20.5.2026
7	DG Methods: Introduction	-	-	3.6.2026
8	DG Methods: DGSEM, Entropy-stable methods	-	-	10.6.2026
9	Particle-based methods: SPH, Vortex methods	-	-	17.6.2026
10	Particle-based methods: DSMC	-	-	24.6.2026
11	Guest lecture	-	-	1.7.2026
12	Uncertainty quantification, sensitivity analysis	-	-	8.7.2026

1.3 Exercises

#	Topic	Topics	Date
1	Introduction (Shell, Git, Finite Difference, Repo Template)	Shell, Git, Finite Difference and Repo Structure	21.4.2026
2	FEniCSx/Gmsh project preparation, post-processing	Gmsh geometry and boundary tags, FEM, Paraview	05.05.2026

1.4 Projects

#	Topic	Sheet	Deadline	Submission
0	Finite Differences	Project 00 (example)	-	21.4.2026
1	Open FEM Project with FEniCSx	Notes · Slides · PDF · Notebook	01.06.2026 (end of date)	Via Moodle as Link to repo and PDF

1.5 Skills

#	Topic	Notes
1	Bash for Simulation Workflows	Skills 01
2	Git for Simulation Software Development	Skills 02
3	Gmsh Geometry for FEM	Skills 03
4	Paraview for FEM Output	Skills 04

1.6 Local Installation and Execution

The local workflow below uses the FEniCSx/DOLFINx stack used by Lecture 03 and Project 01: `dolfinx 0.10.x`, PETSc, Gmsh, Jupyter, and Quarto.

1.6.1 1. Create local conda environment

```
conda create -n fenicsx010 --override-channels -c conda-forge -y \
  python=3.12 fenics-dolfinx=0.10.0 ipykernel pyyaml matplotlib gmsh
```

If the conda solve does not provide the Python `gmsh` or `pyvista[jupyter]` module on your platform, install it with pip inside the environment:

```
conda run -n fenicsx010 python -m pip install --no-cache-dir gmsh pyvista[jupyter]
```

1.6.2 2. Register Jupyter kernel for Quarto

Quarto notebooks in this repo use `jupyter: fenicsx`, so register that kernel name:

```
conda run -n fenicsx010 python -m ipykernel install --user \
  --name fenicsx --display-name "Python (fenicsx 0.10.0)"
```

1.6.3 3. Install Quarto (if needed)

Check if Quarto is available:

```
quarto --version
```

If not installed, follow the official instructions: - https://quarto.org/docs/get-started/

1.6.4 4. Render the site locally

```
quarto render
```

Output is written to: - `_site/index.html`

The site render includes Quarto notebooks such as:

- `lectures/03.ipynb`, producing notes, RevealJS slides, PDF, and a copied notebook resource.
- `exercises/01-fem.ipynb`, producing `01-fem-notes.html`, `01-fem-slides.html`, `01-fem.pdf`, and a copied notebook resource.

To render only the current FEM project sheet:

```
quarto render exercises/01-fem.ipynb
```

1.6.5 5. Render the combined manuscript PDF

To build the book-like combined PDF with syllabus, lecture notes, exercises, and skills:

```
quarto render --profile manuscript --to pdf
```

Output is written to: - `manuscript/_book/mssd.pdf`

1.6.6 6. Quick sanity checks

```
conda run -n fenicsx010 python -c "import dolfinx, gmsh, petsc4py, mpi4py; print(dolfinx.__ver
```

You should see DOLFINx `0.10.0`.

1.7 Links

- ACoM Website
- RWTHOnline Course Page
- Moodle Page