ChE-312

Numerical methods

Miskovic Ljubisa

Cursus	Sem.	Type
Chemical Engineering	BA6	Obl.
Chemistry	BA6	Obl.
HES - CGC	E	Opt.

Language of teaching	English
Credits	3
Session	Summer
Semester	Spring
Exam	During the semester
Workload	90h
Weeks	14
Hours	**3 weekly**
Courses	2 weekly
Exercises	1 weekly
Number of positions	

Summary

This course introduces students to modern computational and mathematical techniques for solving problems in chemistry and chemical engineering. The use of introduced numerical methods will be demonstrated using the Python programming language.

Content

- Numerical differentiation (Euler forward, backward, Richardson extrapolation, error analysis)
- Numerical integration (Trapezoid rule, Simpson rule, composite rules, Romberg integration)
- Methods for solving nonlinear equations (bisection, Regula-Falsi, Newton-Raphson, error analysis)
- Methods for solving ordinary differential equations (notion of stability of solutions, stiffness, Euler methods, Runge-Kutta methods, Adams-Bashfort-Moulton, adaptive methods)
- Boundary value problems (finite difference method, FTCS scheme, Crank-Nicolson method, Finite difference methods in 2 and 3 spatial dimensions, Transient Boundary value problems)
- Basic notions of data analysis/processing

Keywords

Numerical differentiation and integration, nonlinear equations, ordinary differential equations, partial differential equations

Assessment methods

Two written evaluations during the semester (mid-term and end-of-term).

Supervision

Assistant.e.s	Yes
Forum	Yes

Resources

Moodle Link

- https://go.epfl.ch/ChE-312