

**Instructor:** Prof. M. A. Stadtherr, 118A Cushing Hall, markst@nd.edu

**Course Description and Aim:**

This course provides a survey of numerical methods and other computational algorithms used in steady-state chemical process simulation and optimization. For the most part, these are nonlinear equation solving and optimization (nonlinear programming) methods that are applicable not only in the context of chemical process engineering, but also in a wide variety of other engineering problems. The aim is to introduce the student to the basic concepts and strategies used, providing a foundation from which the student can develop or learn new methodologies, and to provide the student with problem solving tools that can be used in a wide variety of applications in engineering and science.

At the conclusion of the course, it is anticipated that you will have a basic understanding of:

- How calculations are organized in a process simulator (partitioning and tearing)
- How a process simulator actually solves (converges) calculations
- Numerical methods for solving nonlinear equation systems, including Newton, quasi-Newton and hybrid methods
- The importance of sparsity in solving large problems
- Optimality conditions for unconstrained optimization problems
- Numerical methods for solving unconstrained optimization problems, including Newton and quasi-Newton methods
- Optimality conditions for constrained optimization problems
- Numerical methods for solving constrained optimization problems (nonlinear programming), including GRG and SQP.
- Strategies for solving some special types of optimization problems (e.g., LP, GP, MINLP)
- Strategies for solving global optimization problems