M475 - Spring 2022

Industrial Mathematics

Modeling, Analysis, and Computation of interesting scientific / technological / industrial problems commonly known as **Computational Science**

Prof. Vasilios ALEXIADES Ayres 213 974-4922 alexiades@utk.edu
Office Hours: TR 1:10-2:00 and by arrangement (email me: alexiades@utk.edu)

- Prerequisites: Calculus (M141,142,241), ODEs (M231), and **familiarity with a programming language** (Matlab, Python, Julia, R, Fortran, C/C++)
- **Attendance is mandatory.**
- No textbook to buy!
- Work and Grading: No exams!
  8-10 Lab/Homework assignments: 40% , Project assignments: 40% , Term/Team Project: 20%
- Do not hesitate to talk to me if you are facing difficulties.
- **Do not fall behind!** Several things need to be done concurrently. Faster pace in the beginning, slower later...

- All incidents of academic misconduct will be reported to the Student Judicial Affairs office.
- If you need an accommodation based on the impact of a disability, please contact me privately.
  Contact the Office of Disability Services (2227 Dunford Hall, 974-6087) to coordinate reasonable accommodations for documented disabilities.

- **Computational Science :** doing Science by means of computation ("in silico").
  Involves: scientific problem → math problem → computational algorithm → numerical solution → implications for original scientific problem. CSE-HPC.jpg
  It has become the 3rd pillar of Science, complementing Theory and Experiment.
- Real scientific/technological/managerial problems canNOT be solved explicitly/exactly.
  Need to be solved numerically (approximately), so need *effective* approximations/algorithms and to understand effects of errors in the calculations.
- Want algorithms to be: ***effective, accurate, reliable, efficient*** and ***robust*** !
  These aims often play against each other, so trade-offs need to be made...
- Issues of *verification, validation, uncertainty quantification* are becoming increasingly important.

The course will simulate the core aspects of ***Computational Science*** including: • *modeling and computational simulation of physical phenomena*
• *writing reports* • *writing proposals* • *collaborating with colleagues on a Team/Term project* • *and presenting your work.*
Start thinking about a Term project topic right away!

Topics / Content

```
I.  Crystal precipitation
  - physical model leading to ODE system
  - about ODEs - well posedness of IVP
  - equilibria - root finding (Newton method) - plotting
  - analysis of the model
  - Euler scheme - computational errors
                 - consistency-stability-convergence
                 - implementation
  - classical RK4 and other numerical schemes

II. Air pollution: Advection and Diffusion Processes
  - the general conservation law  u_t + div F = 0
                     - derivation from first principles
                     - conservation of species
```

- advective and diffusive fluxes
- continuity equation
- constitutive laws (for non-advective fluxes)

- finite volume discretization of $u_t + F_x = 0$ - explicit/implicit
- diffusion ($F = -Du_x$) - parabolic PDEs - boundary conditions
  - explicit scheme - CFL condition
  - super-time-stepping acceleration
- advection ($F = uV$) - explicit upwind scheme
  - CFL condition - implementation
- linear advection - wave propagation
  - 1st order PDEs - method of characteristics
- advection-diffusion ($F = uV - Du_x$)
  - explicit scheme - CFL condition
  - effect of small/large Peclet number
- a few words about Lax-Wendroff and other schemes

III. Chemical reactions via mass action kinetics

IV. Uncertainty Quantification and parameter estimation

Some other possible topics:

V. Melting and Freezing
- phase-change basics, moving boundary problems
- Stefan Problem, exact solution, analytic approximations
- enthalpy formulation, explicit scheme

VI. The catalytic converter
- diffusion-reaction model
- control problem
- calculus of variations - Euler-Lagrange equation
- numerical scheme for the forward model

VII. Electron beam lithography (inverse problems)
- forward scattering (dose to exposure)
- inverse problem (exposure to dose) - ill posed problem
- Fourier-Poisson integral solution of diffusion equation
- Fourier series solution of diffusion equation
- Fourier series approximation of the inverse problem
- Discrete Fourier Transform, FFT

---------- Some comments from happy students ----------

- ***"Thank you for a very interesting and informative class. I looked forward to taking it and am incredibly glad I did."***
- ***"You made this class very interesting, challenging, and (dare i say it) fun ... I REALLY enjoyed the final project and feel more confident in my abilities because of this class."***
- ***"This class was one of the best, if not the best, of my college career. I really enjoyed it."***
- ***"Extremely relevant course material, broken down in a very understandable method by instructor"***
- ***"... the best math class I've had so far.... I really learned a lot and plan to use it."***
- ***"Loved it. It's the best class I've ever taken"***
- ***"... For someone who enjoys programming, and has a real desire to see what all this math can be used for, it has been a terrific course."***