MATH768: Mathematical Modeling I

An exploration of the synthesis of continuum mechanics with stochastic machine learning

Course syllabus

Times	MWF 2:30-3:20PM, Phillips 385
Office hours	MWF 12:30-2:00PM, and by email appointment, Chapman 451
Instructor	Sorin Mitran

1 Motivation

This course presents the theory of continuum mechanics from both a classical and contemporary perspective. Classical continuum mechanics is usually presented using the tools of differential calculus and provides a complete description for linear media with no memory effects, as exemplified most prominently by the Cauchy elasticity equations. While sufficient for the purposes of traditional mechanical engineering relying on small deformation of crystalline metals, vast classes of important materials encountered in plastics processing, paper processing, non-Newtonian flow or biological materials are only awkwardly described through the mathematical apparatus of partial differential equations (PDEs) mainly due to four causes:

Nonlinearity. Many materials of practical contemporary interest exhibit intrinsic nonlinear behavior, typically arising from a *mesoscopic* underlying structure instead of a *microscopic* one. Whereas the mechanical behavior of metallic monocrystals arises from electrostatic interaction acting at the length scale of the crystalline lattice of $\ell \sim 10^{-10}$ m along all directions, cytoskeleta exhibit an underlying structure with an average actin filament length of $a_1 \sim 10^{-8}$ m with a radius of $r_1 \sim 10^{-9}$ m, while muscle tissue fibers are of length $a_2 \sim 10^{-2}$ m with a radius of $r_2 \sim 10^{-5}$ m. When averaging out, or *homogenizing*, the behavior of the constituent elements of the medium to a macroscopic length scale of practical interest, say $L \sim 10^{-2}$ m, the large number of interactions in materials with microscopic structure often leads to isotropic and linear partial differential equations, but anisotropic and nonlinear behavior is obtained for materials with mesoscopic structure.

Active behavior. In classical continuum mechanics the underlying microscopic structure is typically considered to be fixed in time, a good approximation of the slow rate of chemical reactions (e.g., oxidation of iron) within the range of materials of interest. In contrast, conformational changes in flowing polymers or cellular dephosphorylation of ATP into ADP leads to markedly different mechanical behavior in viscoelastic flow or cellular motility. Such materials are said to be *active*, and typically exhibit very complex and incomplete mathematical descriptions within the framework of differential equation theory.

Stochastic behavior. Active materials tend to rearrange their mesoscopic structure, typically under the influence of random excitation (i.e., thermal bath) from the surrounding medium. This leads to the need for stochastic processes to describe the response of the medium to application of external forces.

Memory effects. The reorganization of mesoscopic structures due to chemical activity or external forces often occurs at time scales longer than those of observation, such that the prior history of the medium influences the observed behavior. Such memory effects can be modeled by differential equations of fractional order (i.e., integro-differential equations), and when combined with random thermal forcing require the consideration of non-Markovian stochastic processes.

The conundrum facing both the instructor and the student is how to efficiently explore the considerable achievements of classical theory synchronously with consideration of how gaps in its descriptive capability can now hope to be filled by developments within machine learning. The approach taken in this course is to present two tracks:

Track I (Mathematics oriented). This track follows the classical development of continuum mechanics. After introduction of the theory of mechanical deformation, elasticity, plasticity, and rheology are introduced as separate topics based upon a hypothetical relation between displacements and forces known as a *constitutive relation*. This leads to standard PDE descriptions of continuum mechanics such as the Cauchy equations of elasticity, Navier-Stokes equations for Newtonian fluids, or Oldroyd-B equations for viscoelastic flow. The nature of the PDEs for each case is considered along with presentation of some canonical solutions.

Track II (Applications oriented). This track starts from the basic conservation laws of physics, but eschews pre-formulated hypotheses on the link between displacements and forces in favor of a *data-driven* approach in which the tools of machine learning are applied to numerous experiments to extract appropriate constitutive relations. Such data-driven constitutive equations can be updated to take into account stochastic changes in the medium.

2 Course topics

The target population for Track I are mathematics graduate students who would benefit from a rigorous investigation of PDE modeling of mechanical behavior of continua. Track II is oriented for advanced undergraduates and graduate students with a background in biology, chemistry, computer science, engineering, or physics. Since course lectures regularly switch between the two tracks, all students will gain exposure to both approaches. Course homework is differentiated between the two tracks, and allows more in-depth study of topics within each track.

2.1 Track I topics

TEN. Tensor algebra and calculus

KIN. Kinematics of point masses, rigid bodies, deformable bodies

CON. Conservation laws (mass, momentum, energy) applied to continua

ELS. Elasticity, reversible small-amplitude deformations of a solid

PLS. Plasticity, irreversible deformation of a solid

NSF. Navier-Stokes flow of a Newtonian fluid

VEF. Viscoelastic flow

NET. Fiber networks

ACT. Active media

2.2 Track II topics

LSQ. Review of least squares approximation, seen as a particular example of machine learning

ANN. Review of artificial neural networks, seen as a particular example of approximation theory

DNN. Deep neural network models of constitutive equations:

- **DNN-ELS.** Classical elasticity theory recovered from a deep neural model of linear deformation
- **DNN-PLS.** Deep neural model of plastic deformation
- **DNN-NSF.** Navier-Stokes equations recovered from deep neural model of Newtonian flow

    - **DNN-VEF.** Deep neural models for viscoelastic flow
    - **DNN-NET.** Deep neural models of fiber networks
- **SNN.** Stochastic neural network models of active media
    - **SNN-VEF.** Polymeric fluids with changing connectivity, reptation.
    - **SNN-NET.** Fiber networks with changing connectivity
    - **SNN-ACT.** Fiber networks with active elements

3 Grading

3.1 Required work

- Homework, 7 assignments x 12 = 84 points
- Readings, 2 topics x 8 = 16 points

3.2 Mapping of point scores to letter grades

Grade	Points	Grade	Points	Grade	Points	Grade	Points
		H-,B+	86-90	P-,C+	71-75	L-,D+	56-60
H+,A	96-100	P+,B	81-85	L+,C	66-70	L–,D-	50-55
H,A-	91-95	P,B-	76-80	L,C-	61-65	F	0-49

4 Course policies

- This is a graduate-level course. Students are expected to undertake independent work to deepen their understanding of course material, as exemplified by the suggested reading topics
- Students are free to establish their own schedule; there is no need to inform instructor of absences. Course attendance is highly recommended to gain insight into course topics
- Late homework is not accepted.
- Homework is to be submitted in typeset, electronic form through Sakai. Templates will be provided.

5 Course materials

5.1 Bibliography

There is no single course text. Topics are drawn from the following sources that are available in electronic form from the course repository or UNC library.

- *Course lecture notes*, S. Mitran
- *Continuum Mechanics: Foundations and Applications of Mechanics*, C.S. Jog
- *Continuum Mechanics*, Andrus Koppel and Jaak Oja
- *Elements of continuum mechanics*, R.C. Batra
- *Deep Learning*, I. Goodfellow and Y. Bengio and A. Courville

Additional material is available in the course material repository (`/biblio` subdirectory)

5.2 Class slides

Slides are posted prior to class time. Additional notes are posted as needed. Read slides and notes before class to gain a first exposure to lecture material.

Week	Dates	Monday	Wednesday	Friday
01	08/19-23	-	Lesson01: TEN	Lesson02: TEN
02	08/26-30	Lesson03: LSQ	Lesson04: LSQ	Lesson05: KIN
03	09/02-06	(Labor Day)	Lesson06: KIN	Lesson07: ANN
04	09/09-13	Lesson08: ANN	Lesson09: CON	Lesson10: CON
05	09/16-20	Lesson11: ELS	Lesson12: ELS	Lesson13: DNN-ELS
06	09/23-27	Lesson14: DNN-ELS	Lesson15: PLS	Lesson16: PLS
07	09/30-04	Lesson17: DNN-PLS	Lesson18: DNN-PLS	Lesson19: NSF
08	10/07-11	Lesson20: NSF	Lesson21: DNN-NSF	Lesson22: DNN-NSF
09	10/14-18	Reading	Reading	(Fall Break)
10	10/21-25	Lesson23: VEF	Lesson24: VEF	Lesson25: DNN-VEF
11	10/28-01	Lesson26: DNN-VEF	Lesson27: SNN-VEF	Lesson28: SNN-VEF
12	11/04-08	Lesson29: NET	Lesson30: NET	Lesson31: DNN-NET
13	11/11-15	Lesson32: DNN-NET	Lesson33: SNN-NET	Lesson34: SNN-NET
14	11/18-22	Lesson35: ACT	Lesson36: ACT	Lesson37: DNN-ACT
15	11/25-29	Lesson38: DNN-ACT	(Thanksgiving)	(Thanksgiving)
16	12/02-06	Lesson39: SNN-ACT	Lesson40: SNN-ACT	-

5.3 Homework

Homework assignments present practical application of course concepts

Nr.	Issue Date	Due Date	Topic	Problems	Solutions
1	08/26	09/06	LSQ, TensorFlow	Homework01	
2	09/09	09/20	ELS	Homework02	
3	09/23	10/04	PLS	Homework03	
4	10/07	10/25	NSF	Homework04	
5	10/28	11/08	VEF	Homework05	
6	11/11	11/22	NET	Homework06	
7	11/25	12/04	ACT	Homework07	

6 Computational resources

Though the course concentrates on concepts within continuum mechanics and machine learning, the computational implementation of these concepts is essential to an appreciation of the utility of the considered approaches. Templates are provided for all computational applications, typically comprising:

1. Generation of data for constitutive relations;
2. Definition of deep neural networks that approximate the constitutive relation data;
3. Numerical methods (finite element, finite volume) that solve the classical formulations of continuum mechanics, e.g., Cauchy elasticity equations, Navier-Stokes flow equations.

6.1 SciComp@UNC Linux environment

This course uses a customized Linux environment named SciComp@UNC available to students as a virtual machine in which all course software is preinstalled, and course applications are preconfigured. Download Virtual Box and the SciComp@UNC virtual machine image.

Various software tools for carrying out and documenting practical scientific computation will be successively introduced:

- TeXmacs: editing of documents containing live computation
- SciPy: scientific Python environment
- TensorFlow: machine learning platform accessible from Python

- Mathematica: system for numerical, symbolic, and graphical computation with DNN support
- Gnu compilers (Fortran, C++): high-performance compiled code development
- Julia: a high-performance interactive environment
- Paraview: data visualization
- BEARCLAW: a package for solving PDEs using finite volumes
- FreeFEM++: a package for solving PDEs using finite elements

The Mathematica commercial package is accessible to students while connected to the campus network (either directly or remotely through the UNC VPN server).

6.2 Course material repository

Course materials (lecture notes, workbooks, homework, examination examples) are stored in a repository that is accessed through the subversion utility, available on all major operating systems. The URL of the material is http://mitran-lab.amath.unc.edu/courses/MATH768.

The initial svn checkout is made using commands:

```
mkdir ~/courses
cd ~/courses
svn co svn://mitran-lab.amath.unc.edu/courses/MATH768
```

On SciComp@UNC the initial checkout can be carried out through the terminal commands:

```
cd ~/courses
make MATH768
```

Update the course materials before each lecture by:

```
cd ~/courses/MATH768
svn update
```

Links to course materials will also be posted to this site, but the most up-to-date version is that from the subversion repository, so carry out the svn update procedure prior to each lecture.