Mesoscale Modeling of Complex Fluids (ME 580B) Spring 2015

Instructor: Dr. Xin (Frank) Yong, email: xyong@binghamton.edu

Office Location: Engineering & Science Building, Room 1320

Office Hours: Monday, Wednesday 1:00 pm-2:30 pm, and by appointment

Lecture Session Time: Monday, Wednesday 6:00 pm-7:25 pm for 15 weeks

Location: Nelson A. Rockefeller Center 161 (RC 161)

Out-of-class Learning Time: Students are expected to devote 6 hours per week to this course, including time required for readings and assignments.

Course Description: Complex fluids, i.e., polymeric liquids and melts, colloidal suspensions, and micelle solutions, are of great importance in nanotechnology, biomedical engineering, food science, and petroleum industry. This advanced fluid mechanics course will provide an overview of the structure and rheology of complex fluids from a computational modeling perspective, covering fundamental and applied topics relevant to current frontier research. The first half of the course will introduce various complex fluids and their physical behavior. The second half of the course will focus on surveying the state-of-the-art computer simulation methods (such as molecular dynamics, dissipative particle dynamics, lattice Boltzmann methods, and others) and their applications to model complex fluids.

Course Prerequisites:

- Analytical Methods ME 535;
- Introduction to Fluid Dynamics ME 550;
- Engineering Computational Methods ME 403 or equivalent.

Course Objectives:

- Introduce the structural and rheological properties of several complex fluids;
- Introduce computational methods for simulating complex fluids on the mesoscale.

Desired Course Outcomes: Upon completion of this course, students should be able to:

- Analyze kinematics and stresses for different flow geometries (shear and shear-free);
- Discuss basis properties of polymers, colloidal suspensions, and liquid crystals;
- Identify appropriate simulation techniques for specific complex fluid systems;
- Model a complex fluid system of interest using at least one simulation technique.
- Analyze and assess simulation results

Textbooks and Other Required Material:

- Required (recommended) textbooks:

- Supplemental materials: In addition to the above textbook, we will use portions of other textbooks (some listed below as references) and recent journal articles. These will be distributed in class as needed and posted on Blackboard.

- References:

**Course Format:** Class sessions will be used to develop topics, discuss applications and solve example problems. The Blackboard course management system will be used to post class scheduling and class materials. Students are expected to constantly check the Announcements Section and Content Section for any updates.

**Tentative Course Schedule:**

<table>
<thead>
<tr>
<th>Week(s)</th>
<th>Topic(s)</th>
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<tbody>
<tr>
<td>1</td>
<td>Introduction to complex fluids/review of math and fluids background</td>
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<tr>
<td>2</td>
<td>Rheometry</td>
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<tr>
<td>3</td>
<td>Basis forces in complex fluids</td>
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<tr>
<td>4-5</td>
<td>Polymers</td>
</tr>
<tr>
<td>6-7</td>
<td>Colloidal suspensions</td>
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<tr>
<td>8</td>
<td>Liquid crystals</td>
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<tr>
<td>9-10</td>
<td>Molecular dynamics</td>
</tr>
<tr>
<td>11</td>
<td>No class (spring recess)</td>
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<tr>
<td>12</td>
<td>Brownian dynamics/dissipative particle dynamics</td>
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<tr>
<td>13</td>
<td>Lattice Boltzmann method</td>
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<tr>
<td>14-15</td>
<td>Oral presentations of final projects</td>
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</tbody>
</table>
Course Grading: Class participation (5%), homework (20%), in-class quizzes (10%), mini-projects (25%), and final course project (40%).

- Homework will be assigned every 2-3 weeks. Due at the beginning of class one week later unless otherwise stated.
- Multiple-choice quizzes (10 minutes long) will be given every 2 weeks at the beginning of class on Monday. The lowest quiz grade will be dropped.
- Mini-projects will be assigned every 2-3 weeks. Due at the beginning of class two weeks later unless otherwise stated.
- The final course project will consist of an original paper and an oral presentation. The students are expected to apply the concepts and simulation methods from the class to a topic of interest.

All students are expected to abide by the Honor Code for Binghamton University and the Watson School. See link below:

http://www2.binghamton.edu/watson/about/honesty-policy.pdf