Instructor: Derek Elsworth & Roozbeh Foroozan  
Time: Tu, Th – 4.40-6.00  2 Deike Building  
Credits: 3  
Web: www.ems.psu.edu/~elsworth/  
Objective: To develop an understanding of methods of modeling important physical and chemical phenomena involved in natural and engineered systems. These include both separate and mixed solid (solid mechanics) and fluid (computational fluid mechanics) systems, including reactive components. The emphasis is on finite element methods.  
Students will develop working MatLab and FemLab modules of simple-through-complex models of interactive physical systems.  

COURSE OUTLINE  

1. Review of Important Physical Systems and their PDE’s  
   a. Terminology  
   b. Conservation of Mass and Energy (Scalar quantities)  
   c. Conservation of Momentum (Vectorial quantities)  
      i. Fluid Mechanics  
      ii. Solid Mechanics  
   d. History of Finite Element Methods  

2. Finite Element Representation of Important System Types (MatLab)  
   a. Mass and Energy Transfer  
      i. Fluid Flow and Diffusion  
         \[ A \frac{\partial c}{\partial t} + \nabla \cdot (-D \nabla c) = R \]  
         1. 1-D elements  
         2. Petrov-Galerkin formulation  
            a. 2-D triangular elements  
            b. 2-D isoparametric elements  
            c. 3-D generalization  
         3. Time-dependent behavior  
      ii. Advective Flows  
         \[ A \frac{\partial c}{\partial t} + \nabla \cdot (-D \nabla c) = R - \mathbf{v} \cdot \nabla c \]  
         1. 1-D elements  
         2. Petrov-Galerkin formulation  
            a. 2-D triangular elements  
            b. 2-D isoparametric elements  
            c. 3-D generalization  
         3. Time-dependent behavior  
         4. Reactive transport  
   b. Momentum Transfer - Fluid Mechanics  
      \[ \rho \frac{\partial \mathbf{v}}{\partial t} + \rho(\mathbf{v} \cdot \nabla)\mathbf{v} = \mathbf{F} - \nabla P + \eta \nabla^2 \mathbf{v} \]  
      \[ \nabla \cdot \mathbf{v} = 0 \]  
      1. 1-D elements  
      2. Petrov-Galerkin formulation  
         a. 2-D triangular elements  
         b. 2-D isoparametric elements  
         c. 3-D generalization  
      3. Time-dependent behavior  
   c. Momentum Transfer - Solid Mechanics  
      \[ -\nabla \cdot (\mathbf{c} \nabla \mathbf{u}) = \mathbf{F} \]
1. Virtual work formulation
   a. 1-D elements
   b. 2-D triangular elements
   c. 2-D isoparametric elements
   d. 3-D generalization

2. Time-dependent behavior

3. Coupled Process Models (FemLab)
   a. Fully-coupled solutions using FEM
      i. System coupling via governing equations
      ii. System coupling via Level-set methods
   b. Externally-coupled solutions
      i. Sequentially-coupled overlapping meshes
      ii. Meshes at multiple scales – linked FEM-MD models

4. Alternative Numerical Methods
   a. Integral methods
   b. Meshless models including SPH
   c. Discontinuum methods
      i. Block and Granular mechanis models
   d. Automaton Methods
      i. Simple models of Nature
      ii. Lattice-Gas Automata

ASSIGNMENTS & GRADING
1. Theme 1 – Individual MatLab Assignments (self-graded and subset presented 50%)
   a. Diffusive flow
      i. Steady state 2-D
      ii. Transient 2-D
   b. Advective-Diffusive Flow
      i. Steady state 2-D
      ii. Transient 2-D
   c. Navier-Stokes Flow – Steady – 2-D
   d. Solid Mechanics – Steady – 2-D

2. Theme 2 – Individual or Group Research Investigation (50%) (~30 hrs per person)

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<tr>
<td>Tentative Topic</td>
<td>Assign/Select Problem</td>
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<tr>
<td>1. Introduction &amp; 6. References</td>
<td>Research topic and complete and report literature review</td>
<td>One page narrative and at least 20 references</td>
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<tr>
<td>2.1 Governing Equations</td>
<td>Define conservation equations, constitutive relations, and boundary and initial conditions</td>
<td>One page max plus figures</td>
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<td>2.2 Formulation</td>
<td>Formulate using FemLab</td>
<td>One page max plus figures</td>
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<td>2.3 Solution</td>
<td>Solve using FemLab</td>
<td>One page max plus figures</td>
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<td>3. Validation</td>
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<td>One page max plus figures</td>
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<td>4. Parametric Study</td>
<td>Complete parametric study</td>
<td>One page max plus figures</td>
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<td>5. Conclusions</td>
<td>Distill significant results</td>
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<td>0. Abstract and 10 min Presentation</td>
<td>Complete paper and present results</td>
<td>10 minute presentation with one slide for each of 1; 2.1; 2.2; 2.3;</td>
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<td>A 28 &amp; A30</td>
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Grading – As above.

REFERENCES

_A compiled notebook and various resources are available online via Angel._

3. FemLab User’s Guide. ComSol. (Available on Angel and online with software)
4. FemLab Modeling Guide. ComSol. (Available on Angel and online with software)

Books on reserve at the library include:


Academic Conduct

Penn State’s policy on academic integrity applies to all aspects of course deliverables. Students are encouraged to work together, in groups, but to submit independent work. Further details are available at: [www.ems.psu.edu/students/integrity/index.html](http://www.ems.psu.edu/students/integrity/index.html)