EME 521 – MATHEMATICAL MODELING OF ENERGY & MINERAL ENGINEERING SYSTEMS

Coupled Processes of Deformation, Flow and Transport

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Modality: Web

Credits: 3

Online Materials: https://personal.ems.psu.edu/~fkd/courses/EGEE520/index.html

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 but also includes other continuum methods (LBM, SPH), integral methods and discontinuum methods.

Students will develop working MatLab modules of simple-through-complex models of interactive physical systems and research materials on some form of computational methods.

COURSE OUTLINE

1. **Review of Important Physical Systems and their PDEs**
    a. Terminology
    b. Conservation of Mass and Energy (Scalar quantiites)
    c. Conservation of Momentum (Vectoral 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 $-\nabla \cdot (c\nabla \mathbf{u}) = \mathbf{F}$

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 (Comsol-Multiphysics)

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

c. X-FEM

4. Alternative Numerical Methods

a. Integral methods

b. Meshless models including SPH

c. Discontinuum methods
    i. Block and Granular mechanics models

d. Automaton Methods
    i. Simple models of Nature
    ii. Lattice-Gas Automata

ASSIGNMENTS & GRADING

1. Theme 1 – Individual MatLab Assignments (self-graded with group discussion 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

e. Poromechanics
    i. Steady state 2-D
    ii. Transient 2-D

2. Theme 2 – Group presentations of exotic methods – BIEM/DEM/SPH/LBM …… (50%)

a. SPH – Smoothed particle hydrodynamics
    https://en.wikipedia.org/wiki/Smoothed-particle_hydrodynamics

b. LBM – Lattice-Boltzmann Method
    https://en.wikipedia.org/wiki/Lattice_Boltzmann_methods

c. Phase Field Methods
    https://en.wikipedia.org/wiki/Phase_field_models

d. X-FEM – Extended Finite Element Method
    https://en.wikipedia.org/wiki/Extended_finite_element_method

e. BEM – Boundary Element Methods
    https://en.wikipedia.org/wiki/Boundary_element_method

f. DEM – Discrete Element Methods
    https://en.wikipedia.org/wiki/Discrete_element_method

g. Lattice Methods
    https://onlinelibrary.wiley.com/doi/pdf/10.1002/nag.2249

h. Peridynamics

https://en.wikipedia.org/wiki/Peridynamics

REFERENCES

A compiled notebook and various resources are available online via Angel.

1. Elsworth, D. 2005. Companion Notes.
2. MatLab. 2005. User's Guide. Mathsoft. (Available online with software)

Books on reserve in the library include:

3. Kattan, P.I. 2003. MATLAB guide to finite elements : an interactive approach. Springer. pp. 385. TA347.F5K38 2003.
4. Kwon, Y.W. 2000. The finite element method using MATLAB. 2nd Edition. TA347.F5K86 1997.
5. Zienkiewicz, O.C. 2005 The finite element method: its basis and fundamentals. Elsevier. TA640.2.Z52 2005
6. Bathe, K.J. 1996. Finite Element Procedures. Prentice Hall. TA347.F5B36 1996

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: http://www.ems.psu.edu/current_undergrad_students/academics/integrity_policy