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Integrating COMSOL into a Mathematical Modeling Course for Chemical Engineers

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Premise

- Mathematical Modeling has been traditionally taught using:
  - Analytical methods (Laplace transforms, Fourier series etc.)
  - Pencil and paper
  - Linear problems in simple geometries
- Engineering students need to learn how to formulate models of realistic physical situations, how to solve them and how to interpret results
- Want to introduce our engineering students to problem-solving with modern engineering tools, such as COMSOL
- **Key issue: How can we give students a powerful package like COMSOL for their models, while teaching them to be informed and critical users?**

Specific Teaching Questions

- Are we giving students right background to use COMSOL?
  - Keep sight of the physical and chemical phenomena being modeled
  - Mathematical tools – calculus, differential equations, etc.
- Are we effectively teaching students how to use COMSOL?
  - Do they see it as a black box?
  - Similar concerns for process simulators e.g. Aspen
- Are we teaching students to be informed and critical users of computer packages?
  - Need to verify and validate
  - Guard against tendency to accept results at face value
  - Willingness to critically examine their own efforts

May need to re-focus course objectives and re-structure course content

Course Environment

- Four 7-week terms / year (A & B Fall terms, C & D Spring terms)
  - Students take 3 courses/term
  - “Applied Math for Chemical Engineers” meets 5 hours per week
  - Is a core course (12 of 14 required)
    - Only course that integrates all transport areas and reactors
  - Offered in final term (D) of year; taken by juniors and seniors (19 in class discussed here)

- Student preparation
  - Calculus and differential equations; not all have had matrices or vectors/tensors
  - Separate courses in Fluids, Heat Transfer, Mass Transfer and Kinetics & Reactors (usually concurrently)

Course Structure

- First 3 weeks:
  - Derivation of models for transport and reaction (“shell balances”)
    - 1st-order IVP and 2nd-order BVP
    - Elliptic, parabolic and 1st-order (convection) PDEs
  - Background mathematics classes
    - Matrices, vectors & tensors
  - Evaluation by exam and homework problems
- Last 4 weeks (focus of this talk):
  - COMSOL lab sessions
    - “watch & do” – instructor demo then worksheet for students
  - Theory classes in FEM (in parallel with lab sessions)
  - Evaluation by in-lab exam, final exam and computer exercises
- COMSOL demos and worksheets associated with the lab sessions based on books by Finlayson and Plawsky (not required)

COMSOL in-class examples and homework

Lab	Demo and *Worksheet*	Homework exercise
1	Conduction in a slab with k(T) *Conduction in cylinder, k(T), Q(r)*	Diffusion across membrane with D(C), reaction
2	Isothermal diffusion/reaction in sphere *Diffusion/reaction in sphere + heat effects*	Nonisothermal 1D tubular reactor
3	Pipe entry flow – Newtonian fluid *Pipe entry flow – Non-Newtonian fluid*	Flow in 2D microfluidic device
4	Conduction in 2D – regular & irregular domain *Conduction in combustion chamber*	Heat transfer in microchannel reactor
5	Transient conduction / Convective diffusion *Unsteady reaction/diffusion / 3D flow past heated sphere*	Dispersion/reaction in microfluidic device
6	Advection tube flow – artificial diffusion *Chromatography column – convection/diffusion*	Convection-dominated reactors

Lab Demo 2: Diffusion/Reaction in Sphere

The following equations govern diffusion and reaction in a catalyst with significant heat effects. Solve for $\phi = 1.1$, $\gamma = 30$ and $\beta = 0, 0.01, 0.03, 0.07, 0.10, 0.12, 0.15$.

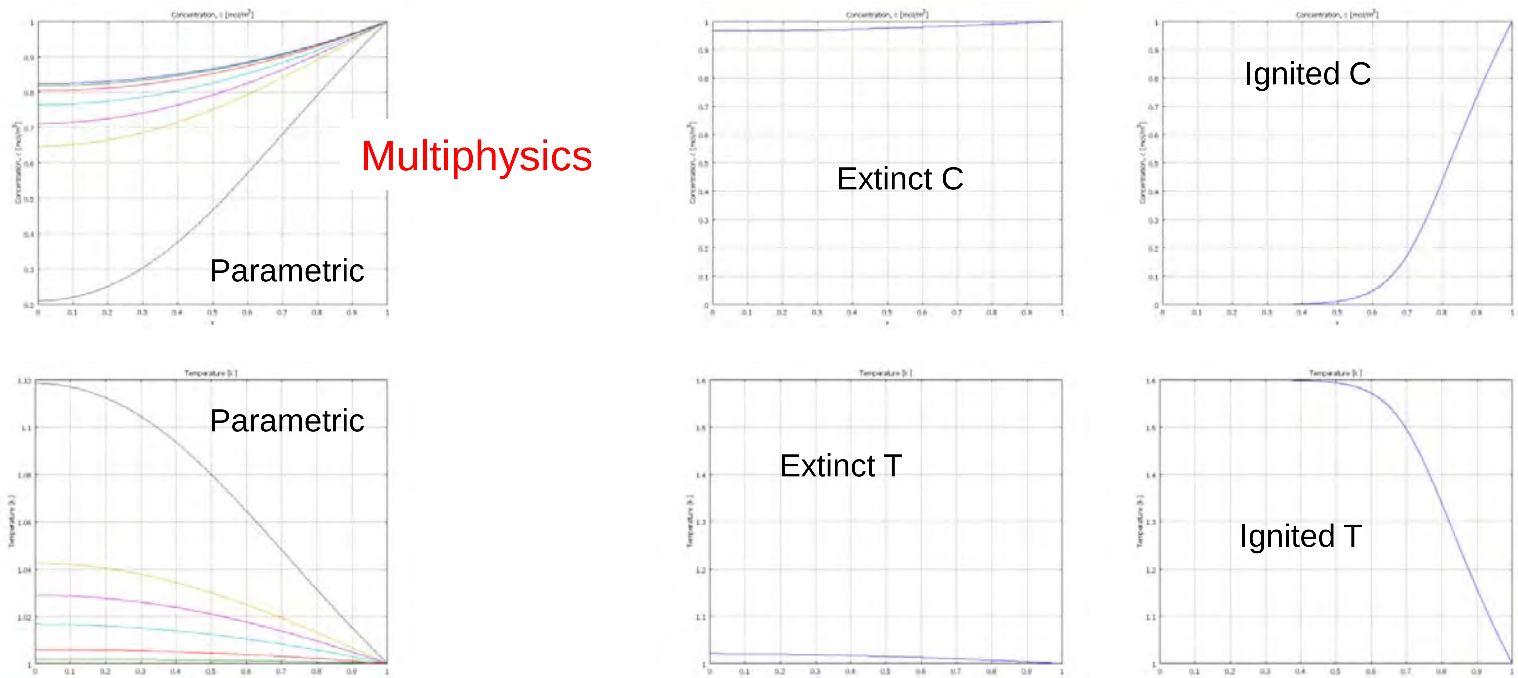
$$\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}c}{\mathrm{d}r}\right) = \phi^2 R(c,T), \ \frac{\mathrm{d}c}{\mathrm{d}r}(0) = 0, \ c(1) = 1$$

$$\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}T}{\mathrm{d}r}\right) = -\beta\,\phi^2 R(c,T), \ \frac{\mathrm{d}T}{\mathrm{d}r}(0) = 0, \ T(1) = 1,$$

$$R(c,T) = c\,\exp[\gamma(1 - 1/T)]$$

(From Finlayson (2006))

Multiplicity



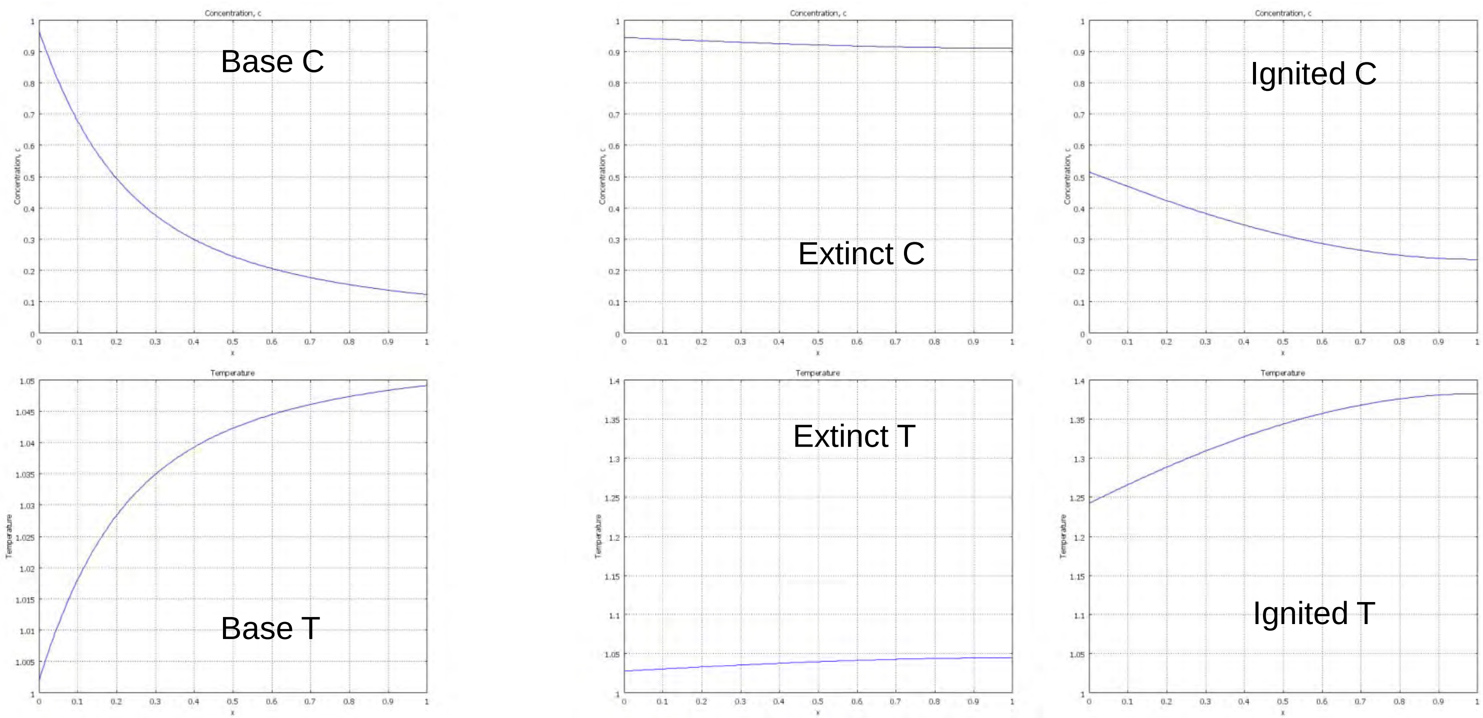
Exercise 2 – Nonisothermal 1D tubular reactor

- multiphysics
- multiple solutions, depending on values of $\beta = \dfrac{(-\Delta H)c_0}{\rho c_p T_0}$

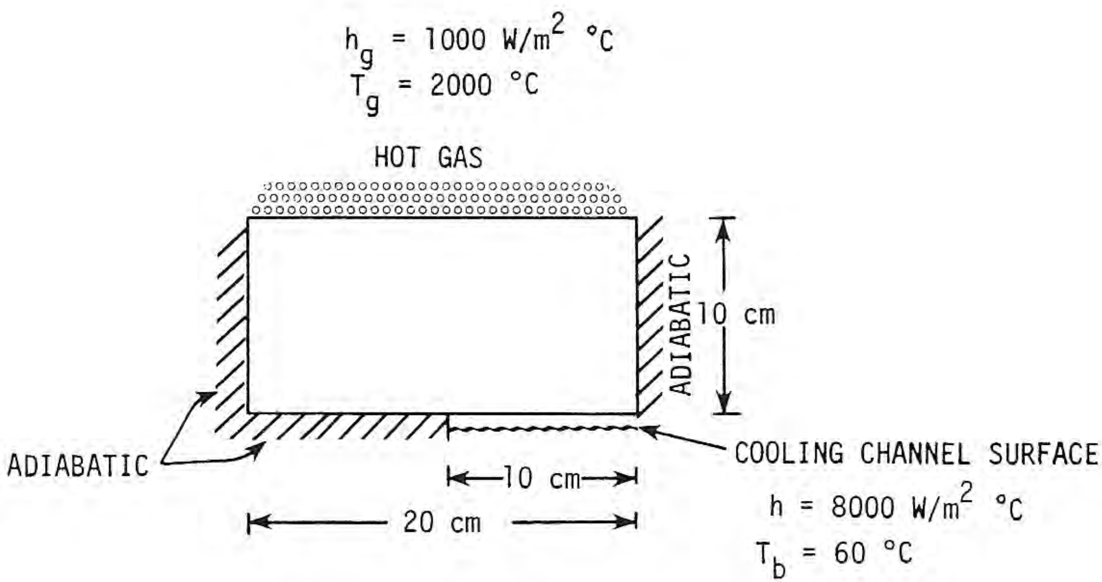
$$\frac{1}{Pe}\frac{d^2c}{dx^2} - \frac{dc}{dx} = Da\, R(c,T), \qquad -\frac{1}{Pe}\frac{dc}{dx}(0) = 1 - c(0), \quad \frac{dc}{dx}(1) = 0$$

$$\frac{1}{Pe_H}\frac{d^2T}{dx^2} - \frac{dT}{dx} = -Da\, \beta\, R(c,T), \qquad -\frac{1}{Pe_H}\frac{dT}{dx}(0) = 1 - T(0), \quad \frac{dT}{dx}(1) = 0$$

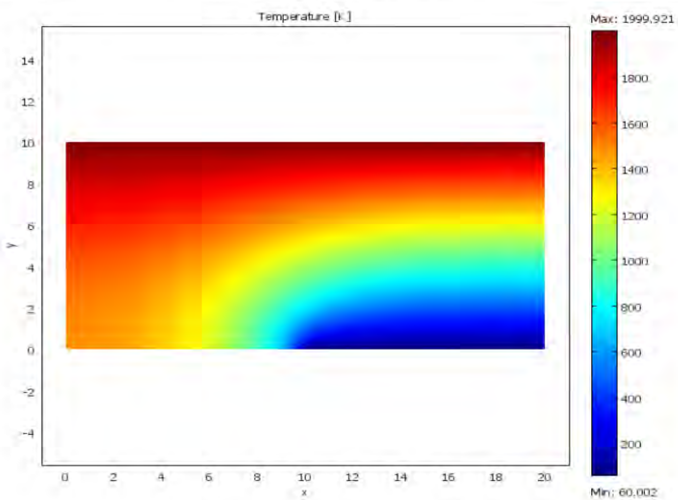
$$R(c,T) = c^2 \exp\left(\gamma - \frac{\gamma}{T}\right)$$

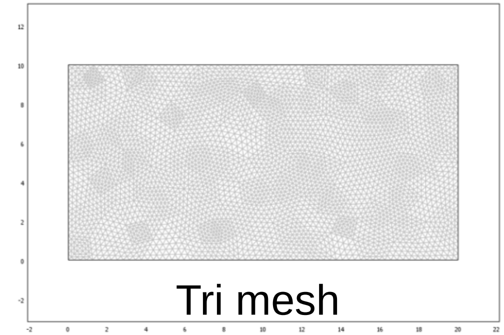


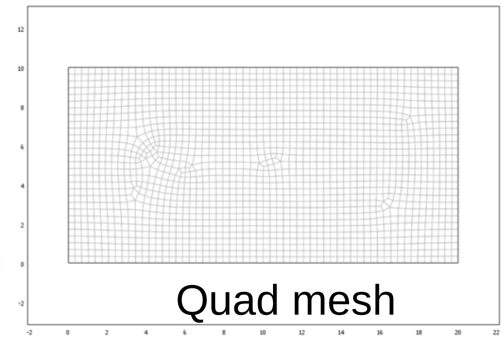
Lab Demo 4: 2D Conduction in Chamber

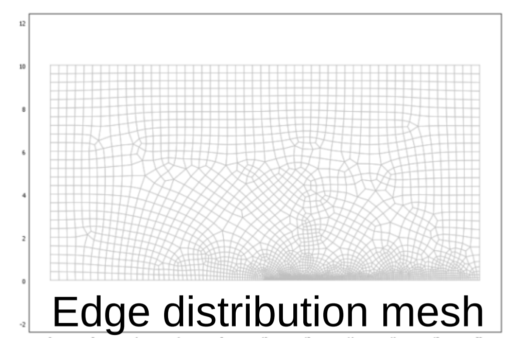


Students learn to:
– set up boundary conditions
– check energy bal. in 2D
– use different mesh strategies




Tri mesh

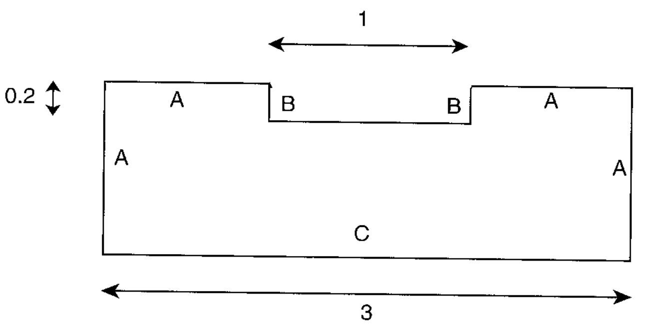

Quad mesh


Edge distribution mesh

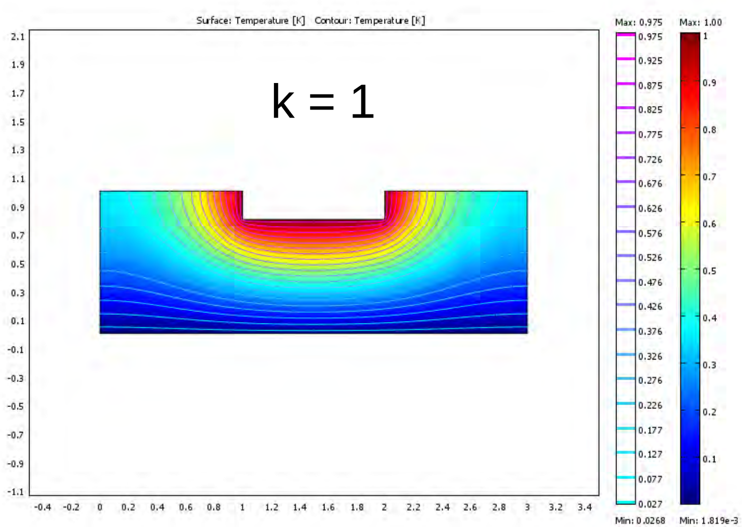
Exercise 4 – Heat transfer in microchemical reactor

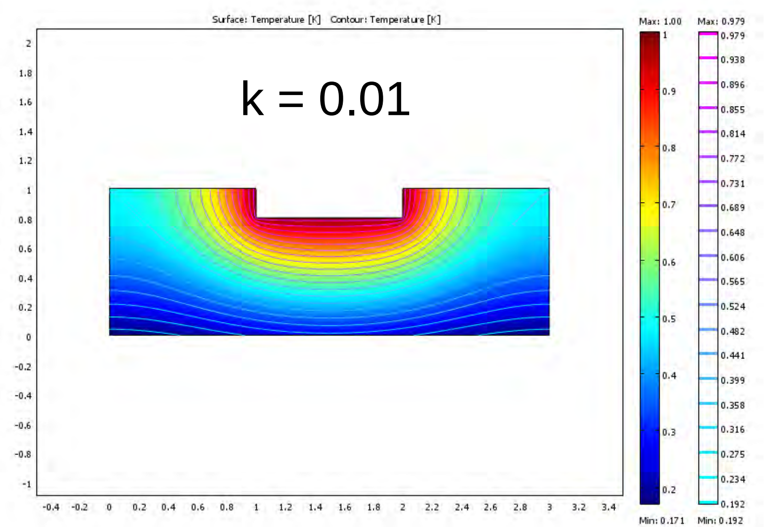
Heat transfer takes place in the geometry shown. Boundaries A are insulated; along boundary B the temperature is 1.0; the boundary condition at C is

$$-k\frac{\partial T}{\partial n} = hT$$



(From Finlayson, 2006)



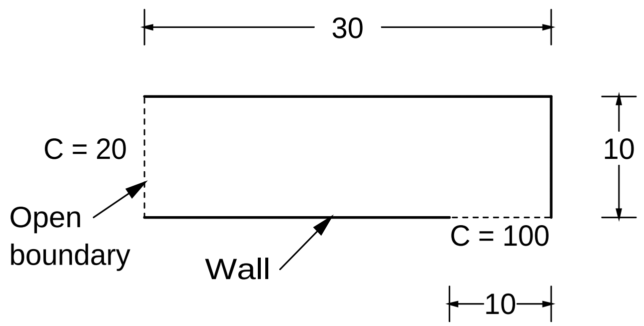


Students checked energy balances and refined tri and quad meshes

FEM and Numerical Methods

Class	Topic
1	Discretization for BVP and IVP, Galerkin method
2	FE basics, weak form, natural and essential b.c.
3	Computation of matrix elements, matrix assembly in 1D
4	2D weak form, meshing, shape functions, matrix assembly, heat equation, Galerkin-Petrov
5	Systems of linear equations, direct methods (GE, LU, sparse methods)
6	Systems of linear equations, indirect methods (Jacobi, Gauss-Seidel, preconditioning, multi-grid)

Evaluation: Midterm exam



$$D\left(\frac{\partial^2 C}{\partial x^2}+\frac{\partial^2 C}{\partial y^2}\right)-kC=0$$

Boundary conditions as shown on diagram

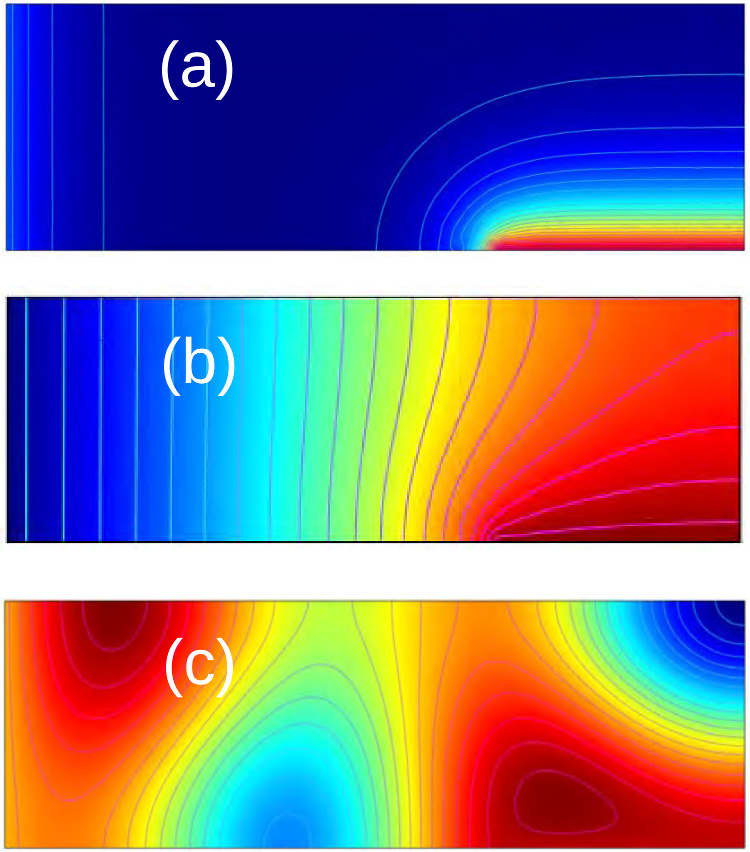
- Skills tested
  - Translate given equation into vector/tensor form for COMSOL
  - Input geometry, define mesh, solve, make surface plot and export for grading
  - Use subdomain and boundary integration to compare transport into domain to volumetric consumption by reaction – close mass balance
  - Refine mesh to improve mass balance
- Grading
  - Individual *k*, *D* values for each student
  - Students submit a bitmap plot and .mph file via e-mail

Evaluation: Midterm exam results

- Student contour plots
  - Top one (a) shows generally correct answer
  - In (b), mis-set boundary conditions produce this map.
  - The picture in (c) won class award for "most colorful"

- Statistics
  - Class average was 82
  - $\sigma = 14$, Range 52 – 98

- Basic COMSOL skills satisfactory
  - Problems with vector/tensor
  - Problems with boundary, domain integration



Evaluation: Final exam theory questions

Question topic	Average	Standard Deviation
1. Given vector/tensor equation for incompressible Navier-stokes model, write it in component form	4.68/10	1.72
2. Given a 2^{nd}-order BVP and a first-order trial function, get an expression for the residual and apply Galerkin's method	7.53/15	5.05
3. Derive the weak form for a 2^{nd}-order BVP with essential boundary conditions	10.10/15	2.13
4. System matrix assembly for a two-element 1D domain with linear basis functions, given the element mass and stress matrices	7.37/15	4.77
5. Complete the LU factorization for a given symmetric 3×3 matrix, from the lower-diagonal factor U	11.26/15	3.61

- Students struggled , except for weak form which they saw a few times
- Need to tie theory in to lab exercises and give more practice

Evaluation: Final exam concept questions

Question topic	Average	Standard Deviation
6. Critical examination of numerical results - non-isothermal diffusion-reaction problem in a slab, four answers given illustrating errors, multiplicity	3.84/10	1.69
7. Verification of numerical method - laminar flow around a golf ball (dimpled sphere). Ideas of mesh and domain independence, test mesh on smooth sphere model.	7.42/10	2.78
8. Model validation – how to validate a simulation of non-Newtonian flow through a triangular structured packing 	4.84/10	2.62

– Students all failed to recognize the possibility of multiple solutions despite seeing it earlier in course, for #6
– Most students could not interpret wrong answers in #6 to suggest possible sources of error
– Ideas of verification and validation reasonable – “refine mesh”

Survey Question - 1

Question topic (1 – Strongly disagree 2 – Somewhat disagree 3 – No strong feeling 4 – Somewhat agree 5 – Strongly agree)	Average Response	Standard Deviation
Mathematics background		
1. One class on matrix algebra was enough	4.78	0.71
2. One class on vector/tensor calculus was enough	4.28	0.56
3. The background in calculus and differential equations was enough for the course	4.11	0.94

- Students were overly optimistic about vector/tensor calculus, from their responses to exam questions
- Background in calculus and differential equations adequate but responses suggested a problem with retention

Survey Question - 2

Question topic (1 – Strongly disagree 2 – Somewhat disagree 3 – No strong feeling 4 – Somewhat agree 5 – Strongly agree)	Average Response	Standard Deviation
Computer in-lab instruction – more time was needed on		
1. geometry set-up in 2D	1.89	0.87
2. correspondence between COMSOL format and model equations	3.06	1.13
3. post-processing for plots	3.33	1.15
4. post-processing for boundary and domain integration	2.83	1.26
5. subdomain settings	2.33	1.10
6. boundary settings	2.33	1.15

Exam results suggest student confidence in #4 is too optimistic

Survey Question - 3

Question topic (1 – Strongly disagree 2 – Somewhat disagree 3 – No strong feeling 4 – Somewhat agree 5 – Strongly agree)	Average Response	Standard Deviation
Background theory on Finite Element Methods		
1. don't need FEM theory to use COMSOL	3.28	1.32
2. more information would make theory easier	3.33	1.05
3. theory was ok but too much in too few classes	4.39	0.89
4. needed more worked examples and homework	4.50	0.83

- Most students felt more homework and worked examples would be beneficial
- No-one wanted to positively recommend a higher workload
- A vocal minority felt "we don' need no stinkin' theory"

Survey Question - 4

Question topic (1 – Strongly disagree 2 – Somewhat disagree 3 – No strong feeling 4 – Somewhat agree 5 – Strongly agree)	Average Response	Standard Deviation
General aims of course and course structure		
1. better to spread COMSOL material out over entire course	3.06	1.39
2. should go back to finite differences using Excel	1.28	0.93
3. course helped me be a better/more careful computer user	4.39	0.49
4. more worked examples and homework problems on theory would aid understanding	4.28	1.10

- Expected students to endorse more time on COMSOL and spread out over full seven weeks
- Resistance to this idea rooted in desire to preserve “model development” part of course

Conclusions

- Students demonstrated reasonable competence in using COMSOL
  - Strongly appreciative of in-lab demonstrations, one-on-one help
- Positive student reaction to COMSOL
- Student understanding of theory behind numerical method was poor
  - Need to integrate FEM material more tightly, focus on what really connects with the COMSOL application
- Need to find ways to emphasize and reinforce ideas on verification, validation and more thorough scrutiny of results