With COMSOL, That Time is Now

Presented by:

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Outline

• Early simulation tools
• Career inspiration
• Engineering choices
• Projects prior to COMSOL
• Current COMSOL-involved projects
• Inspiring others to use COMSOL
1972 Freshmen Engineering Students Learned How To Use a Slide Rule

- Last year of slide rule course at VPI&SU.
- The instructor used “teaching” slide rules.
- Calculators became common the next year.
- COMSOL could not be envisioned yet.
1972 Freshmen Engineering Students Learned How To Program in FORTRAN

- FORTRAN is still in use today.
- Many legacy FORTRAN codes.
- Now is a good time to replace legacy code with COMSOL models.
1977: My Initial Inspiration for a Career in Simulation

- Senior Lab UTK-NE: ORNL Health-Physics Research Reactor (HPRR)
- Compared pulse experiments to FORTRAN code
- Stack of FORTRAN cards about 4-inches deep, tweaked coefficients to match data

These experiments could not be repeated today, but this would have been perfect for the COMSOL application builder!
1984: RELAP5 Nuclear Power Plant Simulation and Testing of Gamma Thermometer Level Monitoring

- In response to the TMI accident, need improved level monitoring.
- An NRC code RELAP5 was used to simulate tests for the new instruments.
- RELAP5 and similar codes are still used today.
- COMSOL Pipe Flow Module has demonstrated similar models (Wang et al.)
Engineering Choices: Technology that Works Requires High Quality

- 1972: Nuclear Engineering (NE)
- 1977: computer simulation
- 1979-1982: utilized codes that needed a lot of improvements
- received excellent mentoring
- 1983-1992: finite element (FE) methods, PhD research
- continue to apply this FE-based simulation in NE
- used advanced software tools such as LaTeX and Linux
- 1994-2004: sought a code that met established goals
- 2004-2014: the code became COMSOL
- 2014-future: expand COMSOL usage to new problems
1992: PhD Graduation, the Mentoring Finalized

- Many long discussions together.
- We envisioned an ideal computer software environment.
- Numerical Analysis Digest announced release 3.0 of COMSOL.
- After graduation, I asked AJ if he ever heard of COMSOL.
- His response: “Sure! My students do their projects using COMSOL.”
- I guessed that the number of incomplete grades (I) for the semester has been reduced!
- I have often desired to go back and repeat my own “wine-glass problem” using COMSOL.
- So, that is how I started with COMSOL.

Calculated Transverse Momentum for the Ideal-Gas Viscous Solution of the GAMM Double-Throat Nozzle Problem (Fig. 8.84 of Ref #3).
A Brief Description of the ORNL High Flux Isotope Reactor

- HFIR is a DOE research reactor
- Does not produce power
- Main product is neutrons
- HFIR core (shown at the right) consists of 2 fuel elements, 9.4 kg of 93% enriched U$_{235}$
- HFIR has 4 primary missions:
  1. Neutron scattering,
  2. Irradiation materials testing
  3. Isotope production
  4. Neutron activation analysis
2004: The First COMSOL Project for HFIR at ORNL

- used COMSOL to design the pressurizer component
- connects ambient to 20 K supercritical para-hydrogen loop
- pressure and temperature dependent material properties
- weak statement provides a thin-shell for the structure
- COMSOL simulations match the instrument outputs
- has been operating successfully for over 7 years
- Could revisit with present versions and computing capability

COMSOL simulated internal natural convection flow streamlines

COMSOL simulated surface temperature distribution

Installed HFIR cold source pressurizer
2011: HFIR Fuel Plate Thermal Deflection Validation

- Validation case for the HFIR LEU fuel conversion project
- Demonstrates COMSOL can simulate thermal-structural interaction sufficiently for this project

Jain, et al. ORNL/TM-2012/138, June 2012

COMSOL Applied to Nuclear Reactor Kinetics, David Chandler et al.

- equation-based modeling, space-time kinetics in 2D axisymmetric geometry.
- demonstrates COMSOL could be a major tool for modeling reactor physics.

\[
\begin{align*}
\frac{1}{v^g} \frac{\partial \phi^g}{\partial t} - \nabla \cdot (D^g \nabla \phi^g) + \left( \sum_{g=1}^{G} \phi^g - \sum_{g=1}^{G} \phi^{g+1} \right) \phi^g = (1 - \rho_{\text{eff}}) \chi^g \sum_{g'=1}^{G} \phi^{g'} + \sum_{g'=1}^{G} - \sum_{i=1}^{I} \lambda_i \chi^g C_i
\end{align*}
\]

\[
\frac{\partial C_i}{\partial t} + \lambda_i C_i = \beta_i \sum_{g=1}^{G} v \Sigma_f^g \phi^g
\]

Fast Flux  Epithermal Flux  Thermal Flux

neutron flux distribution

Free mesh + boundary layer mesh

Solved for power excursion transient with control element feedback
COMSOL Applied to Pu-238 Production for NASA COMSOL
Freels, Jain, Hurt, et al.

single bare pellet, 2nd irradiation cycle, COMSOL 4.2a, 3D, ¼ pie slice

reduced-length bare pellet, 2nd irradiation cycle, COMSOL 4.2a, 3D, ¼ pie slice

partially-loaded (8 pellets) prototype production target, 2 irradiation cycles, COMSOL 4.3

fully-loaded prototype production target (52 pellets), COMSOL 4.3, 2D axisymmetric

individual pellet at maximum temperature in stack:
stress contour with 10000x deformation
2009-Present: COMSOL is providing fundamental support for the conversion of HFIR to LEU fuel

- Provide best-estimate and safety-basis accurate 3D simulations of:
  - fluid flow into, through, and out of the core flow channels,
  - fuel-plate and coolant heat transfer,
  - structural response due to thermal expansion (TSI),
  - structural response due to fluid interaction (FSI),
  - oxidation of the fuel-plate surface and subsequent geometry changes,
  - fuel shrink and swell due to radiation effects,
  - hot spot and hot-streak effects due to manufacturing defects,
  - additional physics as necessary.

- The approach has been a multi-step process that includes:
  - develop physics test bed in 2D to feed results to the 3D models,
  - develop 3D geometry, mesh, and property inputs,
  - perform separate-effects simulations in 3D to V&V physics goals (heat transfer, FSI, TSI).
  - provide perturbed estimates and/or separate safety-basis models from the best-estimate models to answer safety-analysis questions (hot spots, buckling potential, reduced flow, decay heat, etc.).
  - combine separate effects models into the all-physics model
  - provide input data for other parts of the HFIR safety analysis (transients using RELAP5, etc.).
Typical LEU Fuel COMSOL Safety-Basis Case (from Prashant K. Jain, see poster) Inner Fuel Element under 100 MW Nominal Conditions

- **Volumetric Heat Source (kW/cm³)**: 61.1
- **Clad Surface Heat Flux (W/cm²)**: 450
- **Clad Surface Temperature (°C)**: 120
- **Plate Deflection (mils)**: 7
- **Coolant Pressure (psia)**: 460
Typical LEU Fuel COMSOL Separate Effects Case
(from Franklin G. Curtis)
Fluid-Structure Interaction Flat Plate Analysis Results

Results for Run 1 from Kennedy’s report with a plate thickness of 40 mils. No comb on leading or trailing edge (data courtesy of John Kennedy, University of Missouri, Columbia, Mechanical Engineering Department).
Typical LEU Fuel COMSOL Best Estimate Case
HFIR Inner Fuel Element Plate – Old Reference Design

\( T_{\text{max}} \) axial cut line mesh convergence history of temperature

\( T_{\text{max}} \) cut plane height-enabled velocity

\( T_{\text{max}} \) normal cut line mesh convergence history of temperature (left) and velocity (right)

wetted surface temperature

\( T_{\text{max}} \) cut plane temperature

SST turbulence model, temperature-dependent properties
COMSOL has enabled research and employment opportunities for graduate students and professionals through our group on ORNL projects

- Kirk T. Lowe, PhD ME dissertation, Bettis Atomic Power.
- Prashant K. Jain, PhD NE post-doc, full-time ORNL staff.
- David Chandler, PhD NE dissertation, full-time ORNL staff.
- Vaibhav Khane, PhD ChE, summer intern at ORNL, Intel.
- Isaac T. Bodey, PhD ME dissertation, Savannah River Remediation.
- Franklin G. Curtis, PhD candidate ME, finishing up soon.
- Christopher J. Hurt, PhD candidate NE, currently supported.
- Several intern students have used COMSOL in their research while supported by ORNL projects.
- We engage through user groups and workshops to encourage COMSOL usage at ORNL.
In the 1980’s, when computers became more common in the workplace, my colleagues and I would often marvel and say “someday we will be able to solve time-dependent, 3D, Navier-Stokes equations right on our desktops.”

-with COMSOL, that time is now.

Today, I think that, someday, we will be able to solve most any physics we want in full 3D to the resolution that we desire. Perhaps then we will reexamine the fundamental equations of physics that we currently hold true.

-with COMSOL, we will be able to test these new theories and equations.
Oak Ridge National Laboratory: Meeting the challenges of the 21st century

Thank you for your attention!
List of References

8. J. D. Freels et al., *Design and Nuclear-Safety Related Simulations of Bare-Pellet Test Irradiations for the Production of Pu-238 in the High Flux Isotope Reactor using COMSOL*, COMSOL Conference Boston 2012.