CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT

SUBJECT: FEMLAB Training Courses
(06002.01.011.026)

DATE/PLACE: August 8–9, 2005; Albuquerque, New Mexico

AUTHOR: S. Stothoff

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PERSONS PRESENT:	Approximately 12 participants attended the course, at least half from Los Alamos and Sandia national laboratories

BACKGROUND AND PURPOSE OF TRIP:

FEMLAB is a software package that is intended to provide easy-to-use multiphysics modeling capabilities. At least six staff members at CNWRA have expressed interest in using FEMLAB in their work. FEMLAB is built on MATLAB, and is an outgrowth of the PDE toolbox available with MATLAB (although orders of magnitude are more powerful). COMSOL, Inc. created both the PDE toolbox and FEMLAB. COMSOL, Inc. offers frequent training opportunities typically organized as a series of three one-day courses in sequence at specific locations scattered about the United States and Canada. The first two days in the sequence are called "Introduction to FEMLAB" and "Advanced Modeling Features." The third day focuses either on a particular module supplied with the code (e.g., "Heat Transfer Modeling") or additional advanced features.

The purpose of the trip was twofold: (i) to evaluate the code for potential use at CNWRA by engaging in training, and (ii) to have a staff member familiar with how the code is used should FEMLAB be purchased. For this purpose, only the first two days of the sequence were deemed sufficient.

SUMMARY OF PERTINENT POINTS AND ACTIVITIES:

The introductory course focused on interacting with the Graphical User Interface (GUI) while running through a series of lectures and workshop exercises illustrating how the multiphysics capabilities of the code are implemented. The first exercise was coupled three-dimensional Navier-Stokes flow with deflection of a rod in the current. Other exercises considered thermal effects of electrical currents, transport of heat due to Navier-Stokes flow, thermal stresses, radiative transport of energy between separated subdomains, and parametric studies.

The advanced course presented much more of the details of how the numerical modeling is performed and how to select options driving the code. The lectures focused on selecting solvers, coupling techniques, accurate flux calculations, adding algebraic equations, and weak form mathematics. The workshop exercises demonstrated topics in the lectures.

An analysis of the strengths and weaknesses of the FEMLAB software for the purposes of CNWRA and NRC is attached.

CONCLUSIONS:

The courses were extremely beneficial for finding out how to use the FEMLAB code. The introductory course provided a good overview on how to interact with existing features, while the advanced course provided a good introduction into the capabilities for adding additional user-specific modeling features. These courses are likely sufficient for users that will be using and modifying existing applications. The code is sufficiently powerful that users interested in developing new applications might benefit from an additional day of advanced training (this option is available for a training course in November in Palo Alto, California, and December in Burlington, Massachusetts).

PROBLEMS ENCOUNTERED:

None.

PENDING ACTIONS:

None.

RECOMMENDATIONS:

The FEMLAB code is recommended for purchase based on the observations from this course. Attending a training course is highly recommended for staff intending to use FEMLAB. It is recommended that, if possible, staff should try the code out ahead of time to get somewhat familiar with it before attending the course.

Note that training is offered at reduced rates to license-holders and COMSOL, Inc. will provide onsite training. If the FEMLAB code is purchased, it might be attractive to arrange for a course to be held at Southwest Research Institute®.

SIGNATURES:

S. Stothoff
Senior Research Scientist

8/26/2005
Date

CONCURRENCE:

G. Wittmeyer
Assistant Director, Earth Sciences

8/26/2005
Date

Patrick C. Mackin
Director of Administration

8/26/2005
Date

ATTACHMENT

Evaluation of FEMLAB Software

S. Stothoff

Overview

The FEMLAB software is a general-purpose multiphysics analysis code built upon the MATLAB analysis platform. The developer is COMSOL, Inc., a Swedish company with offices in the United States. The code can be run completely from a script, but it is designed to be used with a Java-based graphical user interface (GUI).

The FEMLAB code considers one-, two-, and three-dimensional subdomains, including axisymmetric and radial domains, and allows different subdomains to be linked together. Within each subdomain, a wide variety of partial differential equations (PDEs) can be considered based on the classical set of PDEs and extensions important for science and industry. The PDEs can be static (no time derivative) or transient (1st-order and 2nd-order time derivatives). Any particular subdomain can implement any subset of the available PDEs; the equations can be coupled within a subdomain and between subdomains.

The FEMLAB code uses a finite-element discretization. Typically the elements have low-order geometry (i.e., line segments, triangles, tetrahedral) but a variety of basis functions (e.g., linear, quadratic, cubic). The code allows quadrilaterals only in a so-called map mode; however, mixing quadrilaterals and triangles is planned for an upcoming release. Numerous tools are provided in the GUI to create meshes.

The FEMLAB code reduces the equation set to differential algebraic equations, hence transient analyses use the method of lines. In essence, the method of lines discretizes the spatial component of an equation set (using finite elements for FEMLAB) and uses a robust ordinary differential equation solver to handle the time derivatives. This approach is known to be quite powerful for adaptive time stepping. The code allows mixtures of transient and static PDEs during the same analysis.

A variety of solvers can be used to solve the set of linearized equations. Four direct solvers are provided, as well as several iterative solvers. FEMLAB offers sophisticated options for sequencing the solution of equations. The equations can all be solved simultaneously, in a user-specified sequence, or any mixture of the above. A scripting capability is provided to fine tune equation solution sequences. In addition, equations can be solved through a parametric approach that allows a difficult solution to be obtained by varying a parameter (e.g., solving a high-Reynolds-number problem by using the solution from a low-Reynolds-number problem as the initial condition). The same parametric approach can be used to sequence a number of simulations where the sensitivity to the parameter is of interest.

Powerful analysis and visualization capabilities are part of the package, including all of the standard tools for visualization (arrows, streamlines, isosurfaces, cross sections, transparency, etc.). It is also possible to have the code do integrals along lines, boundaries, and domains; such integrals can be used during simulations as well as in post-processing.

A variety of core applications are provided with the base FEMLAB package, and an additional set of six more-powerful module packages are available for the core applications. A set of model libraries further extends each package. The module packages include

- Chemical engineering module—specialized equations for momentum, energy, and material balances suitable for chemical engineering applications
- Earth science module—specialized equations for earth sciences, such as heat transport, Darcy's law, Richards' equation, Brinkman equation, Navier-Stokes equations, and solute transport
- Electromagnetics module—specialized equations for electrical engineers, including electrostatics, magnetostatics, and wave equations
- Heat transfer module—specialized equations for heat transfer applications, such as surface-to-surface radiation, nonisothermal flow, and bioheat
- Microelectromechanical systems module—specialized equations for electromechanical, thermo-mechanical, fluid-structural, and microfluidics applications, including deformations and moving boundaries
- Structural mechanics module—specializations for structural mechanics, primarily in enhancements for structural applications (e.g., material libraries, elements) and a more specialized interface

Strengths of the FEMLAB Code

The FEMLAB code offers a quite powerful and flexible environment for rapidly setting up multiphysics problems, solving them, and analyzing the results. The GUI is well suited to creating, solving, and analyzing problems falling within the suite of applications for a wide variety of domain geometries. The FEMLAB code was apparently developed from the standpoint of handling engineered features, and is quite powerful in this area. Strong built-in capabilities exist for equation solvers and a variety of element types are supported. PDEs and parametric relationships not available in the code can be fairly straightforwardly included, through the built-in interface or through MATLAB files. Note that legacy FORTRAN and C modules can be accessed by writing MATLAB wrapper files in a straightforward way.

The FEMLAB code and its modules offer some features that are not available in codes currently available at CNWRA or are labor-intensive to incorporate. Examples include

- Surface-to-surface radiative transfer
- Nonlocal flux boundary conditions during simulations
- Integrals and coordinate mappings can be used during simulations
- Nonconformal elements can be used at subdomain interfaces

For example, it would be straightforward to consider radiative transfer at the drift scale. Nonlocal flux conditions would make it possible to consider dripping from the drift ceiling onto a drip shield and invert, by mapping where fluxes leave the ceiling to where they land, without modeling the falling water explicitly. And it might be possible to model a fault using adjacent subdomains without requiring that the meshes align.

Weaknesses of the FEMLAB Code

The FEMLAB code does not appear to be as well suited to modeling natural systems as it is to modeling engineered systems. My take on FEMLAB's weaknesses are summarized as follows:

- Thin features appear to require many elements to maintain element shape integrity. This may be a concern for modeling fractures or thin strata. The present release apparently allows either quadrilateral or triangular meshes, but not a mixture.
- Future releases reportedly will allow a mixture of quadrilateral and triangular meshes, which might address this shortcoming.
- Heterogeneity is considered by specifying coefficients that are constant by domain, functions of a variable (e.g., dependent on the x coordinate or on pressure), or interpolated based on 1, 2, or 3 variables. It is not clear that the full range of heterogeneity patterns that might be considered in natural systems can be easily accommodated.
- The potential for developing solvers for equations not included with FEMLAB is powerful, but the present environment for equation development appears to be awkward. The user is forced to type expressions into a spreadsheet-like cell that may be much smaller than the expression, and ability to comment is poor.
- It is not clear how well the code is suited to archiving analyses, including inputs, equations, and results. The instructor claimed that an analysis session could be exported into a text file that could be run to repeat the analysis. This may be satisfactory for archival purposes.
- The code assumes that the unit system is self-consistent. The current version does not indicate units for parameters, but this is remedied in the next release.
- It would be difficult or impossible to use FEMLAB without recourse to the GUI, if only to specify boundary conditions and boundary variables, since the boundaries are indicated by number while the numbering order is not transparent.

Summary

The FEMLAB code cannot be considered a *replacement for* existing simulators at CNWRA and NRC at its present state of development. Instead, the FEMLAB code should be considered a *complement to* existing simulators. FEMLAB is ideally suited to considering complex physics on engineered systems. FEMLAB is also well suited for considering natural systems with relatively benign geometric and parametric variability.

I envision the use of FEMLAB to be primarily in the following areas:

- Very strong use in engineered systems
- Analyses with quick turnaround times
- One-off analyses
- Verification of existing codes
- Rapid prototyping of equation sets for inclusion in other simulators

In areas within and bordering my expertise, I would expect to use FEMLAB in the following situations (should the opportunity arise):

- Analyses of drift-scale thermal processes involving convection, conduction, and radiative heat transfer. Some thought would be necessary regarding how boiling would be modeled.

- Analyses of drift-scale moisture processes involving seepage, dripping, film flow, and condensation, especially with temperatures less than boiling.

- Rapid analysis of low-level engineered systems (for example, interaction of the vadose zone with vaults and barrier degradation due to clay colloid transport).

- Landscape processes (for example, soil evolution on Yucca Mountain, vegetation/flow/soil/nutrient interactions in the Everglades)

I strongly recommend that the FEMLAB package and selected modules be purchased for further evaluation.