MAGNETIC LEVITATION

MELT IT IN MID-AIR

NANOWIRES
Spinning the tiniest imaginable threads

INSTRUMENTATION
Revealing unknown effects

WAVEGUIDES
TERAHERTZ: The last frontier in the electromagnetics spectrum
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Welcome to our 2006 technical computing magazine!

This issue features some of the highlights from our recent user conferences as well as information about our new-product introductions that we trust you will find valuable.

The computational power of mathematical modeling keeps evolving, and we are rapidly putting it to work for you. We’ve added 64-bit Windows support that allows very large simulations on standard PCs. Because of this along with new multigrid solver technology—an implementation of the Vanka preconditioner/smaller—we are confident you’ll be equipped to handle tens of millions of degrees of freedom in your simulations. In this issue of the COMSOL News you’ll witness use of multigrid techniques through a great user story—the Mittleman Terahertz Research Group at Rice University used them to seriously cranked up their computing capacity.

Many of you will also be thrilled with the introduction of the COMSOL Reaction Engineering Lab®, which brings together a unique combination of capabilities for the modeling and simulation of reacting systems. We have made it a standalone product for chemists, material scientists, life scientists, and process engineers who can now simulate perfectly mixed systems just by typing in the reaction formulas. We also provide users of COMSOL Multiphysics with a convenient way to include the reacting system’s mass and energy balances in space-dependent simulations. Check out the product news section to learn about the capabilities of this addition to our modeling and simulation products.

Looking back at our first user conferences last fall, we are excited about the burgeoning multiphysics modeling community. In this issue we capture some of the highlights from our user presentations: Melt It in Mid-Air by Roland Ernst and Free Neutrons at ORNL by Jim Freels. This is just the tip of the iceberg—you can get all 229 papers by requesting the free User Presentations CD at www.comsol.com/conference2005/cd/.

This fall you’ll have the opportunity to join one of our upcoming User Conferences 2006—the perfect setting to learn about the latest research results, get training, try out new products, and shape the future of multiphysics modeling.

See you there!
COMSOL MULTIPHYSICS REVEALS UNKNOWN in process instrumentation

Modeling has become invaluable in MKS Instruments’ development of first-class mass-flow controllers for the process industry. We have gained a detailed understanding of the complex gas dynamics in our instruments. With that knowledge we’ve achieved accuracy that clearly stands out as superior in the industry.

BY DANIEL A. SMITH, STAFF SCIENTIST (left), AND ALI SHAJII, R&D MANAGER, MKS INSTRUMENTS (right)
Rate-of-rise device

In new-product and technology development, the first step is to analyze and optimize a basic concept. When working with modeling software, we can quickly obtain initial results by reducing the problem to a 1D model, with which we can often understand a process’ underlying physics. An attractive feature of COMSOL Multiphysics is its ability to solve 1D problems, which reduces the debug time to practically zero when we extend a model to 2D or 3D.

These techniques proved valuable in modeling a next-generation pressure rate-of-rise device (Figure 1). Often used in semiconductor manufacturing, such devices measure the rate of change of pressure in a fixed volume, and this parameter is related to the flow rate into the volume. Our latest product is the π-MFV (mass-flow verifier), a compact diagnostic instrument that provides in-situ verification of mass-flow controller (MFC) performance. This next-generation MFC includes technology improvements to help users in semiconductor and high-purity thin-film applications increase tool throughput. It features real-time accurate flow control that is insensitive to upstream and downstream pressure disturbances. Towards this goal, it runs advanced digital algorithms on an embedded processor and thereby achieves accuracy significantly improved over conventional PID-based digital MFCs.

Indeed, mass-flow verifiers traditionally have not considered the temperature rise of the gas inside the volume during a verification, so rate-of-rise devices can have as much as 10% error associated with them. Modeling and then creating a device that takes this effect into account involved solving the time-dependent compressible Navier-Stokes equations in 3D.

The ultimate goal of this project was to implement these equations in an embedded processor so they could run in real time on the π-MFV, a task we handled with Matlab® (see sidebar on page 7, “Navier-Stokes in real time”). We then needed to gain confidence that the numerics in the embedded code were accurate, so we compared results for the temperature dynamics in the volume from the real-time model, which uses the condensed equations, to the full 3D COMSOL Multiphysics model, which works with the full Navier-Stokes equations. A prerequisite
Another area in which we made great progress was in the design of a throttle valve used in chemical vapor deposition (CVD). CVD is a chemical process by which very thin layers of chemicals are deposited on a given surface, called the substrate, which is usually a large single crystal of a material such as silicon or quartz. The substance to be deposited, called the precursor, enters a CVD chamber in a gaseous state. Often a precursor enters the chamber by means of a carrier gas that is not to be deposited.

Precursors are supplied with a carrier gas, which when at room temperature and pressure can often be liquid. Further, the precursor’s vapor pressure at process temperatures can be as low as several torr (the torr is the standard measure of pressure in the semiconductor industry; 1 torr = 1 mm Hg, and 760 torr = 1 atmosphere = 101.325 kPa). The market is moving towards precursors that have lower vapor pressures, and this trend brings with it a new set of design challenges we could adequately evaluate and overcome with the help of modeling with COMSOL Multiphysics.

One of the key parameters in a CVD process is the pressure in the reactor, which operators control with a throttle valve (Figure 3). The valve chokes off the flow so that a considerable pressure difference can exist on different sides of the valve—it can be as high as 10 torr in the process chamber upstream of the valve compared to only a fraction of a torr downstream. Such a dramatic pressure drop in a distance of just millimeters can lead to a significant drop in the temperature of the carrier gas. In addition, a vortex can form downstream of the valve because its opening is not exactly symmetric, so the flow area is larger on one side than the other. The vortex, in turn, leads to an increase in the local partial pressure of any precursor.

If the process does not use all the precursor, problems can potentially arise. In detail, the pressure drop and the vortex can both result in a drop in the temperature that causes the remaining precursor to condense. That condensate can cause process contamination and clog the valve over time. Before our study, engineers were unable to explain why the condensate was forming, but with the model we could see these effects and take appropriate countermeasures.

Using the Chemical Engineering Module we were able to draw these conclusions using three application modes: Non-Isothermal Flow, Convec-
We will continue to simulate and debug our designs. The ability to solve 1D problems and quickly evaluate a concept, freely manipulate the PDEs, and specify ODEs as boundary conditions give COMSOL Multiphysics a huge advantage compared to other FEA packages. We have been able to discover the cause of unwanted effects. Many of our competitors don’t have this level of modeling expertise and release products to the market without knowing all of the details of what is going on inside them.

In addition, once we have determined that a model agrees with experimental data, we can use it as a “noise-free” laboratory to further refine our designs. Field measurements and experiments by their very nature always involve some amount of noise and uncertainty, but in the simulation we can eliminate these effects and better study the basics behind new control algorithms and systems. Moving forward, the ability to solve large-displacement fluid/structure interaction problems with the ALE method in the latest version allows us to simulate the dynamics of many existing and future products.

**FIGURE 3:** In a simulation of a throttle valve (a), we plot the pressure (surface plot) and the velocity field (streamline and color) across the valve flapper (b). The sudden drop in pressure and resulting expansion of the gas leads to a drop in temperature and an increase in local partial pressure, leading to condensation.

**FIGURE 4:** A postprocessing image of the throttle valve reveals the dramatic temperature drop across the valve. The cross-sectional figure shows the temperature in the middle of the device and in the gap between the wall and the flapper.
CAD Import Module interfaces to all major CAD packages

The process from geometry design to multiphysics model is greatly streamlined with the CAD Import Module. It features a live synchronization between the COMSOL Multiphysics® and SolidWorks® environments, allowing for the real-time updating of your model geometries immediately following any changes to the design in SolidWorks.

The CAD Import Module works with optional add-ons dedicated to a variety of CAD formats: Pro/ENGINEER®, CATIA® V5, CATIA® V4, VDA-FS, and Autodesk Inventor®. Based around the ACIS and Parasolid geometry kernels, the module provides geometry repair and easy import of drawing data in the SAT® and Parasolid® formats—the native formats of many CAD tools such as Solid Edge® and NX™. It also supports the IGES and STEP file formats.

COMSOL Script® – command-line modeling, technical computing, and GUI design

COMSOL Script brings you a general computing environment. You can run it standalone or together with COMSOL Multiphysics. This MATLAB®-compatible computing environment provides basic math and numeric functions, matrix operations, visualization, and object-oriented programming.

Command-line modeling enables you to access all components of a COMSOL Multiphysics model. You can save the model as an M-file. This text-based representation of the model provides great flexibility in conducting batch simulations, optimizations, and non-standard modeling tasks.

Further, COMSOL Script features Java®-based Swing tools for visualizing results and building user-specified interfaces, also for COMSOL Multiphysics models. You can, for example, display edit fields for just those model parameters that need changing—ideal for designing turnkey multiphysics applications.
From chemical formulas to reactor design

The COMSOL Reaction Engineering Lab® is an innovative tool for modeling and simulating chemical systems. Chemical formulas are typed in directly, and the reaction kinetics plus material and energy balances are automatically set up. From here you can calibrate and validate models to experimental data, investigate reaction mechanisms, and export models to COMSOL Multiphysics® for reactor design optimization.

Modeling a reacting system initially involves the study of reaction kinetics under perfectly mixed conditions. The Reaction Engineering Lab provides an interface for quick and intuitive input of chemical reactions, supporting irreversible, reversible, and equilibrium reactions.

Kinetic parameters and reaction rates are defined either automatically (mass action law) or manually, and material and energy balances are consequentially set up. During this process, thermodynamic and transport properties of reacting mixtures can also be calculated.

Solving such models directly in the Reaction Engineering Lab gives chemical composition and temperature that vary in time.

Kinetic modeling studies often involve the calibration of models to experimental data including the assessment of alternative reaction mechanisms. The Reaction Engineering Lab allows for such studies, while its integration with COMSOL Script® provides for parametric studies and parameter estimation.

Once the chemistry of a reacting system is understood, a reactor’s actual geometry must be designed or optimized. Here, the integration with COMSOL Multiphysics is ideal, where you can directly export models from the Reaction Engineering Lab into the Chemical Engineering Module. As embedded kinetic models in this module, the corresponding reaction terms are coupled to species and energy balances. The result consists of chemical kinetic models for reacting flows in complex geometries, where chemical composition and temperature vary in space and time.
64-bit support in Windows

COMSOL Multiphysics® now runs under Windows XP Professional x64 Edition, which supports as much as 128 GB of RAM and 16 terabytes of virtual memory.

On this platform as well as 64-bit Linux, you can expect to find far larger segments of contiguous memory, dramatically increasing the size of problems direct solvers can handle. Thus you can tackle more-complex real-world problems.

New preconditioner boosts solver performance

The geometric multigrid (GMG) technique is the state-of-the-art technology for solving and preconditioning models for a large class of problems.

COMSOL® has fine-tuned its GMG solver/preconditioner for solving 3D flow, adding to its supremacy within structural mechanics and electromagnetics. The implementation of Vanka smoothing techniques has also increased GMG’s great efficiency in the use of both processor time and memory.

Moving mesh makes moving boundaries a breeze

COMSOL Multiphysics® increases its ability to model moving-boundary problems with the new Moving Mesh application mode. Based on the Arbitrary Lagrangian-Eulerian (ALE) method, this feature expands your ability to model phenomena that are fully coupled to the deformation of the model geometry. Fluid-structure interactions, piezoelectric devices, and free-surface flow modeling are just some of the applications that are easier to simulate with this new feature.
Fuel cells compete with conventional power sources

by Almut Seyderhelm

A fuel cell intended just to run a laptop computer requires the management of complex interactions between multiple physical processes. In addition, you must fit everything neatly within the free space inside a sleek exterior packaging. As a consequence, it becomes daunting to design fuel cells that compete, in economic and performance contexts, with conventional power supplies.

At the Fraunhofer Institute for Solar Energy Systems in Freiburg (Germany), scientists including Christoph Ziegler use COMSOL Multiphysics to simulate processes inside fuel cells and optimize them for efficiency in portable applications. Their models combine mass and heat transport in porous media, charge transport, and electrochemical reactions. According to Ziegler, “The Chemical Engineering Module provides predefined application modes that are exceptionally well suited for these multifaceted and often nonlinear couplings between simultaneous PDEs.” With the software’s ability to let users enter equations from the keyboard, he adds, his group also includes new equations that appear in recent books or the scientific literature.

The COMSOL Multiphysics model on this page describes a lightweight self-breathing fuel cell useful in, for example, a GPS. The Fraunhofer researchers use it to pin down the physics behavior inside the cell so that it becomes easy to identify and exploit areas for improvement. For example, heat transport corresponds strongly to the physical configuration of the fuel cell and system.

How much power these fuel cells put out depends extensively on the oxygen distribution. Because these thin passive self-breathing cells rely almost entirely on diffusion, a goal in modeling is to optimize the geometric features that can otherwise obstruct oxygen transport.

The rib or white block on the right side of the model geometry mechanically stabilizes the cell and provides an area for electron transport. It also blocks oxygen transport through the cell. The COMSOL Multiphysics model results shown in the bottom figure illustrate how the small rib gives rise to a significant oxygen depletion in the active zone ($4 < x < 5$).

The Fraunhofer researchers also use COMSOL Multiphysics simulations to test other innovations. Explains Ziegler, “We try out different materials with mathematical modeling. In fact, one method under study uses lightweight circuit-board stock as a base material.” He adds enthusiastically, “With COMSOL Multiphysics’ versatility, our engineers also adapt the models to the special requirements of new research findings that appear continually.”
Amsterdam Water Supply (AWS) of the Netherlands produces some of the cleanest drinking water in the world using an environmentally benign ozone disinfection approach. To clean up the 100 million cubic meters per year they handle requires giant turbulent disinfection reactors. COMSOL Multiphysics simulations help AWS researchers Dr. Jan Hofman and colleagues fine tune what happens inside these big rigs.

BY LEIGH SOUTTER
Ozone reactions are the primary disinfection step at AWS (Figure 1). Conventional chlorine disinfection produces unwanted byproducts: a chemical soup containing trihalomethanes, haloacetic acids, and chlorite. These compounds require such a slate of monitoring and mitigation measures that it begs the question of whether the cure is worse than the pollution. For its part, ozone transforms organic substances, pathogenic organisms such as viruses and bacteria, and pesticides into benign substances that subsequent treatment steps can filter off. Considered perhaps the most environmentally feasible tool to disinfect water at large scales, ozone (O₃) is a pure oxygen molecule with an extra oxygen atom attached. Inherently unstable, it readily drops one oxygen atom to react with micropollutants. It reverts to oxygen in minutes, so the unused ozone vanishes without trace. COMSOL Multiphysics simulations make it easy to avoid or remedy the one byproduct that ozone reaction produces, bromate.

**It begins as Alpine runoff**

AWS transforms water from the Rhine River into potable water for approximately 800,000 people in Amsterdam and surrounding areas. The Rhine River begins in the Rheinwaldhorn glacier in Switzerland and flows to the North Sea. Along the way, the river collects runoff from the dense cities, open fields, and vast farms it passes.

The 14 steps of the purification process at AWS distill into three main phases. The initial phase removes solid particles through coagulation and settling plus filtration in the Amsterdam dunes and manmade sand filters. The next phase targets various micropollutants using ozone in a turbulent reactor, water softening, and biologically activated carbon filtration. In the final polishing phase the water passes through a string of fine filters before going to consumers.

The ozone-approach proves especially effective for AWS. It significantly raises the plant’s disinfection capacity since the ozone-treated water is so pure it requires no chlorination. In fact, last year AWS received an honor for providing the highest quality drinking water in the Netherlands.
In a turbulent reactor
At its treatment plant in Leiduin, AWS operates five turbulent ozone reactors in parallel. Water coming from earlier filtration steps feeds into a header system (Figure 3), which mixes the incoming water and distributes it to multiple turbulent reactors through pipes known as “streets.” Inside a reactor, water winds around partial walls or baffles to create turbulent flow. The turbulence mixes the water with ozone gas that enters through diffusers just long enough to inactivate micropollutants. Then the water leaves the reactor through a pipe, and the remaining purification steps filter off or otherwise remove the reacted pollutants.

There is no way to look inside a turbulent reactor when it is working, so until now AWS engineers deduced the operation from scattered measurements. They collect velocity data using flow meters and sample concentrations. They also examine time tracers en route from inlets to outlets to ascertain mixing and residence times. With simulations, Dr. Hofman and his colleagues fill in the gaps with models of turbulent flow as well as chemical transport and reaction. According to Dr. Hofman, “The COMSOL Multiphysics environment is so easy to understand and use, it didn’t take long before several of us could model with it and collaborate.”

Once the simulation matches collected data, the team iteratively changes and solves the tested model to find retrofits that improve how the reactor and header assembly perform. As Dr. Hofman explains, “Our simulations of the reactors and header assembly save us tremendous amounts of money and time. Because we test our ideas on a computer, we don’t waste manpower or material costs on trial-and-error retrofits. Besides, the modeling results come in handy when we report to government officials.”

Mapping the flow field
A turbulent reactor at AWS resembles a maze about the size of a house—it’s a big concrete structure with baffles that divide the space into room-sized compartments. The reactor in Figure 1 is 40 m long, 5 m high, and has seven compartments of varying width created by baffle spacing. Filtered river water enters the reactor and winds around baffles until it exits through a pipe.

“The COMSOL Multiphysics environment is so easy to understand and use, it didn’t take long before several of us could model with it and collaborate.”
In this reactor, a flowmeter straddles the fourth U-turn, taking samples in the gap between the fifth baffle and the reactor wall. For the flow component of his models, Dr. Hofman uses the k-ε Turbulence Model application mode. To get a fast, accurate solution, he uses the parametric solver to obtain and solve for better and better initial pressure and velocity fields. The results almost exactly match the flowmeter velocity of 0.17 m/s towards the middle of the reactor (Figure 4).

With a working flow model, the team switched gears and began tracer experiments. They injected fluoride at the inlet and measured the concentration as it passed through the outlet. Comments Dr. Hofman, “The fluoride works well as a tracer because it travels with the water but does not react with the ozone. We modeled the tracer movement by adding convection and diffusion inside the existing model file. Then we got the average outlet concentration at each time using the integration tools, and the model matches the concentrations we measured.” He elaborates, “Because the COMSOL Multiphysics model did such a nice job of matching the experimental data, we could rely on it to rethink the reactor design and achieve greater uniformity in the flow field.”

Eliminating bromate production
Accurate estimates of the flow field are critical for managing the ozone disinfection that Dr. Hofman and his colleagues model (Figure 5). As he explains, “Once we know how long the water spends in the reactor and where it flows, we fine tune the reactor and diffuser setup so that the contaminants stay in contact with the ozone for just the right amount of time and not long enough for bromate to form.”

The researchers started modeling complex chain reactions beginning with bromide and ozone using the prewritten COMSOL Multiphysics example “Turbulent Ozone Reactor” for a simple reaction chain with a flawed reactor design. According to Dr. Hofman, “What-if modeling on simple reactors with obvious design flaws such as this one gave us intuition when we began investigating ozone reaction in our real reactors. It was so easy to open the model and change it. We used it to see how certain baffle arrangements and diffuser setups limit bromate production. Now we use an altered version of the model to simulate real reactor geometries.”

Taking it to the next level
Dr Hofman continues, “Being able to set up computational fluid dynamics models quickly and easily proves invaluable to understanding processes inside the ozone reactors, optimizing them in existing reactors, and also designing new ones.”

“One way the team will take its modeling to the next level is by adding bubbly flow. The ozone comes in as a jet of bubbles that eventually dissolves into the water. This means that near the diffuser there actually are two phases: ozone gas and water. Dr. Hofman elaborates, “Extending our model to 2-phase turbulence will let us examine how the ozone bubbles disturb the flow field and determine whether the dissolving of the bubbles affects the chemical reactions.”

His team is also adding 3D models to investigate other purification steps including a fluidized bed water-softening reactor. Says Dr. Hofman, “When we started the modeling for the real reactors, we focused on 2D simulations. But when the 3D turbulence application mode appeared in an earlier update, we added the z-direction to our models.”

FIGURE 5: This COMSOL Multiphysics plot gives a snapshot of ozone concentrations in the turbulent reactor. AWS uses results like these to position ozone diffusers that improve the ozone mixing.
I want to access the time derivatives of my solution, perhaps to use in equations. Is there an easy way to do that?

Certainly, and in fact, in COMSOL Multiphysics 3.2 we enhanced the notation to handle time-dependent problems in many ways. Now you can just type in \( ut \) if you want to work with the term \( \frac{\partial w}{\partial t} \). This also simplifies the use of mixed space and time derivatives. For instance, to invoke \( \frac{\partial}{\partial t} \left( \frac{\partial w}{\partial z} \right) \) simply enter \( uxt \). You can use this syntax both in equation coefficients and in postprocessing.

I have a 2D axisymmetric model. I would like to plot the solution in a 3D plot. Can I do that, and if so, how?

Use the extrusion-coupling variable, which helps you extrude the 2D solution to a 3D geometry. I illustrate the concept in the nearby figure. The general approach is to add a new 3D geometry to the existing 2D model and then make an appropriate mapping of the solution between the geometries. The entire procedure is described in a knowledgebase article at [www.comsol.com/support/knowledgebase/982.php](http://www.comsol.com/support/knowledgebase/982.php).

In this example, the figure on the left shows the actual 2D axisymmetric solution that is the default when you click the Solve button. The image on the right is what you can create by extruding the 2D geometry into a 3D representation and then modifying some of the plotting parameters.
I am solving a fluid-flow problem and can get convergence for a coarse mesh but not for a fine one. What could be the problem?

There is probably a discontinuity somewhere in the inflow boundary condition, or perhaps the flow field is turbulent. In the first case with a discontinuity, try setting up a parabolic inflow profile. In the second case, try working with a turbulence model such as one that employs the k-ε Turbulence Model application mode.

Another possible cause of instability, if the flow is incompressible, is a high reference pressure, which in most cases is governed by the outlet pressure. It is often good to try an outlet pressure of zero.

I often import 3D geometries into COMSOL Multiphysics from the CAD Import Module. It works out very well, but when the geometry features very thin faces, there are sometimes a meshing problem. Why?

This is because you are using an import tolerance that is too low. In most cases you can remove these faces by increasing the relative repair tolerance in the CAD Import Options dialog box. The default value is 1e-4; changing it to 1e-3 often resolves the problem.

I am solving a fluid-flow problem and can get convergence for a coarse mesh but not for a fine one. What could be the problem?

If you are doing time-harmonic analyses in the frequency domain, COMSOL Multiphysics uses complex numbers to represent the dependent variable a(t). A harmonic quantity can be seen as a sum of a cosine and a sine function, or simply as a cosine function with a phase shift φ. a(t) = A \cos(ωt + φ). This can also be seen as the real part of a complex function, a(t) = Re(Ae^{jωt}). Here, j is the imaginary unit, ω the angular frequency and t is time. Now, let's identify A = a_0e^{jφ}. A is a complex amplitude that contains both amplitude and phase information.

Another possible cause of instability, if the flow is incompressible, is a high reference pressure, which in most cases is governed by the outlet pressure. It is often good to try an outlet pressure of zero.

2.4*exp(j*30*pi/180) since φ = ωΔt expressed in time, the expression would be 2.4*exp(j*omega*dt). j can be swapped with i in COMSOL Multiphysics.

When plotting a quantity, say V, in a time-harmonic problem, you see the real part of the solution as a default. You can type operators to see other functions of the complex solution, like abs(V), imag(V), angle(V). On the General tab of the postprocessing dialog box, you can set the phase angle (in degrees) of your plot. Plotting V and setting the phase to 90 is the same thing as plotting V*exp(j*90*pi/180).
THIS PAST FALL, COMSOL held its first-ever international conferences, and the feedback has been overwhelmingly positive. Meetings in seven countries in the US and Europe gave COMSOL users and other interested parties an opportunity to learn about the latest product developments, exchange ideas and tips, as well as meet the development and support teams. In all, roughly 1000 attendees heard almost 250 user presentations along with keynote speeches from notables in various fields.

THE DEMO AREAS WERE FILLED with people who wanted to learn about the products’ latest capabilities, and our support room was completely booked with users looking to get input on their modeling projects. The attendees packed the minicourses to the point where we added extra sessions.

Those who couldn’t make it last year can catch up on much of the technical content. Simply request our Conference CD, which contains the user presentations, some including the actual model files, along with slides from speeches and keynote addresses. Contact your COMSOL representative or go to www.comsol.com/conference2005/cd.

Conference Proceedings CD

42,000 requested and counting —a world record!
The support room was a popular destination.

Keynote speakers:
- Bruce Finlayson
- Carl Meinhart
- David Burnett
- Howie Stuart
- Amy Duwel
- Svante Littmarck
- Bruce Finlayson

MELT IT IN MID-AIR

FIGURE 1: COMSOL Multiphysics results showing the electric current (arrows), induced magnetic field (streamlines), and temperatures (color plot) in the crucible and solid charge.
Dr. Ernst develops cold crucibles that melt incredibly hot metals and other materials without letting the melt touch the container walls. With these methods he can refine ultra-pure titanium and other materials. His approach combines electric currents, induction, heat transfer, and magnetic levitation.

EPM-Madylam Laboratory specializes in designing strategies for the electromagnetic processing of materials for a wide range of uses. Aeronautics and other industries, such as the biomedical industry, require highly pure materials including titanium alloys, silicon, or pure glass. Simply heating a raw material in a container has obvious limitations, most notably that containers made of fireproof graphite or ceramic leave impurities when the melted raw material comes in contact with the container wall. Wouldn’t it be ideal to both levitate the contents and use electromagnetic fields to melt the raw materials in mid-air (Figure 1)?

Dr. Ernst successfully developed setups of this nature. His cold crucibles consist of a cylindrical insulator with an electrically conductive coil wrapped around it (Figure 2). Inside the insulator is a circle of evenly spaced sections made up of conductive materials such as copper. The raw material to be heated, known as the “charge,” is placed within this circle of sections (Figure 3). Sending a high current through the coil induces a current within each of the sections. This in turn induces a current in the charge to incur Joule heating and a melting of the charge.

A skewed magnetic field arise from the fields coming from the coil and the sections, concentrating the total field into the charge. This leads to the levitation of the charge.

A trick in getting the cold crucible to work lies in determining the best size and spacing of the sections. Regarding the electromagnetic component, Dr. Ernst explains, “The models are easy to set up and especially efficient with COMSOL Multiphysics’ impedance boundary condition, even with the low-skin-depth high-frequency conditions we use. The results show me how the electromagnetic fields behave over whatever full 3D geometry I need.”

With the coupling of the electromagnetic fields to heat transport in the charge, temperatures in the charge rise (Figure 1). Dr. Ernst comments, “Now I’m adding the solid-to-liquid phase change plus the fluid flow and deformation that comes with the melting.”

He adds, “COMSOL Multiphysics allows me to efficiently model the full 3D problem, and that’s especially important for the melting part. We must understand the asymmetries inside the melted charge to avoid the risk of contact with the crucible wall.”
“Free” neutrons are hardly free at all when it comes to money—actually, it takes enormously sophisticated equipment to create them, and only a handful of places on earth do it. Who needs free neutrons, anyway? Developers of advanced materials, new biotechniques, and cold fusion make just a few candidates. Now more than ever, cutting-edge experimentalists like these turn to the High-Flux Isotope Reactor (HFiR) at the Oak Ridge National Laboratory in Oak Ridge, Tennessee, to satisfy their needs. With COMSOL Multiphysics, senior safety analyst Dr. Jim Freels ensures that these powerful neutron streams enter equipment slow, cold, and trouble free.
Right now, the HFIR (Figure 1) is one of the most powerful research reactor facilities in existence. Established in the 1960s, its unique design currently uses moderated nuclear fission to produce free neutrons for researchers and industrial users. The neutrons are termed “free” because they exist outside the nucleus of atoms after reactions break them into subnuclear constituents: protons, electrons, and antineutrinos. Being electrically neutral, the free neutrons penetrate deep because they pass unhindered through electrical fields within atoms and slow primarily when they collide with atomic nuclei. With only one proton and neutron encased in its nucleus, hydrogen makes an excellent refrigerant for the fast-moving free neutrons.

At HFIR, neutron production is most intense in the hot center of the 2-foot diameter reactor core, where rare isotopes such as californium-252 form. HFIR collects whatever free neutrons form outside the core to produce a dense or “bright” flux for scattering studies and other experiments at a new beam facility named HB-4 (Figure 1). When their new low-temperature hydrogen system comes on line to cool the neutrons, the flux coming out of this beam tube to experimental equipment will be as slow and bright as the current best in the world.

“The hydrogen from the new cold source must not only cool the neutrons, it also must cool all of the equipment it passes through,” explains Freels. The new hydrogen cold source at HFIR maintains approximately 5 kg of the gas at between 18 and 21 K and circulates it continually in a transfer-line loop. Three variable-speed circulators move the hydrogen from the cold source into the line. The circulators spin fast enough to pump the hydrogen through at 0.074 kg/s. Even though they operate by magnetic levitation, the spinning still generates considerable heat. The pressurizer (Figures 2 and 3) picks up some of this heat while it maintains 14 to 15 bar absolute along the line, a level that prevents subcooled nucleate boiling. When the hydrogen circulates through the moderator vessel at the outer extent of the loop, the neutron beam coming from the reactor passes through it. The free neutrons pass down empty guide halls to experimental equipment, traveling like a dense invisible laser beam. The flowing hydrogen, however, returns from the moderator vessel to the pump module for recirculation.

With the nuclear reactions, the variable-speed circulators, and intrinsic heat leaks, the hydrogen must dissipate 2200 W of heat. “This is where COMSOL Multiphysics comes in: to give us an accurate estimate of the cooling process,” he adds. The components of greatest concern have the steepest temperature drops—the pressurizer that receives the heat from the ambient surroundings and the moderator vessel with an outer wall that absorbs a dense neutron flux.

**A pressure-volume-temperature balancing act**

The simulations that Freels conducts often involve significant temperature and pressure changes. Typically they include heat transfer in solids with non-isothermal hydrogen flow, at times laminar and at other times turbulent. Complicating the models is the fact that material properties vary strongly with temperature and pressure. Says Freels, “We use COMSOL Multiphysics because it lets us efficiently design one-of-a-kind physics and makes it straightforward to incorporate varying experimental data in our models. Most of the software programs we see require intensive training just to set up even the
most artificially simple problems. With COMSOL Multiphysics I could use tools that come standard to solve real problems with real materials right from the start.”

A pressurizer (Figure 3), housed within a safety-first pump module, generally interfaces the ambient outside world and the cold cryogenic world within the HFIR. If air and heat leak in and create just the right mixture with hydrogen, a fire or explosion could result. To prevent such a disaster, the pressurizer sits within a vacuum chamber housed inside a safety-first pump module that Freels helped design. The two chambers of the pressurizer stack one above the other and interact through heat-resistive tubing. Near the variable-speed circulators, at the top of the pressurizer, temperatures reach approximately 300 K. The base of the pressurizer connects by a vertical tube to the main transfer line where hydrogen at 18 K moves at 8.1 m/s through a pipe diameter of 1.25 cm. Inside the pressurizer, the hydrogen remains relatively still.

When the HFIR shuts down for regular maintenance or during a power outage, the hydrogen in the transfer line essentially shrinks, which sucks some of the gas from the pressurizer into the transfer line. If the hydrogen in the pressurizer is too hot, it heats up the mass already in the transfer line. The mixing lowers the density, which could trip the variable-speed circulators or unnecessarily damage other loop components. Sufficient hydrogen at temperatures below 33 K in the lower chamber of the pressurizer prevents such disruptions.

Freels uses COMSOL Multiphysics to determine if the pressurizer will contain enough hydrogen at a sufficiently low temperature to prevent trouble when the HFIR shuts off. His models combine the Non-Isothermal Flow and the Convection and Conduction application modes for the hydrogen, with the Thin-Conductive Shell application mode for the pressurizer walls. He handles the nonlinear changes in the hydrogen properties by importing experimental data with COMSOL Multiphysics’ automatic interpolation feature. He uses cubic spline or linear interpolation and reads in experimental data through text files. With the data, COMSOL Multiphysics finds the right material value at each iteration step. As Freels explains, “Simply using the interpolation functions, it was very easy to set up these nonlinear material properties in the provided tables.”

A major boost in computational efficiency came from using shell elements for the thin walls of the pressurizer. Representing the pressurizer walls with a thin 3D layer would require an enormous quantity of tiny elements. COMSOL Multiphysics’ shell elements model physics along a boundary instead of across it. In Freel’s case, the walls of the pressurizer became 2D surfaces represented by a relatively coarse mesh.

Freels also combined the parametric solver with solver scripting to set up an iterative-relaxation scheme. By automatically integrating the density of the gas in the lower chamber, his model determines if the mass of hydrogen in the cold lower chamber is enough to ensure the HFIR operates safely.
The second time around…

flexibility and ease of use

When Freels started using COMSOL Multiphysics, he already had an HFIR pressurizer model built on conduction alone, but he needed to model non-isothermal turbulence in the moderator vessel. He started with a few examples in the model library and then tackled a problem he knew inside out: the conduction-only model of the HFIR pressurizer (Figure 3b). He reports enthusiastically, “Building the model was amazingly easy. I created the 3D pressurizer geometry in the user interface with the built-in CAD tools. I then parameterized the model using intuitive type-in expressions. The temperatures I got from that first model matched my results from the different simulations with other packages including Abaqus, Nastran, and our own Heating program. The COMSOL Multiphysics model gave as good or better results and took a lot less effort.”

It’s easy to see why Freels completely tossed out his early conduction-only work once he added the non-isothermal flow and the nonlinear material properties to his model. This showed that slow buoyant recirculation actually produces much more cold hydrogen than predicted with conduction alone. As Freels notes, “We are validating the non-isothermal simulation results by comparing them with results from a testing program that includes temperature sensors on the pressurizer walls. These temperatures are temperatures at a heated wall obtained with the simulation and NASA data (squares) from a rocket engine test."

Figure 5 shows his match to NASA test data for a similar case—a rocket jet engine with heating on a side wall.

Commenting on his experience with the software, Freels says, “COMSOL Multiphysics modeling is amazingly easy, especially when you consider how hard it is to use other software. Once I sorted out the non-isothermal turbulence strategy, I had the models up and running in pretty short order. The project wound up contracting outside experts to build the same Fluent and CFX models since it just takes too long to set up even simple problems with them. For instance, we found that interfacing experimental material properties with Fluent required a separate coding development. But in COMSOL Multiphysics, we did it all from the graphical interface.”

“I had the models up and running in pretty short order.”

simulations potentially circumvent tremendous trouble and definitely saved us a pressurizer redesign. I wish we had done it with COMSOL Multiphysics from the start.”

The moderator vessel (Figure 4) gets its name because hydrogen passing inside it “moderates” or lowers the temperature of the neutron flux that crosses through it. It is a pouch-shaped aluminum flow-through bend at the outer end of the transfer loop, just at the entry of HB-4 (Figure 4). The outer wall of the vessel heats when it absorbs free neutrons, so the hydrogen inside picks up approximately 2.7 kW of heat. The temperature rise is enough to trigger nonlinear hydrogen behavior along the boundary layers near the aluminum walls. Even when the reactor shuts down for maintenance, it remains so hot that flowing hydrogen is required to cool it (Figure 5).

While modeling non-isothermal turbulent flow with nonlinear material properties is understandably tricky, Freels can still build his simulations straight from the COMSOL Multiphysics user interface. His models couple the k-ε Turbulence application mode with the Convection and Conduction application mode, and he adds an extra equation to account for the non-isothermal effects.

Commenting on the necessity for the modeling described in this article, Freels says, “When it comes to safety at ORNL, a single analysis is very rarely acceptable. In our extensive review process, we check all analyses against other codes capable of performing similar calculations.”

User Profile:

Dr. Jim Freels

Dr. Jim Freels, a nuclear engineer with a mathematical science background, is no beginner to numerical modeling. He wrote his own finite-element code for computational fluid dynamics during PhD research at the University of Tennessee, Knoxville, with Dr. A. J. Baker as his advisor. He’s managed a wide variety of scientific software programs beginning with his work at SAIC (Oak Ridge, TN), Technology for Energy Corporation (Knoxville, TN), and during his 14-year career at Oak Ridge National Laboratory.

Commenting on the necessity for the modeling described in this article, Freels says, “When it comes to safety at ORNL, a single analysis is very rarely acceptable. In our extensive review process, we check all analyses against other codes capable of performing similar calculations.”
Spinining

OF THE TINIEST SIZE IMAGINABLE

The process of manufacturing nanowires—the smallest possible threads—is not wholly understood. Sophisticated modeling is helping researchers better understand this revolutionary process and prepare it for commercialization.

BY PAUL SCHREIER

Pick up a human hair, and then realize that a nanowire can be a thousand times thinner. Made of materials such as semiconductors, polymers, and carbon, these incredibly thin threads can have diameters < 10 nm, just tens of atoms across. Early laboratory findings indicate that these ultra-fine wires will open up a variety of remarkable applications. But until we learn how to manufacture them efficiently, these commercial uses will remain only dreams. Researchers thought they had a good grasp on how nanowires grow, but recent mathematical models along with laboratory observations have uncovered evidence that a completely different growth mechanism might be at work.

Because of their unique and unusual properties, nanowires offer an amazing range of potential applications. They could serve as wound dressings or drug-delivery systems; allow the design of solar sails and mirrors for outer space; develop innovative agricultural pesticides; act as structural elements in artificial organs; and strengthen reinforced composites. A bed of “nanograss” could result in low-friction surfaces on which substances simply glide off. One near-term use is to implement the interconnects needed to wire together the next generation of integrated circuits, which are shrinking so small that conventional packaging techniques are large and cumbersome in comparison; they can themselves even implement digital logic gates. In the future we can expect to see untold numbers of products and devices that exploit these tiny structures.

A totally new way of looking at the process

In the semiconductor area, the most common method of creating a nanowire is known as the vapor-liquid-solid (VLS) growth mechanism (Figure 1). The process supplies the reactants in a vapor phase. They react with a liquid metallic seed particle placed on a substrate, and a nanowire grows perpendicular to the substrate. The VLS mechanism implies that the solid wire forms through precipitation on a droplet of metal that acts as the seed. The driving force for
crystallization is supersaturation within the droplet, which is established by catalytic absorption of the gaseous reactants from the surroundings.

The manufacturing process (Figure 1) starts with a single crystalline GaAs substrate. The next step is to precisely deposit gold nanoparticles on the substrate, which then goes into a reaction chamber. The chamber is evacuated and heats up to $540^\circ$C. The process then introduces reactants into the chamber as molecular beams of gallium and arsenic. Under the right conditions, GaAs forms under the gold particle but not anywhere else on the surface. The resulting nanowire can grow to be as long as 0.5 to 10 µm. Researchers are concentrating on the parameters that control nanowire growth so it forms semiconductor compounds with desirable properties. Among the factors to control are pressure in the reaction chamber, the concentrations of arsenic and gallium, and the diameter of the gold seed.

In some cases, however, this explanation of nanowire growth leaves many unexplained phenomena and inconsistencies. Scientists clearly need a better understanding of the mechanisms governing semiconductor nanowire growth to enable the development of this promising field. One group of researchers investigating this area comes from the Nanometer Structure Consortium at the Lund Institute of Technology (Lund, Sweden). Members of the physics, materials chemistry, and chemical engineering departments believe that the actual growth mechanism in some cases involves solid-phase diffusion rather than the VLS mechanism. To study this concept, they perform laboratory experiments and compare the results to finite-element calculations of the mass transport and expected growth rates using COMSOL Multiphysics. In this way they hope to clarify the alloying situation and the aggregation state of the seed particle, which is a key to a more complete understanding of the nanowire growth mechanism.

A close look at the seed

To better understand what happens in the reaction zone, the consortium enlisted the assistance of Prof. Stig Stenström from the Chemical Engineering Department, who created a model of growth including transport and the formation of the GaAs compound. This single-physics problem in 3D sets up the material balance and calculates the mass-transfer rate using the Convection and Diffusion application mode. This mode’s PDE templates provide the necessary description of the mass-transfer equation, but Prof. Stenström had to add a custom equation that accounts for the reaction rate at the substrate layer. Further, he modeled the gold droplet to consist of a short cylinder topped with a half-sphere.

He also had to apply special techniques when creating the model geometry. The gold spray results in a semispherical droplet on the substrate, and the diffusion at the outer edge is far faster than the diffusion in the middle of the droplet. The resulting model has 4600 nodes and 23,000 elements and solves in just two or three minutes.

Figure 2a shows a typical output plot from the model showing the gallium concentration in the seed particle and the nanowire’s growth rate. By integrating the flux of gallium it is possible to calculate the growth rate of GaAs for different process conditions.

One thing that this model showed the researchers was that the previous generally accepted theory of nanowire growth, the vapor-liquid-solid (VLS) mechanism, should be replaced by a vapor-solid-solid (VSS) mechanism.

Commenting on these results, Prof. Stenström says, “At this time, our model deviates with experimental data by only a factor of two. When I say ‘only,’ I admit that in many situations that amount would be unacceptable, but in this case we think it is quite good given the limited amount of data we have for this process. Part of the reason for these deviations comes from the fact that we don’t fully understand what is going on in the reaction, so we have to make a number of assumptions.”

Prof. Stenström is familiar with COMSOL Multiphysics from previous work, and he was happy to use it for this application. “It’s easy to create the geometry, set up the boundary conditions, and enter the physical data for the system. I was also able to enter my own expressions for the reaction rate, whereas other codes would require us to write our own equations in a much more cumbersome fashion. Further, COMSOL Multiphysics offers good plotting facilities and visualizes results very well. Overall, the package fits in well for problems in chemical engineering such as this.”

REFERENCE
The least-explored region of the electromagnetic spectrum consists of terahertz waves, which at 100 GHz to 10 THz fall between microwaves and infrared light. Only in recent years has the development of suitable waveguides for the technical maturation and widespread commercialization of T-ray technology started. Researchers at Rice University have made important discoveries in this regard and are using COMSOL Multiphysics to study how their approach to waveguides works, and how best to connect these waveguides to antennas and other system components.

**Promising applications**

With the development of efficient and effective waveguides and interfaces, T-ray technology should enjoy wide use due to the unique nature of the radiation. Metals and other electrical conductors are opaque to them, but T-rays can penetrate plastics, paper, dry lumber, and glass just like X-rays. Unlike X-rays, though, they are not hazardous radiation. This combination of attractive traits make T-rays well suited for applications such as the detection of explosives or contraband, defect analysis, moisture monitoring, medical diagnostics, trace-gas detection, and biomedical imaging. In fact, NASA has even used this technology to inspect the foam on the Space Shuttle’s external tank, part of the return-to-flight requirement following the Columbia tragedy.

Today’s systems, though, are mostly large and stationary due to the lack of suitable waveguides that can carry terahertz waves. Thus, it was a major step forward when a research team at Rice—headed by Prof. Daniel Mittleman with the assistance of Dr. Jason Deibel, graduate students Kanglin Wang and Zhongping Jian, and undergraduate student Matthew Escarra—discovered that a simple cylindrical metal wire can act as a low-loss, low-dispersive waveguide at terahertz frequencies. However, for the development to be fully realized, the team also needed to develop a new type of terahertz antenna,
one that better matches to wire waveguides.

The first terahertz photoconductive antennas were essentially linear dipole emitters that produced primarily linearly polarized radiation. With horizontally polarized terahertz pulses focused onto a 0.9-mm stainless-steel wire waveguide, the team found that they could only couple approximately 1% of the incident power to the waveguide. In an effort to improve performance, they then simulated the coupling efficiency of a configuration of two perpendicular wires with a minute gap between them and found that it was even less at 0.42%.

More recently the team discovered that they could produce radially polarized radiation and couple that radiation very efficiently to a simple metal-wire waveguide. Because the wire’s length is many times that of the wavelength, they excite the structure in a small region—then that energy propagates along the wire’s surface at the speed of light. When the energy moves, it causes the conduction electrons to oscillate, creating an effect known as a surface-plasmon polariton. At the end of the wire, that polariton radiates its energy into free space as a terahertz wave. With modeling they learned about various effects, and they are currently employing FEA techniques to better understand the loss mechanisms affecting terahertz propagation as well as investigating the effects of curvature and dielectric coatings.

**Simulating new antenna concepts**

As noted earlier, this breakthrough in waveguides also required a novel antenna. With COMSOL Multiphysics they examined potential designs in the hope that they could produce a radially polarized field. With a multiphysics model that combined the 3D Electromagnetics Wave Propagation application mode (implemented in the Electromagnetics Module) along with an electrostatic analysis of the DC fields in the antenna, they were able to model a proposed photoconductive antenna with radial symmetry.

“In a first model of the radial terahertz antenna, the researchers used an idealized antenna and defined the boundary conditions as being low reflecting. The image shows simulation results for the radiation power.”
Not only did they show that the proposed design could produce a radially polarized beam, the results agreed perfectly with the analytical model they had developed concurrently. While a simulation showed that the actual radial antenna does not generate a terahertz beam with perfect radial polarization, the beam is largely radially polarized.

They then modeled the coupling of the radial antenna’s output to a wire waveguide and found that the coupling efficiency reached approximately 56%, an improvement of more than two orders of magnitude over the dual-wire configuration.

**Many millions of DOFs**
The modeling of terahertz wave propagation and phenomena can be quite challenging, reports Dr. Deibel. To properly simulate wave propagation, the largest mesh element size must be no larger than 1/10th of the radiation’s wavelength.

To model an EM wave propagating at a frequency of 100 GHz (wavelength of 3 mm), the largest mesh element can be no larger than 300 microns; for a wave at 1 THz, this critical element size shrinks to 30 microns. However, a real-world model involves devices and waveguides with feature sizes not only that small but also as large as centimeters. Thus a small critical mesh-element size results in a model with a huge number of mesh elements and subsequently a huge number of DOFs. Comments Dr. Deibel, “While this requirement makes for a difficult model to develop and solve, with proper knowledge of good FEA modeling techniques and the use of its iterative and multigrid solvers, COMSOL Multiphysics can be effectively and efficiently used to model engineering problems and phenomena associated with terahertz wave propagation.”

More specifically, he reports that “as we learned more about FEA modeling and better utilizing the software, we made a significant upgrade to our computing capacity with a Sun workstation consisting of dual-AMD 64-bit processors with 16 GB of RAM. Using a direct solver, the workstation could solve a 3D electromagnetic wave model consisting of 700,000 mesh elements and 1 million DOFs in 36 hours. Upon switching to the GMRES iterative solver and an SSOR vector preconditioner, a similar model with slightly less than 800,000 mesh elements and 1.1 million DOFs could be solved in 24 hours. Most recently, we learned how to apply the multigrid solver. We now routinely solve very complex and large 3D EM models where the refined mesh consists of 1.5 million mesh elements and 4 million DOFs in less than 12 hours. Further, when we can take advantage of models with axial symmetry, we can solve models that have more than 14 million DOFs, which we are starting to do in our efforts to study propagation of the terahertz pulses along waveguides.”

Continues Dr. Deibel, “we’ve pushed the software into completely new regimes, and the people at COMSOL have been very supportive in these efforts.” Along these lines he says, “in each upgrade I’ve found something of substantial use.” For instance, the Electromagnetics Module added a transient-propagation application mode. In the past, he’s had to work in the frequency domain, but now he can “launch” a time-domain pulse and observe it propagating down the wire.

These results were instrumental in the Rice University group winning an NSF grant to further develop this waveguide technology and to develop a compact and easy-to-use terahertz spectrometer to be used in industry and chemistry labs. “It’s our hope,” says Dr. Deibel, “that one day such a spectrometer will be just as common as a FTIR spectrometer in most chemistry labs.”

To read the full paper that Dr. Deibel presented on this topic at the 2005 COMSOL Multiphysics Conference in Boston, order a copy of the Conference CD, which contains this along with more than 200 other papers. ■
Recognizing the rapidly growing importance of scientific computing in research and engineering, KTH (the Royal Institute of Technology) in Stockholm, Sweden, is one of an exclusive group of educational institutions around the world to offer a masters degree program in this subject, which until now has traditionally been the domain of doctoral students.

The KTH Master’s Program in Scientific Computing was initiated in 1997 by Prof. Björn Engquist, and is one of many master’s programs taught in English in a variety of technical disciplines. Until now it has been a 1-1/2 year program, but starting in the fall of 2006 it becomes a 2-year program.

The KTH program is open to students from around the world; the tuition is free, but students pay for educational materials and living expenses.

The applicant should have a BSc/BEng with a solid background in mathematics; knowledge of numerical analysis; be experienced in programming; and have a good overview of at least one application area, a few examples being fluid dynamics, electromagnetics, or materials science. The program consists not only of lectures and classes but also a large part of the course work is devoted to computer labs, projects, and presentations to encourage collaboration among students. The last semester is spent writing a thesis.

The scientific Computing program, which presently has roughly 30 students, is hosted by the Department of Numerical Analysis at the School of Computer Science and Communication, KTH. The course program covers mathematical modeling, numerical methods for PDEs and SDEs (stochastic differential equations), numerical algebra, visualization, high-performance computing, computational fluid dynamics, and computational electromagnetics. Many of the courses make use of modern modeling tools, and one of the program coordinators, Dr. Lennart Edsberg, explains that “COMSOL Multiphysics and COMSOL Script will be important computational tools in the program.”

More information is available on KTH’s web page for Master’s Programs: www.kth.se/eng/education/programmes/master_english/scientific_computing.html or from the coordinators, Dr Lennart Edsberg, edsberg@nada.kth.se and Dr Katarina Gustavsson, katarina@nada.kth.se.

New Books Introduce Students to Engineering Analysis with COMSOL Multiphysics

Introduction to Chemical Engineering Computing (John Wiley & Sons), Bruce A. Finlayson

The problems that chemical engineers must solve can no longer be answered with programs written on a case-by-case basis. Each chapter in the book describes a physical problem and provides step-by-step instructions for solving it with available software including COMSOL Multiphysics. The book also supplies numerous examples and comprehensive explanations.

The Finite Element Method Basic Concepts and Applications (Taylor & Francis), Darrell W. Pepper and Juan C. Heinrich

This 2nd edition introduces the fundamentals of the finite element method featuring clear-cut examples and an applications-oriented approach. In addition to exercises that can be worked out manually, this edition refers to COMSOL Multiphysics for solving heat transfer, fluid dynamics, and structural mechanics problems.
Multigrid Methods Improve Solvers for Speed and Memory

BY JACOB YSTROM

A key feature in COMSOL Multiphysics is support for geometric multigrid (GMG) methods. Consider that direct solvers, which are generally fine for 2D problems, are typically too memory intensive for larger problems such as those involving complex 3D geometries. In these cases, iterative solvers become attractive as they are much more adept at handling large problems. However, iterative solvers are more complex to use because they require high-quality preconditioners, the choice of which is generally problem dependent.

Among possible preconditioners, the GMG technique has become a very popular choice because it not only handles a large class of problems, particularly those in structural mechanics and electromagnetics (Figure 1), but also because it exhibits great efficiency in its use of both processor time and memory.

Basic multigrid concepts

The basic concept behind the GMG method is simple: a hierarchy of meshes to seek the solution for the finest mesh.

The GMG V-cycle (Figure 2) starts with the finest mesh and applies pre-smoothing on the residual. Often a few iterations with simple iteration methods such as Jacobi, Gauss-Seidel, or the successive over-relaxation method (SOR) are good candidates for these smoothing operations. To map the smoothed residual to a coarser mesh, it next applies an operator called a restriction. This procedure repeats until the scheme reaches the bottom of the mesh hierarchy.

At this level it applies another type of solver—a coarse-mesh solver—that takes care of the low-fre-
quency part of the residual at the coarsest level. To map the coarse mesh’s corrected residual up to a finer mesh, the GMG V-cycle now applies an operator called a prolongation. On the way up to the top mesh level, it applies post-smoothing on the residuals. The V-cycle ends with post-smoothing on the finest level. The combined effect of smoothing and coarse-mesh correction is a substantial reduction of the residual for all frequencies.

Implementations in COMSOL Multiphysics
You can apply COMSOL’s GMG technique as a preconditioner where a fixed number of GMG cycles are applied, or as a standalone linear solver where the GMG cycles are repeated until convergence. You can apply the GMG cycle to a hierarchy of so-called mesh cases, where each consists of both a mesh and a corresponding shape-function set. Further, you can produce the mesh hierarchy manually or have COMSOL Multiphysics create it automatically. Pre- and post-smoothers can be selected from a list of standard preconditioners such as SOR, Jacobi, and incomplete factorization routines, as well as more specialized preconditioners. You can also make a free selection for the coarse-mesh solver.

It is possible to handle many real-world problems successfully with GMG methods and by using standard preconditioners as smoothers. Yet, there exist important classes of problems where standard preconditioners are not suitable. For this reason, COMSOL Multiphysics also supplies two more-specialized preconditioners: the SOR-vector preconditioner, designed for the vector Helmholtz equation as discretized with vector (or edge) elements, and the Vanka preconditioner, designed for the velocity-divergence formulation of the incompressible Navier-Stokes equations.

The Vanka method also applies to other so-called saddle-point problems such as when weak constraints are used or when a divergence-free condition is a part of the equations. For example, this condition is a part of k-ε turbulence models, magnetostatics, and magnetoquasistatic applications.

Multigrid vs. direct solver performance
To demonstrate the power of GMG methods in COMSOL Multiphysics, consider the model of a 3D electromagnetic-wave problem—the Helmholtz equation for a corner cube reflector (Figure 1)—when using three different solvers:

- the SPOOLES direct solver
- the UMFPACK direct solver
- the GMRES iterative method with a GMG preconditioner (GMRES/MG).

The large system of linear equations that results from applying finite-element analysis with linear vector elements is complex-symmetric but not Hermitian. In this comparison, SPOOLES can take advantage of symmetry and work on just half of the matrix, whereas UMFPACK cannot (Figure 3).

When setting up the GMRES/MG solver/preconditioner in COMSOL Multiphysics, you select an appropriate smoother—this example employs the SOR-vector and SORU-vector algorithms as the pre- and post-smoothers, respectively. It also works with a manually created hierarchy of three nested meshes, which you create by starting with a coarse mesh and then
Comsol is expanding its reach. We have opened two offices and also appointed Shanghai-based ZhongFang Information Technology Ltd. as our distributor in China.

Heading up the new office in Palo Alto, California, is Dr. John Dunec, who brings two decades of experience in the application of mathematical-modeling software. Commenting on his new position, he says, “the Palo Alto office is strategically located close to major academic institutions and the numerous high-tech firms in and near Silicon Valley. These represent leading R&D facilities in a wide range of application areas, and Comsol multiphysics provides an exceptional tool to assist in that work.”

In Brescia, near Milan, Italy, Mr. Daniel Ericsson is the managing director of Comsol s.r.l. He earned his masters in civil engineering at the Royal Institute of Technology (KTH) in Stockholm and has been in charge of Italian sales since 2001, working out of the Stockholm office. He is joined by Mr. Gian Luigi Zanotelli, who has been working with computer-aided engineering for 15 years.

Comsol Intensifies its Presence in Key Markets

Comsol developers have implemented a core GMG technology and supplemented it with standard and more specialized smoothers/preconditioners. This is only a start, and in later versions you can expect even more improvements in performance.

In the P.R. of China, Comsol has appointed ZhongFang Information Technology Ltd. as its distributor. This organization is a group of more than 50 engineers within the Chinese Simulation Technique Organization who provide professional solutions for virtual-prototyping industries.
term in Poisson’s equation allowed for the generation of vortices caused by the shearing effect of a non-uniform wind blowing across the lake. A comparison of Figures 1a and 1b shows what we were able to do 20 years ago and what is now possible with COMSOL Multiphysics.

After 44 active years, I retired from regular teaching in 2000 and have, alas, been frustrated that the emergence of COMSOL Multiphysics coincided almost exactly with my retirement. Not all is lost, though—for a few weeks every year since 1995, and even today, I have been teaching at the Petroleum and Petrochemical College at Chulalongkorn University in Bangkok, Thailand, using Comsol Multiphysics. I have also incorporated ten fully documented COMSOL Multiphysics problems into my Prentice Hall book, *Fluid Mechanics for Chemical Engineers* (Ref. 1), just published.

For me, the main virtue of this software is the insight it gives into the physics of the solution. For example, you can readily see the viscosity variations in non-Newtonian flows or the velocity vectors and electric potentials in electrophoresis. We no longer have to be content with solving simplified equations with “nice” geometries and boundary conditions, but can now venture into more realistic and practical situations. Thus, the availability of the k-ε model is particularly welcome as turbulence is a topic often sadly neglected in classroom instruction and some textbooks.

This has all been an incredible change since my first work in numerics on an IBM mainframe. Multiphysics has indeed gone mainstream.

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**Reference**

The development of computing hardware has become a familiar story, but such isn’t the case with finite-element analysis software and techniques. Indeed, we’ve entered a transitional period where the use of mathematical-modeling software has gone from the domain of specialists to where it is now available as an easy-to-use, reliable productivity aid to almost every researcher, scientist, and engineer. Whereas the finite-element method was initially the exclusive domain of structural engineers, it is now used in every discipline and branch of study from chemical engineering, to electromechanics, to MEMS, and even earth science.

It strikes me that in their everyday work many people are new to the concept of mathematical modeling and the enormous benefits that this tool can bring to their work. In contrast to these people, my association with computers and working with the numerical solution of partial differential equations (PDEs) goes back almost half a century, and I believe I have a rare perspective on where this tool has come from and where it is headed. I would like to share those thoughts with you.

**EARLY DAYS**

My association with digital computers is almost prehistoric. Soon after arriving in Ann Arbor, Michigan, from England in 1955, I took the first-ever digital computing course at the University of Michigan using an IBM 650 computer—with punched-card input and output, 2000 words of drum memory, and *biquinary* arithmetic. We were allowed 30 minutes of hands-on machine use every week, and we did our very best to avoid programming errors; otherwise, it was “come back next week.”

In the nearly 50 years since then, my research has specialized in the numerical solution of partial differential equations, using both finite-difference and finite-element methods (FDM and FEM), often with experimental verification, in the areas of natural convection, free-surface flows, zone refining, viscoelasticity, reservoir engineering, paint leveling, and polymer processing.

**EARLY FINITE-ELEMENT WORK**

My computational research started shifting from FDM to FEM in the mid-1970s. The big frustration was in learning the basics of the finite-element method because most previously published work had concentrated on structural analysis.

A typical problem involved flow of water in a lake between the rivers entering and leaving it. The source

Continued on page 35