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Friction Stir Welding

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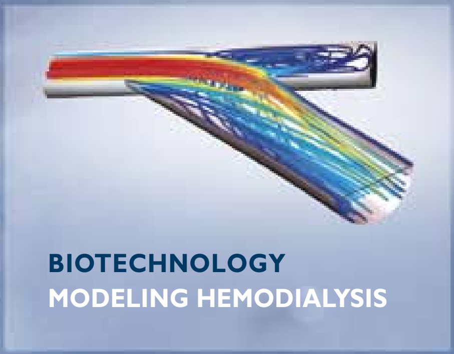

BIOTECHNOLOGY
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CONTENTS

CLICK ON THE HEADINGS TO GO STRAIGHT TO THE STORY

FEATURES

4 AEROSPACE INDUSTRY: Airbus investigates Friction Stir Welding

10 ACOUSTICS-STRUCTURE INTERACTION: SONAR listens to material properties

12 EDUCATION: University brings PDEs to life in undergraduate education

14 SEMICONDUCTOR MANUFACTURING: Multiscale multiphysics modeling in wafer processing

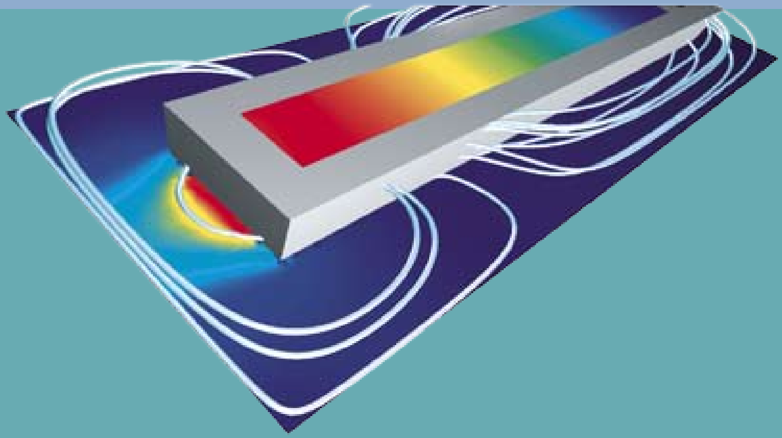
18 PACKAGING: Taking a bearing on quality

19 BIOMEDICAL TECHNOLOGY: Physician moves modeling into patient care

20 AUTOMOTIVE INDUSTRY: Multiphysics modeling sparks innovation in engine design

24 HYDROGEN ECONOMY: Argonne investigates alternate hydrogen-production technique

26 MAJOR SCIENTIFIC BREAKTHROUGH: Duke University presents the world´s first working prototype of an invisibility cloak



29 DEFENSE INDUSTRY: A new approach to railgun operation

30 EDUCATION: Biomedical engineering and multiphysics: Joined at the hip

COMSOL NEWS 2007

CLICK ON THE HEADINGS TO
GO STRAIGHT TO THE STORY

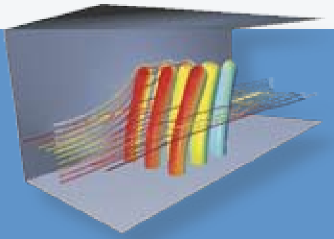
DEPARTMENTS

8 Product news

9 COMSOL Conference 2007

16 support@comsol.com

18 New books



22 APPLICATION BRIEF: Fluid-Structure Interaction

30 ICIAM Conference

30 Certified consultants

31 The Dahlquist Research Fellowship

32 GUEST EDITORIAL Professor Rolf Jeltsch

Multiphysics goes mainstream

The interest in multiphysics simulation is growing fast. A search on Google in August 2004 pulled up 13,000 hits for the term "multiphysics." Now it's at 421,000 hits!

This is just the beginning. We're now seeing the computer simulation industry become even more energized, enabled by the fusion of affordable high-performance hardware and new computational algorithms. A driving factor is that high-tech organizations see multiphysics modeling as an instrumental way to ensure their competitiveness by improving engineering efficiency.

Engineering efficiency can take many forms, a few key ones being research advances, increased understanding for students, and reduced time to market for a new-product introduction. This issue of COMSOL News reports on how your colleagues get the job done using multiphysics simulations.

The feature stories are based on papers that were presented at last Fall's international COMSOL Conferences. More than 300 presentations from the conferences are available on the User Presentations CD, which we have already distributed to more than 100,000 scientists and engineers. Copies are still available at www.comsol.com.

Better yet, you can experience all this excitement in person. Plan on attending one of our conferences this year. The 2007 conference series is shaping up to be the biggest multiphysics event ever. The program includes a major push to welcome first-time users as well as provide in-depth information for those who are already COMSOL users—a unique opportunity to learn about new simulation techniques and boost engineering efficiency.

Welcome to the multiphysics community!

Bernt Nilsson, *VP of Marketing, COMSOL*

ON THE COVER

Friction stir welding shows great potential in manufacturing, particularly in the aerospace industry. Modeling helps engineers understand and optimize the process. Read details about one such study on page 4.

(PHOTO COURTESY OF ECLIPSE AVIATION CORP.)

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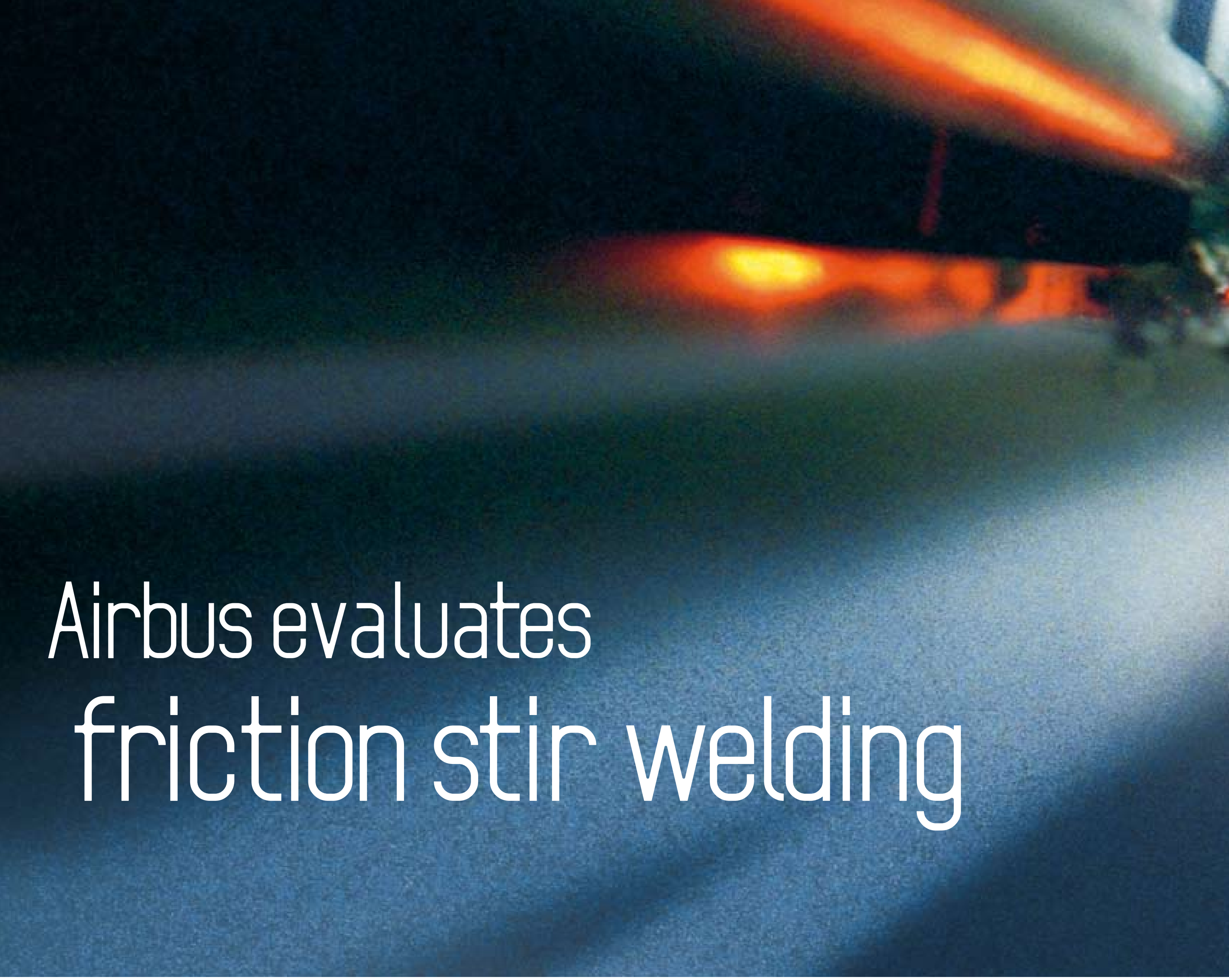


Airbus evaluates friction stir welding

Dr. Paul Colegrove of Cranfield University reports on the benefits of Friction Stir Welding and the modeling conducted by Airbus. A custom user interface to a COMSOL Multiphysics model allows Airbus engineers to quickly determine a weld's thermal properties and strength.

Patented in 1991, Friction Stir Welding (FSW) has since been used widely to create strong joints in aluminum alloys. The aircraft industry has started to adapt this technology, and now the largest manufacturers–including Airbus, an EADS Company–are studying how to cut manufacturing costs with it. First, though, they want mathematical modeling to help them fully understand the process before making massive investments in retooling their manufacturing lines.

As an aluminum-joining technology, FSW offers significant improvements over arc welding or riveted joints. The welds are stronger, lighter, and can be done more quickly. Especially useful in

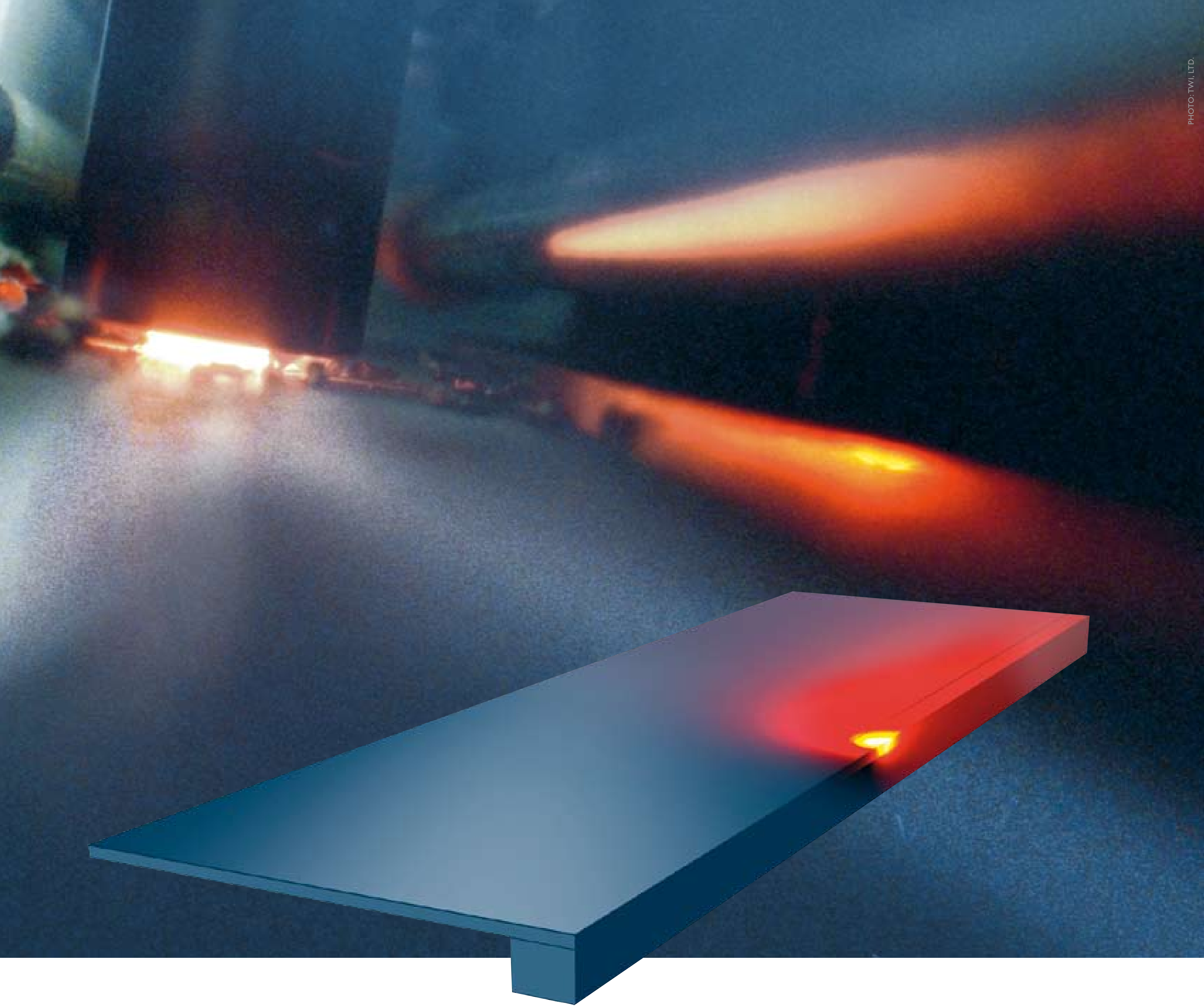


PHOTO: TWI, LTD.

welding aluminum alloys that are otherwise difficult to join, the process results in low distortion, you can weld thick sections in one pass, and produce welds with excellent mechanical properties.

In the FSW process (Figure 1), a cylindrical tool made up of a shoulder and a threaded pin is spun and inserted into the joint between two pieces of metal. The rotating shoulder and the pin generate heat—but not enough to melt the metal. Instead, the softened, plasticized material forms a solid phase made up of a fine-grained material with no entrapped oxides or gas porosity. The crushing, stirring, and forging action produces a joint with a finer microstructure than the parent material. The process can even join dissimilar aluminum alloys, while FSW joints can have twice the strength of riveted joints.

Already in the air

FSW is used in a number of industrial applications, including within the aerospace industry. In commercial airlines, however, its adoption has been slower because those manufacturers must be certain of a process' quality before making the enormous financial investments needed to implement it. Thus far, only one aircraft manufacturer, Eclipse Aviation of Albuquerque, New Mexico, uses FSW. This firm manufacturers the Eclipse 500, a 6-passenger Very Light Jet (VLJ). Its economic advantages are due in large part to FSW, which the firm reports as being energy efficient. One tool can typically be used for 1000 meters of joint length, there is no filler wire or gas shielding, no welder certification is required, and there is no grinding, brushing, or pickling necessary for mass production.

Aware of these advantages, the European manufacturer Airbus is investigating plans to introduce this technology into its manufacturing plants. Riveting is a slow, labor-intensive process, and replacing rivets with a continuous welded joint not only results in faster manufacturing at lower costs, but the distributed load results in a stronger joint. However, because large airliners experience higher stresses and shorter fatigue life, the technology must be brought online carefully. Many aspects of the tool and operating parameters can influence the amount of heat and the quality of the weld: the raw materials, tool diameter, tool geometry, rotational speed, weld travel speed, and down force. This process must be optimized for the materials used in commercial aircraft.

Thus Airbus asked several institutions to join it in a consortium to study FSW. During my time at Cambridge University I developed the heat-generation model presented in this article, while Nicholas Kamp, Joseph Robson, and Andrew Sullivan from Manchester University studied the microstructural aspects.

Closeup examination of a weld

One of the first results was a research project that created a mathematical model of FSW that allows Airbus engineers to look “inside” a weld to examine temperature distributions and changes in microstructures. To enable Airbus engineers to access the model easily, we created a GUI-driven simulation tool so they could look at a weld’s thermal properties and ultimate strength.

The COMSOL Multiphysics model couples a 3D thermal analysis, for calculating heat flow, to 2D axisymmetric swirl flow simulations, for calculating both the flow and heat generation (Figure 2). The thermal analysis calculates the 3D temperature field from the heat flux imposed at the tool surface. It captures the effect of the tool movement, the thermal boundary conditions, and the thermal properties of the material being welded. The model then extrudes the temperature distribution near the tool surface from the 3D boundary to the domain in the 2D model.

That next part of the model, in turn, analyzes the rotational flow of material through a 2D cross section underneath the shoulder. As a final step, it calculates the overall heat flux from this section and sends it back to the 3D analysis.

The analyses use specific modeling interfaces available in the Heat Transfer and Chemical Engineering Modules as well as tools for coupling the variables from the 2D and 3D modeling domains. Use of the 2D modeling domain saved computational memory and time, while results deviated only 1% to 2% from full 3D models of the flow. The analyses are solved simultaneously to guarantee faster and better solution convergence.

As noted earlier, to make this technology easily accessible, we created a custom user interface (Figure 3) using

Figure 1: In Friction Stir Welding, a shoulder sits on the metal surfaces and creates heat through friction, while a pin stirs the plasticized-heated materials to create the weld. *(photo courtesy of Eclipse Aviation, Albuquerque, New Mexico)*

ABOUT THE AUTHOR

Dr. Paul Colegrove earned his PhD at the University of Cambridge on the Modeling of Friction Stir Welding. Most recently he accepted a position as a lecturer in welding engineering at Cranfield University.

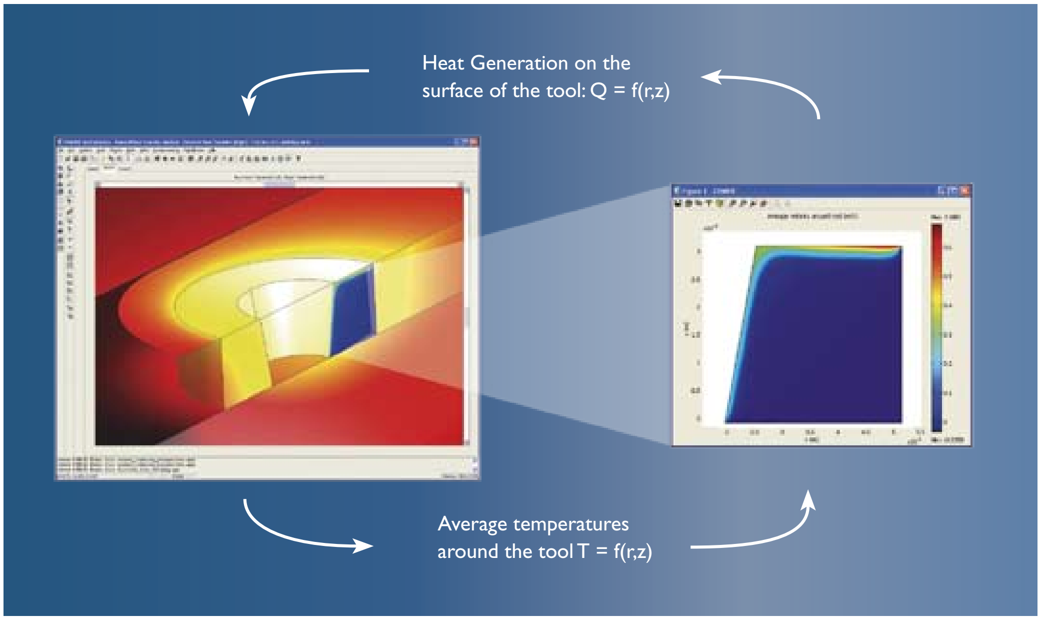
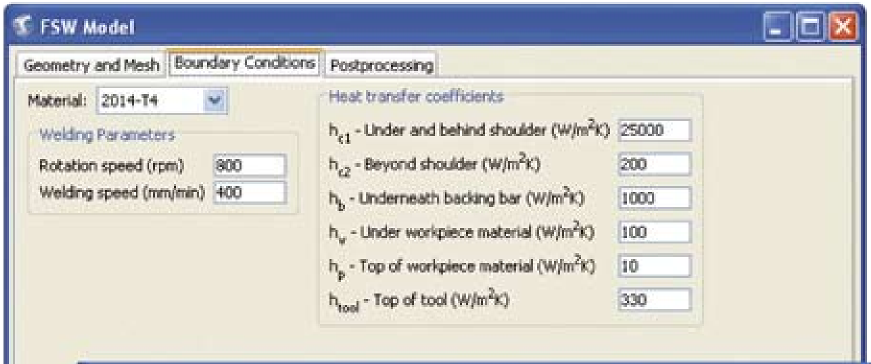


Figure 2: The multigeometric multiphysics model of Friction Stir Welding couples a 3D thermal analysis to 2D axisymmetric swirl flow.



FSW Model

Material: 2014-T4

Welding Parameters

Rotation speed (rpm): 800

Welding speed (mm/min): 400

Heat transfer coefficients

h_{c1} - Under and behind shoulder (W/m^{2}K): 25000

h_{c2} - Beyond shoulder (W/m^{2}K): 200

h_b - Underneath backing bar (W/m^{2}K): 1000

h_v - Under workpiece material (W/m^{2}K): 100

h_p - Top of workpiece material (W/m^{2}K): 10

h_{tool} - Top of tool (W/m^{2}K): 330

Figure 3: A customized user interface to run a mathematical model of FSW to analyze materials and configurations.

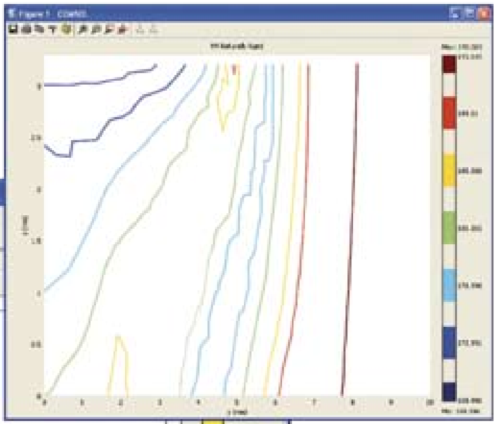
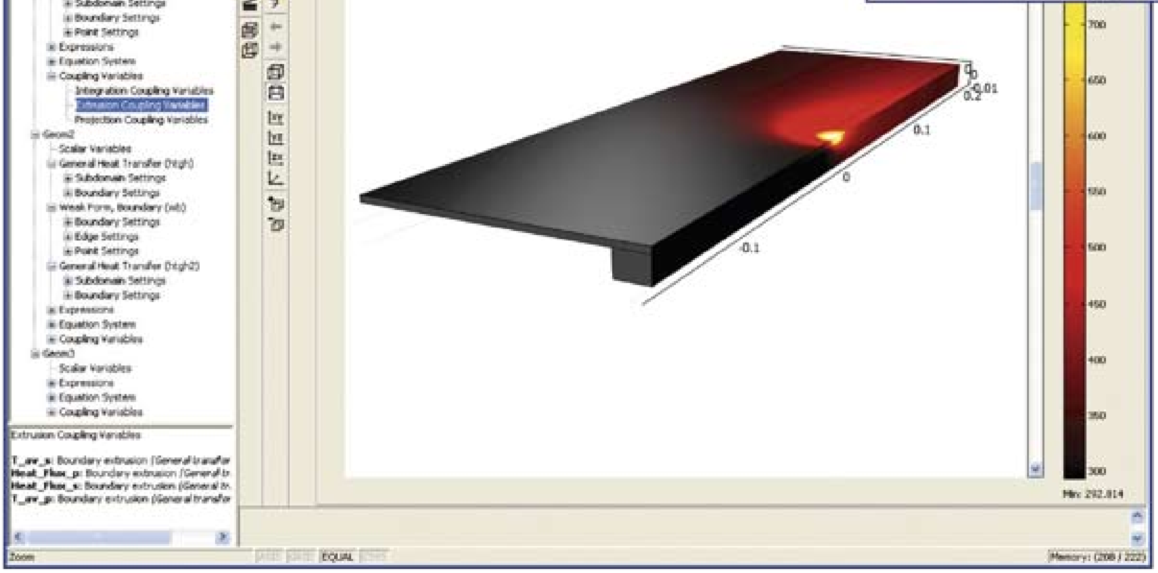


Figure 4: One result that users of the customized GUI can output is this 2D contour plot of the naturally aged hardness measured on the Vickers Hardness Scale. The contour plot is produced by finding the thermal profile at evenly spaced data points in the transverse direction (perpendicular to the welding direction of the tool) and thickness of the weld. The weld never reaches the same strength as the original material, which is the maximum value in the color bar.



COMSOL Multiphysics - Geom2/Heat Transfer Module - General Heat Transfer (htgh) : friction_stir_welding.mph

Figure 5: The 3D thermal profile of the weld.

COMSOL Script. Choosing a material from a pulldown menu selects the microstructural properties associated with that material from a database. The user also gives values for the tool's geometry and operating parameters. The model then creates a contour plot (Figure 4) by finding the thermal profile at various points in the transverse cross section and then calculates the corresponding material microstructure.

The final output plot is the 3D thermal profile (Figure 5). Here an engineer can calculate various statistics such as the temperature of the welded material at the shoulder and tip of the pin as well as the power input (or heat generation).

Obvious choice for modeling

Looking at the model requirements, it's easy to see why COMSOL Multiphysics was the obvious choice. Not only is it easy to use, but we were also able to link the 2D axisymmetric physics to 3D physics – something that would be extremely difficult to do with other packages. It was also easy to link in the microstructural-material aspects, which we developed in MATLAB® (MathWorks, Inc.). Then COMSOL Script brought the tools that allowed us to create the custom user interface that gave Airbus engineers access to the model's functionality.

The model couples a 3D thermal analysis to 2D axisymmetric swirl flow.

Airbus is funding a follow-on project that will allow us to refine the model, both in terms of thermal and microstructural analysis. COMSOL Multiphysics' flexibility and ability to simplify complex physical processes will be an integral part of this work. Furthermore, FSW is a very complex process, and we still want to perform considerable experimentation and validation to make the model as accurate as possible. ■

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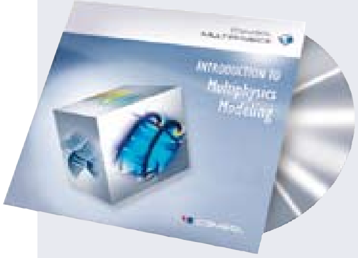
CDs give a quick introduction to multiphysics simulations



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The Material Library features 2500 material properties

New Product!

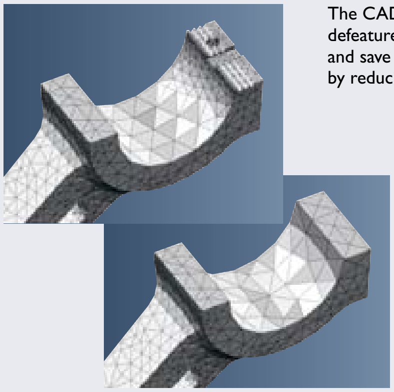
Rather than expect users to enter the massive amounts of data necessary to specify materials in a model, a new product automates the process. The Material Library contains referenced property functions for as many as 24 key material properties for more than 2500 materials.

These property functions allow the material property to depend upon some variable, typically temperature. The properties are then usable in multiphysics models such as structural analysis or quasi-static simulations in electromagnetics—they automatically account for the thermal effects that affect these other properties.

It is also possible to modify or edit the provided property functions, and users can add their own properties and materials.

The Material Library contains property functions for more than 2500 materials. Users simply pick a material from the list to set up the model´s material properties.

CAD Import Module 3.3a



The CAD Import Module can defeature unnecessary details and save computational memory by reducing the mesh size.

The new interactive repair feature in the CAD Import Module makes it possible to remove the gaps or overlaps that often crop up in CAD files. Thus, you can easily create solids and surfaces that are mathematically and physically correct for FEA modeling. To cut down on unnecessary details from a CAD geometry, you also have access to defeaturing tools that easily remove fillets, small faces, sliver faces, as well as spikes or short edges.

The CAD Import Module and its add-ons continue to support the widely used formats from today's CAD community. Specific to this is the live interface between COMSOL Multiphysics® and SolidWorks®.

We recommend the following file formats for import of geometry models from some of the most popular CAD software into COMSOL Multiphysics:

CAD SOFTWARE	RECOMMENDED FORMAT
Autodesk Inventor®	Autodesk Inventor® (.ipt)
CATIA® V4	CATIA® V4 (.model)
CATIA® V5	CATIA® V5 (.CATPart, .CATProduct)
NX™	Parasolid® (.x_t, .x_b)
Pro/Engineer®	Pro/Engineer® (.prt, .asm)
Solid Edge®	Parasolid® (.x_t, .x_b)
SolidWorks®	Parasolid® (.x_t, .x_b)

COMSOL® also supports SAT® (.sat), STEP (.step, .stp), IGES (.iges, .igs), VDA-FS (.vda), GDS (.gds), STL (.stl) and VRML (.vrml) geometry file formats.

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SONAR

Listens to material properties

SONAR has been in use for decades to detect submerged objects, but researchers are finding how to extract new information from its echoes.

BY PAUL G. SCHREIER

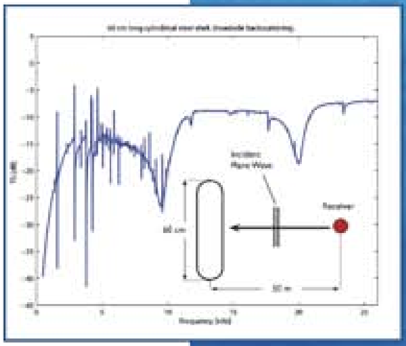


Figure 1: SONAR frequency response of a scuba tank (modeled as an empty cylindrical shell) computed with a model implemented in COMSOL Multiphysics. TS (target strength) is a logarithmic measure of the echo at a large distance from the target.

With the help of multiphysics modeling software, a group of researchers at the NATO Undersea Research Centre in La Spezia, Italy—Dr. Mario Zampolli, Dr. Alessandra Tesei, Dr. Gaetano Canepa, and Dr. Finn Jensen—are studying how to use low-frequency echoes to determine what an object is made of.

SONAR—as its name implies (SOund NAvigation Ranging)—uses sound waves traveling through water to detect and identify objects. The technique is similar to the more widely known RADAR (RAdio Detection And Ranging), which is based on electromagnetic waves instead of acoustic waves. RADAR is not used underwater because radio waves cannot reach very far in that medium due to absorption. During WWII, SONAR was used primarily to detect submarines; today these techniques are used to look for undersea objects such as shipwrecks and for measuring fish abundances and distributions. Similar acoustic techniques are being applied to wide-ranging applications from ultrasonic NDT (nondestructive testing), acoustic-transducer design, and geoacoustics.

SONAR has traditionally used frequencies for which the wavelengths are far smaller than the size of the objects being studied. This makes it possible to discriminate the shape of objects rather well and leads to advanced applications such as underwater acoustic cameras. However, it is difficult to identify the material of an object using high-frequency signals. Thus researchers are turning their attention to low-frequency schemes (Figure 1).

Information in the low frequencies

"Researchers," reports Dr. Zampolli, "have found out that these low-frequency echoes can also contain information that describes other properties of a submerged object such as the physics of its materials. This is because solids, unlike liquids, support not only longitudinal vibrations but also transverse, or shear, vibrations and thus can propagate sound in a number of modes."

Particularly useful is the Lamb wave, a complex wave that travels through the entire thickness of a material layer. Propagation of these waves depends on the material's density as well as its elastic

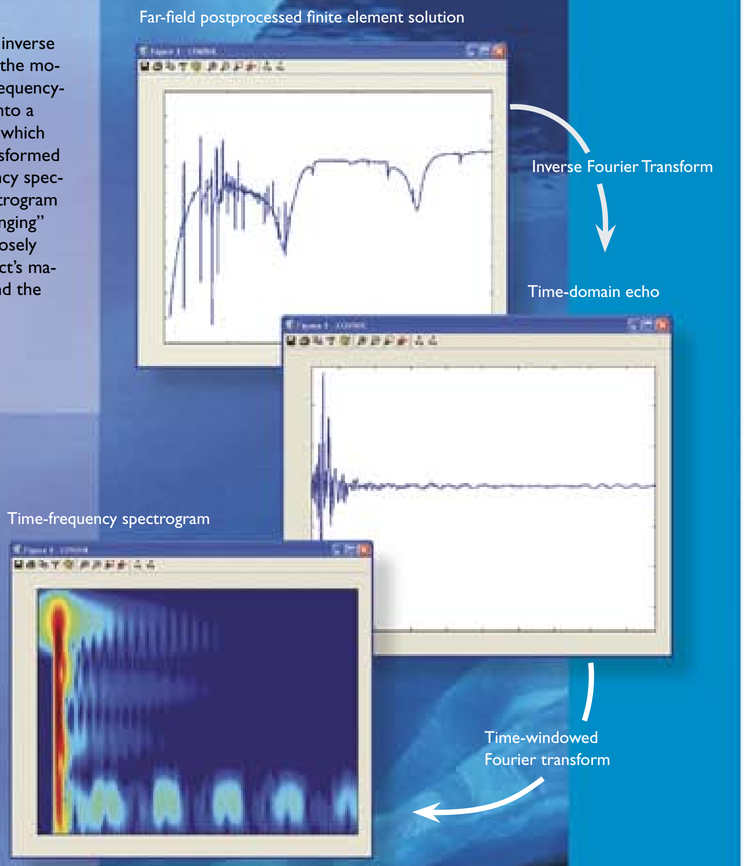


Figure 2: Using the inverse Fourier transform, the model converts the frequency-domain response into a time-domain echo, which can in turn be transformed into a time-frequency spectrogram. That spectrogram exhibits various "ringing" features that are closely related to the object's material properties and the geometry.

and material properties; they are also influenced by the selected frequency and material thickness.

A physical model of the waves' propagation would have to consider that there is more than one relevant wavelength: besides the sound wave that bounces off the structure, there are also the solid-borne waves in the structure. It's also known that the longitudinal wave travels along the interface between the elastic solid and the water more quickly than the shear waves and than the Lamb waves. In fact, the Lamb waves can be up to two orders of magnitude shorter than the wavelength of the sound in water.

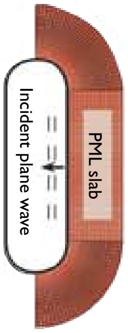


Figure 3: By using Berenger PML boundary conditions, it is not necessary to model the surrounding water.

And yet, the Lamb wave effects in the bounced sound waves contain a great deal of information. For example, you can understand the physical properties of an elastic shell by examining the Lamb wave's resonance effects.

An advanced SONAR receiver must therefore deal with a complex signal made up of multiple waves that taken together determine the echo's resonant structure. Making matters more complex is the fact that there are no analytical models that describe such activity, so it's necessary to unscramble the signal by knowing the underlying physics. In short, you need to know what to look for in such a signal. Only with a mathematical model can a researcher predict the form and structure of the low-frequency waveform emitting from a submerged object.

Fluid-structure interaction

Dr. Zampolli's team built such a model using COMSOL Multiphysics. This multiphysics model describes the frequency-domain elastic-displacement wave equation for a submerged object and couples it to an acoustic-wave equation that describes the waves in the fluid domain. Because the Lamb waves are so short, a finite element model of the object must have many more degrees of freedom than you might expect. "These slow, short waves present a real challenge in the modeling process," notes Dr. Zampolli. "This is a very challenging field," he adds, "and getting a mesh and convergence is difficult."

For their initial model, that of a cylinder with two end caps representing a scuba tank, the team treated the 3D geometry as an axisymmetric 2D problem. They then solved a set of independent 2D problems and added these solutions together through an azimuthal Fourier series to reconstruct the 3D field (Figure 2). "COMSOL Multiphysics' underlying and open structure," comments Dr. Zampolli, "allows us to implement the equations we need to reduce computational memory." Although the target must be axisymmetric, the incident SONAR signal need not be so. Perfectly matched layers (PMLs) absorb outgoing waves, making it possible to simulate efficiently a target immersed in an infinite fluid domain using a finite-sized mesh (Figure 3).

The scheme also employs COMSOL Script for solver scripting and hands-on postprocessing with the Fourier decomposition of the Helmholtz-Kirchhoff far-field integral. Thanks to smart use of COMSOL Multiphysics' features, their modeling method significantly reduces problem size, and now they're even able to model echoes from objects in the mid-frequency regime.

Dr. Zampolli believes that COMSOL Multiphysics is very well suited for such work. "Our studies don't fall into conventional areas, so there are no specialized tools for this type of project. With COMSOL Multiphysics, though, you can tailor virtually everything to your particular needs, and I find the package very impressive. For instance, I use weak-form modeling heavily for the azimuthal Fourier decomposition of the structural-acoustics equations." Now that the software is also available in a 64-bit version, Zampolli feels that "I'd take my first stab at any problem with COMSOL Multiphysics." ■

> "I'd take my first stab at any problem with COMSOL Multiphysics"

READ THE RESEARCH PAPER AT:
www.comsol.com/academic/papers/1009

University brings PDEs to life in undergraduate education

An undergraduate heat transfer course uses COMSOL Multiphysics to help students design the cooling for a motorcycle engine block

BY DR. K. K. BHATIA, ROWAN UNIVERSITY, GLASSBORO, NJ

Although personal computers have brought major changes to higher education, a debate continues as to when is the appropriate time to introduce certain topics that seriously rely on computational power. For instance, is simulating partial differential equations (PDEs) using finite element analysis (FEA) suitable for an undergraduate class? My recent experiences with COMSOL Multiphysics show that it can be done. Such an approach not only gives the students an introduction to a new tool and new knowledge but also motivates them to master these concepts when they later study them in detail.

Engineering education has moved far beyond the traditional chalk-and-talk lectures and examinations. Many programs now incorporate student participation through projects in what is knows as the "paper-poster-presentation" paradigm. Those designs, however, are done on paper, and educators are trying to introduce the concept of "design-build-test" to help students learn by encountering problems, making mistakes, and overcoming them.

Dr. K.K. Bhatia (center) discusses the engine-block simulation with students Chris Rowen (left) and Dave McKenna.

It started with thermodynamics

Last year, along with a colleague, Dr. Eric Constans, I introduced this concept into my first semester junior-level thermodynamics course and his mechanical design course. Student teams built steam engines and air compressors from scratch using raw metal stock. They discovered – through pistons seizing, for instance – that a major part of the task is keeping the cylinders and components cool enough. They tried various methods; one team even used a block of ice.

Keeping an engine running taught thermodynamics concepts, but students didn't yet understand heat transfer effects. I thus decided that for my second semester heat transfer course that I would extend the steam engine idea. However, I found that its cooling requirements resulted in a very simple problem to solve. Therefore, I decided to have them design an air-cooled motorcycle engine block and then study it using modeling software. The cooling requirements of such an engine are not trivial and thus made for a challenging project.

Although finite element modeling is usually absent from undergraduate courses, I saw this as an opportunity to introduce them to a new skill, and even more as a way to help them understand the fundamental physics and practical applications of the PDEs they saw in their textbooks, but never really embraced or even understood.

For this project, the only choice of software for me was COMSOL Multiphysics. True, I could have taught heat transfer modeling with any number of codes or packages, but only COMSOL supplies an intuitive menu structure and graphics-driven user interface where the equations are clearly visible, thus making it suitable for student use. In addition, it also provides direct access to the underlying equations. I wanted to do more than teach them how to use a black box to get pretty pictures; I wanted to teach them the concepts. I decided to start small with a relatively simple project so they could get some experience working with PDEs. Then, when they later take a course in FEA, they will have a stronger motivation for paying attention to aspects such as boundary conditions or solvers that otherwise might seem somewhat arcane.

Let's get to work

Here's the way the project ran: The students first heard a 1 hour introduction to finite element analysis, after which they got a 1 hour introduction to COMSOL Multiphysics focusing on CAD import, manipulating PDEs, boundary and subdomain conditions, getting a mesh and a solution, and generating postprocessing plots.

Next came a half-hour discussion of the project details: to design the engine block for a V-twin air-cooled motorcycle engine. The rough specifications for bore, stroke, vee-angle, and block material came from a Harley-Davidson® engine. The students were to design a block that would stay at a temperature lower than 350 °C while cruising at 60 mph.

The students' real work started with an analysis on paper of a simplified block design, making a first guess at the number of cooling fins, their geometries, and sizes. Then, using assumptions and hand calculations, they arrived at a rough answer for the heat generation and dissipation from the running engine.

Then they moved to actual design. They drew the engine block and its cooling fins in SolidWorks®, which they have access to in our computer lab and had used since their freshman year. After they created the 3D geometry, it was brought into COMSOL Multiphysics using the CAD Import Module.

The results at this stage were already interesting. Roughly half of the teams came up with conventional designs, while the other half let their imaginations run wild and put cooling fins in odd locations. For instance, one team placed huge fins across the cylinders. At times like this I would inject some manufacturing concerns, which sometimes meant they had to do a redesign.

"No risks, no gain"

With the CAD geometry in COMSOL, they could then set up the model and generate a plot of the block's temperature. Some students used the Heat Transfer Module while others simply modeled the steady-state heat conduction equation (Laplace equation) using the Coefficient Form. Next year, I might require all to use the Coefficient Form because it will involve more exposure to raw PDEs. Whether a conventional or unconventional design, in about half the cases the modeling results were within 10 °C of the hand calculations. In fact, comparing the hand calculations to the model results not only made them comfortable with the model results but also drove home the important lesson of not putting blind trust in them.

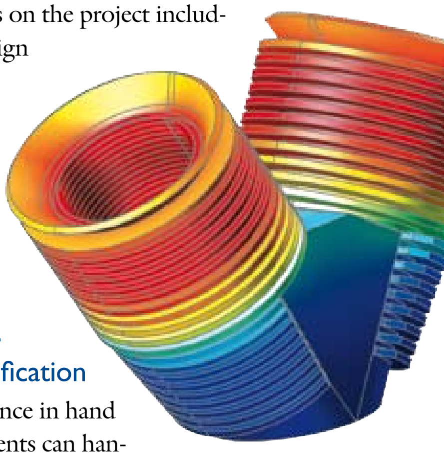
"Bringing modeling and simulation tools into a course has tremendous advantages"

In that regard, I believe that students can learn a great deal through their mistakes, or as I like to say, "no risks, no gain." I wanted my students to have a chance to fail because with SolidWorks and the COMSOL Multiphysics live-connection they can quickly reiterate a modified design.

No black boxes or canned projects

When some of my colleagues learned about this project, they were afraid that it was too ambitious because it wasn't a "canned" project available in a textbook. They also questioned whether there would be enough time to pull it off. In the end, the project was a complete success.

One of my main goals was to make the students comfortable with PDEs so the next time they ran into one they wouldn't be afraid to deal with it. With any other simulation tool except COMSOL Multiphysics this wouldn't have been possible. They'd likely be working with the PDEs "blind" as if the tool were a black box, and they wouldn't have direct access to the equations. It was also great that the students kept within the time plan–the teams spent roughly 15 hours on the project including the CAD design and model analysis. Almost universally, the feeling among the students is that "modeling is really cool!"



Temperature distribution in the engine block of a motorcycle engine.

Adding experiments and verification

With this experience in hand I know that students can handle the software and the PDEs, and so I want to complete the design-build-test cycle. Thus, in my next undergraduate course, on advanced heat transfer, students will not only design something using COMSOL Multiphysics, they will also build it and compare experimental data to model results. One idea is to design a cooling device for a computer CPU. Not only will they go to the machine shop and manufacture a heat sink, they'll later attach thermocouples and take temperature measurements.

It's clear to me that bringing modeling and simulation tools into a course has tremendous advantages. I wouldn't be surprised to see it become a standard element of undergraduate engineering education in the near future. ■

AUTHOR'S BIOGRAPHY

Dr. Krishan K. Bhatia joined the faculty in Mechanical Engineering at Rowan University as an assistant professor after completing his PhD at the Pennsylvania State University. While at Rowan University he has focused his efforts on direct methanol fuel cells and advanced powertrain vehicles.

READ THE RESEARCH PAPER AT:
www.comsol.com/academic/papers/1529

Dr. Jozef Brcka performs modeling to assist in the development of metal containing high-density plasmas utilized for submicron and nanotechnology applications.

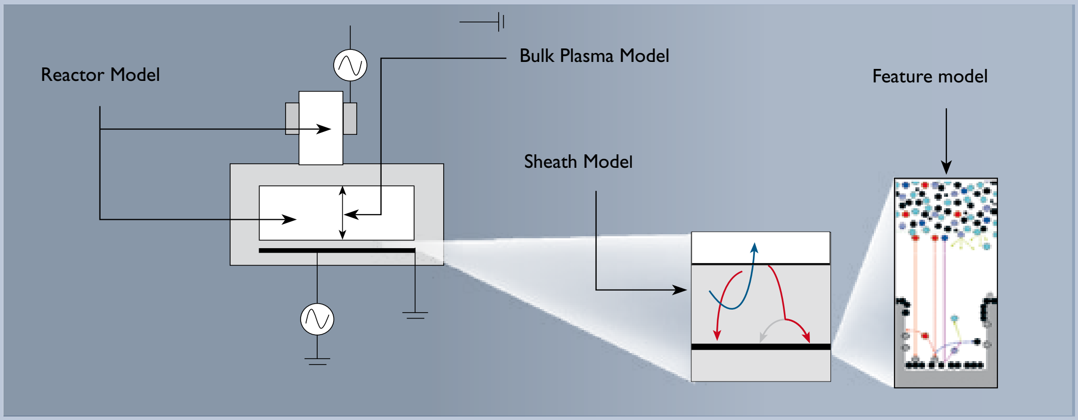


Figure 1: Process for surface preparation and cleaning of silicon wafers using hydrogen.

Finding the one solution

for multiscale multiphysics modeling in wafer processing

BY DR. J. BRCKA, TEL TECHNOLOGY CENTER, ALBANY, NY

Semiconductor wafer manufacturing involves a large number of processes, and the corresponding physics range in size from meters to nanometers. The search for one integrated environment that could handle them all led to COMSOL Multiphysics.

Optimizing semiconductor processing equipment is a complex task because of the large number of aspects that contribute to the whole. First it is necessary to prepare and process materials and thin films, typically in a complex plasma environment. Next, manufacturers deal with flowing and reacting gas mixtures, where it is vital to account for static or RF electromagnetic fields and their couplings to the processing media. A wafer fab represents a true multiscale problem because the reactors in which the wafers are placed can be more than a meter wide, whereas you must account for molecular activity happening in the nanometer range. Further, time scales of interest can range from milliseconds to hours.

In the past, the design of chip manufacturing and processing equipment depended mostly on empirical methods due not only to the rapid pace of innovation but also to the incomplete understanding of the fundamental physical and chemical phenomena. Dedicated codes have been developed at universities, but they require users to master their specifics, and they also often use simplified geometries or analytical approach models.

Yet, without adequate modeling, finding a part that does the job exactly as required under complex chemistry environments, heat or electromagnetic field loads, and with predicted actual impact on process performance, is primarily trial and error. Not only do nonworkable parts turn into expensive scrap, but it can take weeks to get such prototype parts made. With a good model, it's possible to test 10 or 20 cases in just days and thus get a new process online as quickly as possible.

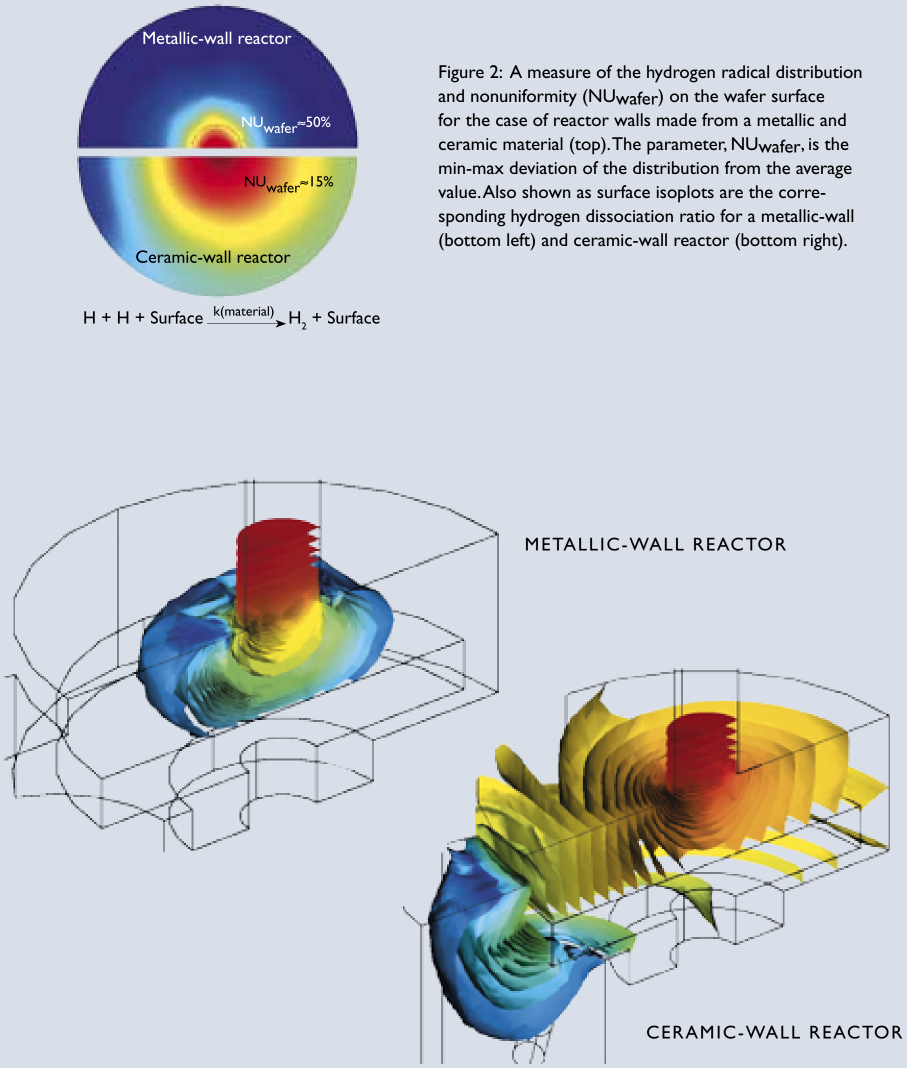


Figure 2: A measure of the hydrogen radical distribution and nonuniformity (NU_{wafer}) on the wafer surface for the case of reactor walls made from a metallic and ceramic material (top). The parameter, NU_{wafer}, is the min-max deviation of the distribution from the average value. Also shown as surface isoplots are the corresponding hydrogen dissociation ratio for a metallic-wall (bottom left) and ceramic-wall reactor (bottom right).

Future manufacturing requirements

We at Tokyo Electron Ltd (TEL) are taking advantage of finite element modeling. TEL, founded in 1963 and today with annual sales near $US 5.8 billion, was the first company to introduce American semiconductor production equipment and integrated circuit testers to Japan. At the TEL Technology Center in Albany, NY, our role is to develop new processes and hardware to meet future semiconductor manufacturing requirements. Working closely with process engineers, we bring the nano and macro scales together. We have found that doing our job is simply not cost effective without modeling because without simulation results, an equipment designer doesn't even know where to start a development project or how to change tool components to satisfy new process or technology requirements.

However, over time a problem arose because we adopted a variety of simulation codes and methods for each manufacturing stage. Consider, for instance, the use of hydrogen for surface preparation and cleaning of silicon wafers and thin films (Figure 1). The first area to study covers the electromagnetic interactions with the wafers and the processing materials; previously we studied what was going on with a commercial package dedicated to EM simulations. Next is the bulk plasma model, for which I was forced to use my own custom code. It is also necessary to develop a sheath model that examines the transport of the chemically active species during the manufacturing process, and here we typically worked with an analytical model. Finally, to look at the feature model that describes events at the molecular level, we again worked with my own code.

I have found this combination quite annoying and counterproductive. I'm dealing with different codes, on different platforms and operating systems, in different time scales. Then problems of moving data between these codes arise. In parallel to this, to create novel technical solutions you want to use a flexible simulation tool and implement new ideas in reasonably short time, in other words to be independent in development work. I came to believe that it would be far more effective to use an all-in-one simulation package. Thus I embarked on a feasibility study to see to what extent I could perform plasma-reactor simulations using COMSOL Multiphysics. In just six months I have come to some very positive conclusions.

Involving the chemistry

There are a couple of different ways in which the wafer surface can be prepared, where one of them uses hydrogen radicals interaction with the wafer surface, eventually low energy ion bombardment stimulation. Even though I was a new user of COMSOL, I felt comfortable modeling the hydrogen's chemistry; and in this study I looked at 15 reactions. The important thing with the chemistry is to achieve as uniform a distribution of hydrogen radicals as possible. Figure 2 shows the effect that the reactor wall has on this parameter. Reactors made with a metallic surface on the walls, typically an aluminum alloy, result in process performance at the wafer surface less uniform than those made with a ceramic wall surface. Further, metallic walls react more with the intermediate species so that there are fewer hydrogen radicals available and the overall chemistry in complex molecular plasma can be negatively affected.

Now that I have completed the bulk-plasma and chemical-reaction model, it's also time to include the full sheath model as well as the feature-level model. Here I hope to include even more of the phenomena that describe the process in full and will provide a self-consistent model solution. I am also reworking my first models to include other aspects and more complex geometries. Yet, just the fact that COMSOL Multiphysics gives me one simulation environment for all the phenomena in my multiscale and multiphysics systems means that I am far ahead of where I could have imagined just six months ago. ■

READ THE RESEARCH PAPER AT:
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support@comsol.com

Application notes

Our technical support team leader, Niklas Rom, has selected a few interesting issues that he's encountered lately and presents them here. We invite our readers to send support questions of any type to him at support@comsol.com.

Modeling turbulence

The modeling of turbulent flow is increasingly popular among COMSOL users (Figure 1).

Both the *k*-ε and *k*-ω turbulence models are available in the Chemical Engineering and Heat Transfer Modules. Of special concern among our users is how to handle the inlet and wall conditions in turbulence models. Because these built-in turbulence models add two equations to the Navier-Stokes equations, they also require additional boundary conditions. Thus you must provide further information about the flow at all boundaries compared to cases based on laminar flow.

Self-contact

Many users ask about mechanical contact problems, and sometimes we get more specific questions about self-contact. The advantage with the contact feature in the Structural Mechanics Module is that it automatically detects contact pairs between parts in an assembly. However, contact pairs that belong to the same part have to be created manually.

Consider a model that treats the rubber seal around a shaft (Figure 1). When the seal is pressed downwards, two of the vertical boundaries significantly deform while also tilting slightly sideways. You can therefore initially identify at least two self-contact pairs, which are marked in Figure 1.

In this case, as in many cases involving self-contact, the structural model must account for large deformations (Figure 2). However, large deformations are inherently treated in the modeling interface for hyperelastic material models found in the Structural Mechanics Module, used here.

You can define the contact pairs under the Physics>Contact Pairs menu item. Here you can select one group of boundaries as the master boundary and the second as the slave boundary. In Figure 3, the green-colored surfaces are the master group while the violet-colored surfaces belong to the slave group.

Once you have manually identified potential self-contact pairs, the next steps are simply meshing and solving the model. The default settings for the contact-solver algorithm are often adequate for good convergence. Yet, in more complex contact problems, you might want to use the parametric solver in order to step cautiously through the deformation so as to gradually and successively calculate the shapes of the contact surfaces. ■

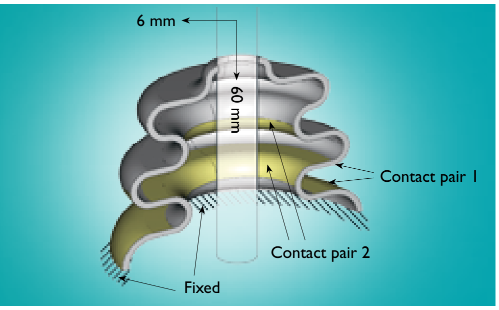


Figure 1: The self-contact regions are highlighted in yellow.

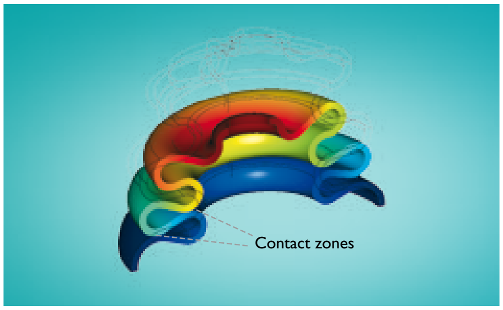


Figure 2: The collapsed rubber seal and the zones of contact.

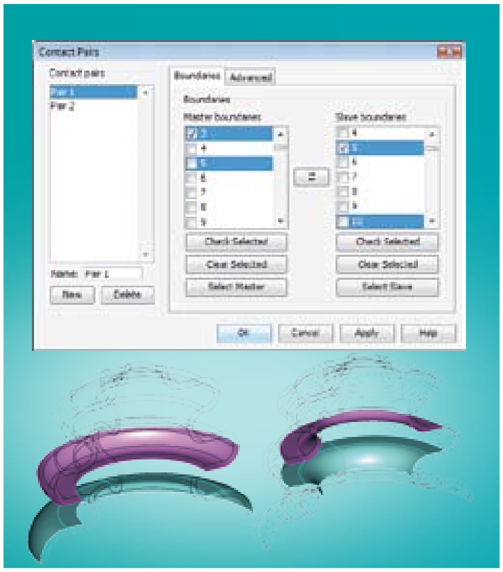
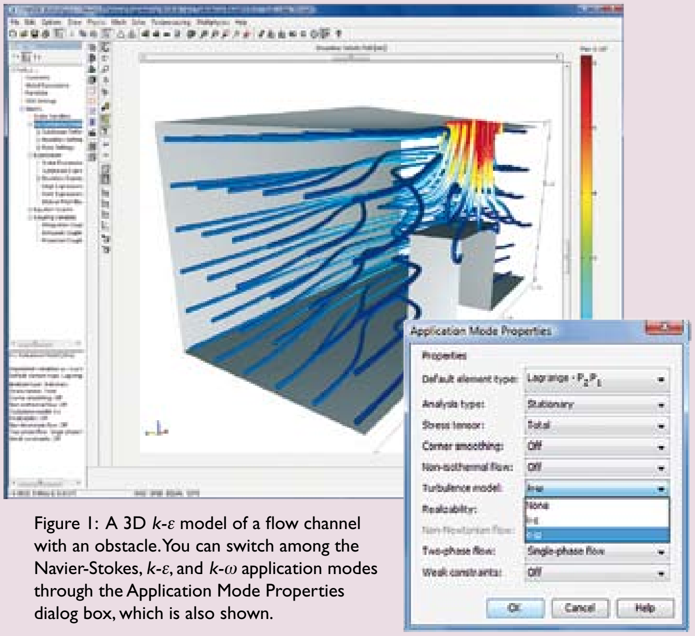


Figure 3: Two expected contact pairs in the rubber seal. These are defined as Pair 1 and Pair 2 in the corresponding dialog box.

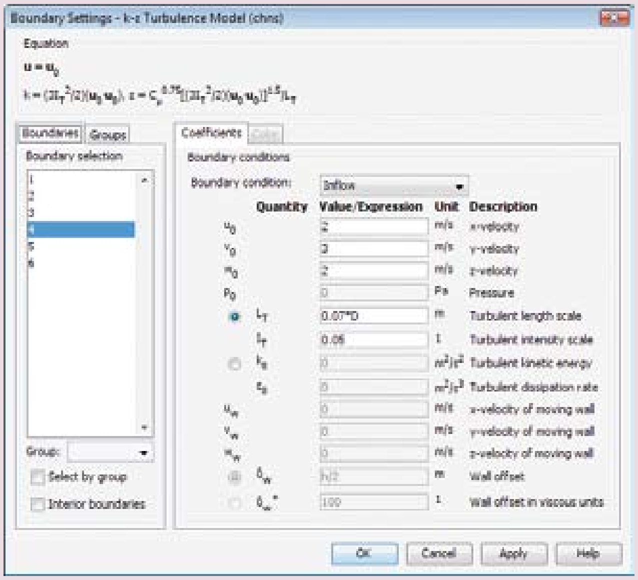


Default element type: Lagrange - P_2P_1
Analysis type: Stationary
Stress tensor: Total
Corner smoothing: Off
Non-isothermal flow: Off
Turbulence model: k-ω
None
k-ε
k-ω
Realizability:
Non-Newtonian flow:
Two-phase flow: Single-phase flow
Weak constraints: Off

Figure 1: A 3D k-ε model of a flow channel with an obstacle. You can switch among the Navier-Stokes, k-ε, and k-ω application modes through the Application Mode Properties dialog box, which is also shown.

Two properties that you can use to set inlet conditions for the turbulent entities (k and ε, or k and ω) are the turbulent length-scale and turbulence intensity. A possible approach is to set these properties to values typical for fully-developed turbulent internal flow. This would correspond to a value for the turbulent length-scale of `0.07*D`, where `D` denotes the typical length of the inlet, and a turbulence intensity of approximately 5%. Typically the turbulence length-scale and intensity for a large number of systems are available in the literature, and you can usually find a system that is similar to the one you are modeling.

For solid walls, you can usually set so-called lift-off wall functions (Figure 2). The computational domain is then assumed to be displaced a small distance, δ_w, from the true position of the surface. If the wall offset is large compared to the size of the geometry, you must redraw the domain accordingly with the wall displaced by δ_w. The wall functions assume that the displacement, expressed in viscous units, δ_w^+, falls between 30 and some upper limit depending on the Reynolds number (typically near 300). In order to check that you are within the interval for δ_w^+ (30 – 300) you can plot the variable **`dwplus_chns`** (δ_w^+) on the boundary. ■



Equation

$u = u_0$

$k = (3I_T^2/2)(u_0 \cdot u_0),\ \varepsilon = C_\mu^{0.75}[(3I_T^2/2)(u_0 \cdot u_0)]^{1.5}/L_T$

Boundary selection
1
2
3
4
5
6

Group:

☐ Select by group

☐ Interior boundaries

Boundary conditions

Boundary condition: Inflow

Quantity	Value/Expression	Unit	Description
u_0	2	m/s	x-velocity
v_0	3	m/s	y-velocity
w_0	2	m/s	z-velocity
p_0	0	Pa	Pressure
● L_T	0.07*D	m	Turbulent length scale
I_T	0.05	1	Turbulent intensity scale
○ k_0	0	m^2/s^2	Turbulent kinetic energy
ε_0	0	m^2/s^3	Turbulent dissipation rate
u_w	0	m/s	x-velocity of moving wall
v_w	0	m/s	y-velocity of moving wall
w_w	0	m/s	z-velocity of moving wall
● δ_w	h/2	m	Wall offset
○ δ_w^+	100	1	Wall offset in viscous units

Figure 2: The inlet boundary condition dialog box.

Q&A

Questions&Answers

from the Support Desk

The following are typical questions we often receive from our customers through support@comsol.com. Many of our suggestions point to the KNOWLEDGE BASE where you can find examples and small tutorials demonstrating the workarounds—visit www.comsol.com/support/knowledgebase

Q1: "How can I implement a B-H curve in COMSOL?"

A1: You can easily implement a B-H curve by defining the relative permeability, denoted μ_r in COMSOL Multiphysics, as a function of **B** or **H**. With the function option you can either type in an analytical expression or a lookup table, or link to an external text file or a COMSOL Script/MATLAB function. In the AC/DC Module you can try the Soft Iron predefined material to see how a B-H curve lookup table works.

You can find more details about B-H curve implementations in Knowledge Base Solution 852, where you can download a tutorial model.

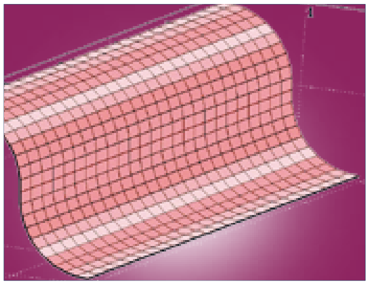
Q2: "I was wondering if anyone knows how I can set up the compressible Navier-Stokes equations in COMSOL?"

A2: There is an application mode named Non-Isothermal Flow, designed for weakly compressible flows at low Mach numbers (<0.3). It is available in the Chemical Engineering Module, the Heat Transfer Module, and the MEMS Module. The Navier-Stokes equations here are stated with the assumption that density can be a function of temperature, pressure, chemical composition, or any other modeling variable.

Q3: "My thin 3D geometry generates considerable mesh elements when I use the default tet-mesh option (in other words, I push the Initialize Mesh button). How can I reduce the number of elements?"

A3: One option is to generate a quadrilateral mesh on one of the thinner faces and then use the swept mesh feature to create a hexahedral volume mesh.

Get more details in Knowledge Base Solution 120, where you can download a tutorial model.



Swept thin layer mesh of hexahedral elements.

Q4: "I want to add an ODE (Ordinary Differential Equation with respect to time) to my COMSOL Multiphysics model so as to simulate rigid-body motion. How is this best done?"

A4: This is easily done through the ODE interface (Physics>ODE settings). Note that in the ODE dialog box you can also specify algebraic equations—just omit the time derivative. This can be useful if you want to specify system-level constraints for a model.

Get more details in Knowledge Base Solution 970 where you can download an example model.

New Books

Accelerate the Mastering of Multiphysics Modeling

The number of textbooks and educational materials based on COMSOL Multiphysics continues to grow. Here are some of the latest works to consider either for professional development or classroom use:

Multiphysics Modeling with Finite Element Methods

William B. J. Zimmerman
World Scientific Publishing Co

Microfluidics for Biotechnology

Jean Berthier and Pascal Silberzan
Artech House Publishers

Numerical Methods for Chemical Engineering: Applications in MATLAB

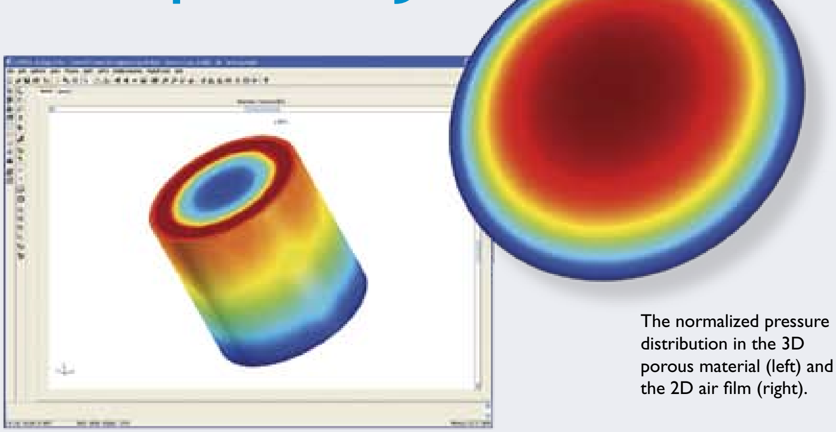
Kenneth J. Beers
Cambridge University Press

The Computational Engineering Sciences

A. J. Baker, University of Tennessee
Knoxville, book and DVD

Full descriptions and ordering information are available at www.comsol.com/stories/books

Taking a bearing on quality

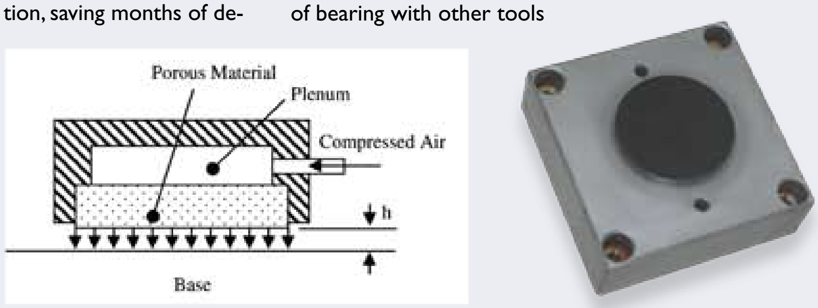


The normalized pressure distribution in the 3D porous material (left) and the 2D air film (right).

Porous air bearings are critical in high-precision machinery thanks to their essentially frictionless operation, high speed, and accuracy. ASM Assembly Automation Ltd of Hong Kong uses them in its electronic-assembly and packaging equipment. Rather than rely on commercial bearings, the company manufactures its own. With COMSOL Multiphysics, ASM engineers eliminated the need for more than one prototype of a new design before going into production, saving months of development time.

Air bearings use a thin film of pressurized air so there is no solid-to-solid contact. Air penetrates into the gap through millions of paths. "The same air gap that makes an air bearing so effective also makes modeling challenging," notes S.W. (Alex) Ng, a senior CAE engineer at ASM. "The model interface between the air film and bearing surface has a non-standard boundary condition that involves a partial differential equation." Ng tried to model this type of bearing with other tools but was unsuccessful because of that PDE. He then found COMSOL Multiphysics, the only package that let him work with nonstandard boundary conditions.

"Without COMSOL Multiphysics," adds Ng, ”you basically cannot solve this kind of problem, not with any other commercial software." Coupling the physics between different geometric dimensions is normally a difficult process to set up numerically, but in COMSOL Multiphysics it is an automatic feature. ■



In an air bearing (photo right), compressed air enters the plenum, passes through the porous material, and forms an air film that creates the bearing's upthrust (load capacity). The model combines 2D and 3D geometries: the bearing subdomain simulates 3D porous media flow using Darcy's Law, while the 2D film domain assumes compressible laminar flow.

BY PAUL G. SCHREIER

READ THE RESEARCH PAPER AT:
www.comsol.com/academic/papers/1043

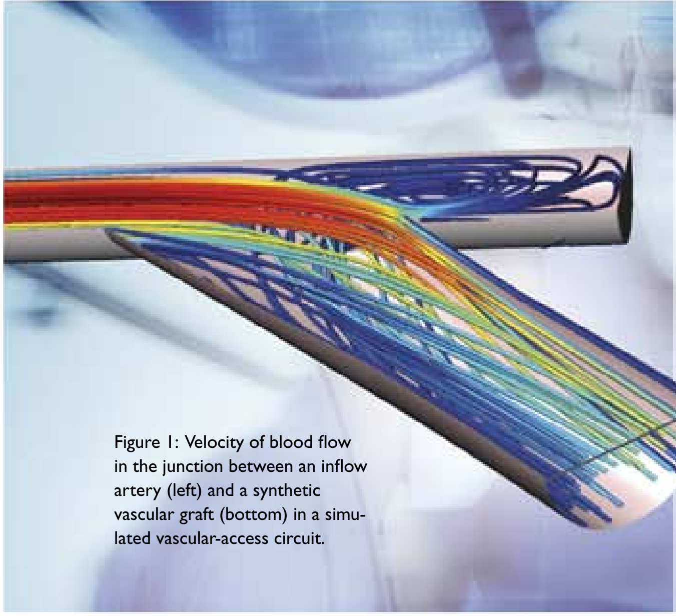


Figure 1: Velocity of blood flow in the junction between an inflow artery (left) and a synthetic vascular graft (bottom) in a simulated vascular-access circuit.

THE IMAGE OF A PHYSICIAN performing a bedside diagnosis might not come to mind when thinking of the typical person doing simulation and modeling. However, this technology has become so accessible to the practicing scientist and engineer that there's hardly a "typical" modeler any more. In his job as a physician, Dr. Steven Conrad has used modeling to refine artificial organs.

Physician moves modeling into patient care

Dr. Conrad graduated from Medical School in 1978 and then completed an MS in Biostatistics and a PhD in Biomedical Engineering from Case Western Reserve University. He joined the faculty of the LSU School of Medicine in Shreveport in 1986 and established a critical-care program.

BY PAUL G. SCHREIER

Dr. Conrad's experience with modeling began when he got interested in simulating physiological systems. In particular, he explains, "until recently, artificial organs were frequently designed empirically without simulation, which I felt could bring them to higher efficiencies. I wanted to model fluid and molecular transport in the fiber membrane of an artificial kidney, but I had no time to write code. With COMSOL, though, I immediately fell in love with the finite element concept. Fortunately, the application modes removed the nitty-gritty details of solving the PDEs so I didn't have to delve into computational methods." Dr. Conrad had to configure the hollow fibers and determine the amount of blood and dialysate flow. He adds, "I want to find which operating parameters can get the best efficiency out of existing designs as well as look at new designs to get even higher efficiency."

Furthermore, the simulations he performed with COMSOL Multiphysics have provided insight into the complexities of fluid and toxin removal with continuous dialysis performed in the ICU, and the results have given him insight into the best ways to apply this therapy to different types of critical illnesses. For instance, Figure 1 depicts the velocity of blood flow in the junction between an inflow artery (left) and a synthetic vascular graft (bottom) in a simulated vascular-access circuit used in patients who require long-term hemodialysis. The 3D Navier-Stokes equation was used to model the fluid flow. The development of complex secondary flows in the ligated arterial segment (right) and swirl flows in the graft segment (bottom) are easily identified. This COMSOL model allows the prediction of pressure losses in the circuit and provides insight into the diminuation of the graft function that can occur over time.

Meanwhile, he has started two other FEA projects. In one he is helping design a blood catheter for extracorporeal life support (ECLS), and in the other he helps analyze complications of the vascular access circuits used for hemodialysis, a process that removes waste products and free water from the blood when the kidneys can't do so. "Vascular access complications," says Dr. Conrad, "represent the greatest cause for hemodialysis patient hospitalizations."

> "COMSOL's flexibility makes it a perfect all-round tool for a doctor."

Results from the FEA models lie close to experiments run on a mock hemodialysis vascular access loop and are superior to previously used analytical models. "COMSOL Multiphysics' flexibility in the systems and physics it can model makes it a perfect all-round tool for the many applications that a doctor can encounter," concludes Dr. Conrad. ■

READ THE RESEARCH PAPER AT:
www.comsol.com/academic/papers/1724

Multiphysics sparks innovation in engine design

Low fuel consumption is a universal goal, and a system that shows great promise is the fully variable electromagnetic valve train (EMVT) that replaces the camshaft. Dethrottling an engine with an EMVT system leads to a fuel savings of possibly 18% compared to camshaft-driven engines. Further, the EMVT can achieve the low-end torque typically known only in diesel engines. Even though EMVT systems are well known they have not yet been brought to market. TRW Automotive in Barsinghausen, Germany, is investigating innovative solutions such as optimizing the system's electromagnets with COMSOL Multiphysics.

BY DR. C. HARTWIG, TRW AUTOMOTIVE,
BARSINGHAUSEN, GERMANY

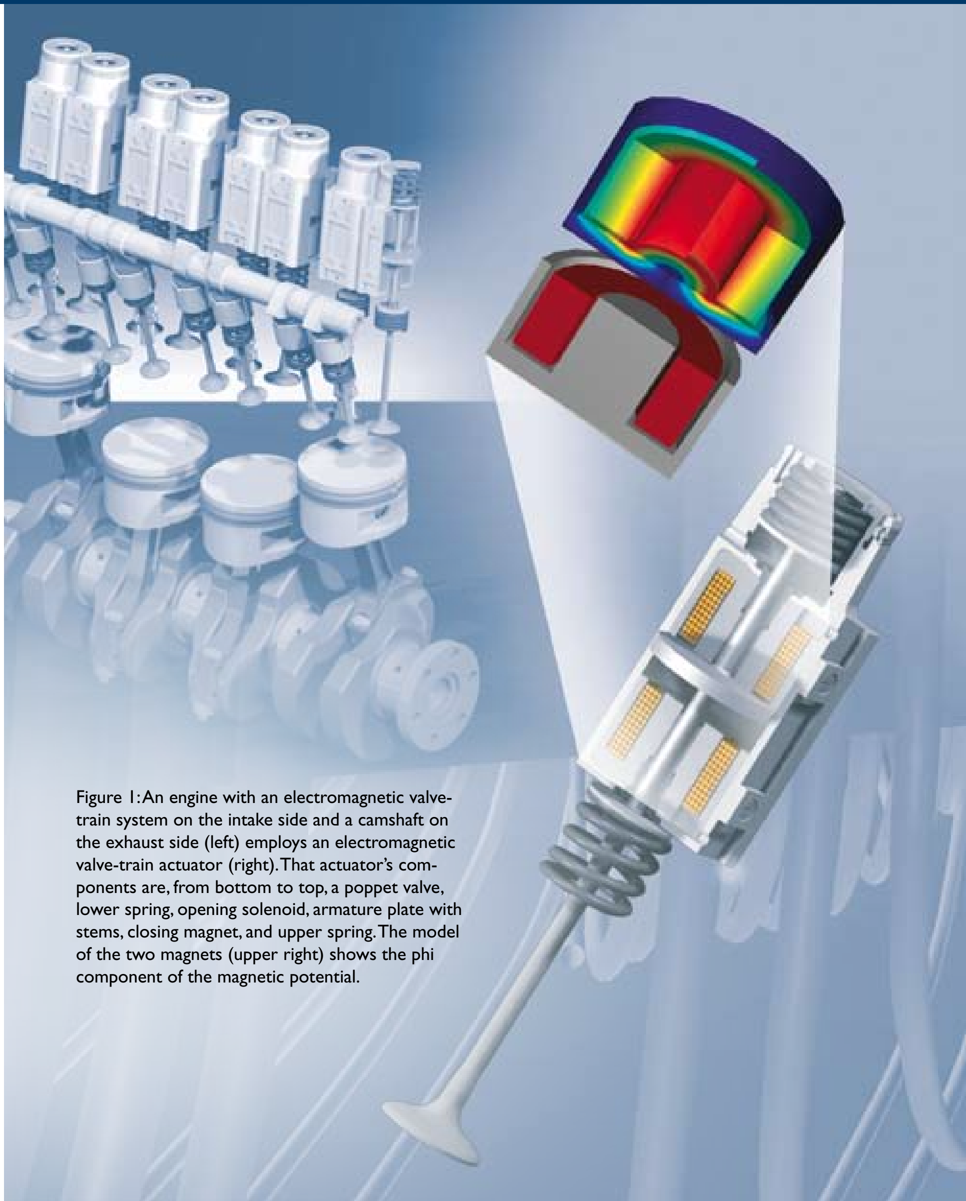


Figure 1: An engine with an electromagnetic valve-train system on the intake side and a camshaft on the exhaust side (left) employs an electromagnetic valve-train actuator (right). That actuator's components are, from bottom to top, a poppet valve, lower spring, opening solenoid, armature plate with stems, closing magnet, and upper spring. The model of the two magnets (upper right) shows the phi component of the magnetic potential.

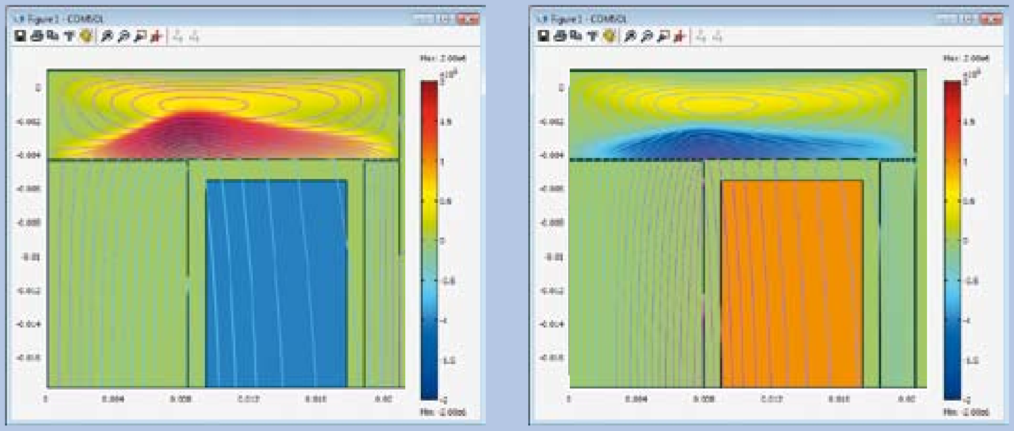


Figure 2: Distribution of eddy currents in the armature plate 2 ms after switch-off of the upper electromagnet, shortly before being caught by the energized lower electromagnet, here shown for two cases: when the currents in the two coils have the same orientation (left) and the opposite orientation (right). The color plot shows the current density.

The electromechanic drive

An EMVT actuator consists of a mechanical oscillator and two electromagnets that hold the valve and the armature open and closed. The transition time from open to closed must be short enough to allow valve timing and control strategies even at high engine speeds. This is achieved through a lightweight design. An appealing solution is the electromagnetic intake valve train (Figure 1). With it, all intake valves can operate individually whereas the exhaust valves are operated by a camshaft. This system has 90% of the advantages of a full EMVT system while avoiding the worst drawbacks.

Nevertheless, the limited space in a cylinder head requires an efficient electromagnetic actuator with a high force density and low losses. For this, COMSOL Multiphysics allows the easy calculation of static force-stroke-current characteristics, which are the starting point for the geometry optimization. Nonlinear material parameters can be provided by tables or functions, and this feature is very useful for examining different soft magnetic materials and reduces the number of prototypes.

Dynamic simulation

Energizing the magnets generates alternating magnetic fields and also induces voltages, which can cause undesirable eddy currents that cause losses and deteriorate system dynamics. Thus the soft magnetic core is laminated to reduce eddy currents. However, the thin armature plate cannot be laminated because doing so would impair mechanical rigidity. Eddy currents can be reduced only by making the material's electrical resistivity high and by disturbing their paths.

A transient simulation calculates the eddy currents as well as the equation of motion and the coupling between them and thereby calculates the electrical power transfer into the actuator. We can identify the distributions in copper losses, eddy current losses, and mechanical losses as well as analyze the impact of material parameters for various soft magnetic materials.

Another interesting experiment is this: The armature is released from one side and accelerates towards the other. When it gets close to the catching magnet, the eddy currents have not decayed. There are two ways to energize the catching magnet: where the current has the same or the opposite orientation as in the releasing magnet (Figure 2). In one case the magnetic field rises more slowly; if the armature plate approaches at a high speed, a control engineer would chose that current orientation to reduce the mechanical impact. The other case could be applied if the armature has been slowed down, such as by gas forces in the cylinder. ■

READ THE RESEARCH PAPER AT:
www.comsol.com/academic/papers/1513

Christoph Hartwig is a research engineer at TRW Automotive, where he is responsible for the modeling, simulation, and design of electromagnetic actuators. He earned both his Diplom Ingenieur and Doktor Ingenieur degrees in electrical engineering at the University of Hannover, Germany.

APPLICATION BRIEF

Modeling Fluid-Structure Interaction in COMSOL Multiphysics

A heart pumping, a plane taking off, or wind blowing in your hair when driving a convertible on a sunny summer day—these are all examples of fluid-structure interaction.

BY ED FONTES, VP OF APPLICATIONS, AND NILS MALM, SENIOR DEVELOPMENT ENGINEER, COMSOL

This group of phenomena is characterized by the flow of a fluid being influenced by the deformation of a solid structure, which in turn is deformed by the forces exerted by the fluid. Modeling fluid-structure interaction (FSI) involves specific multiphysics couplings between the laws that describe fluid dynamics and structural mechanics.

Fluid bends a rubber obstacle

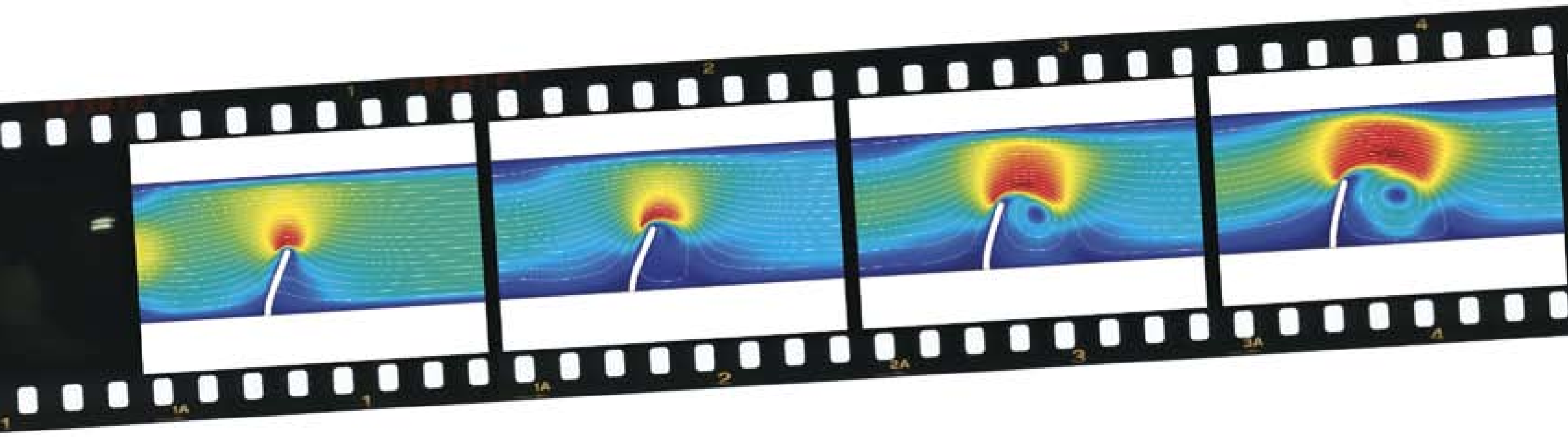
For instance, the images in Figure 1 show the time-dependent solution of the interaction between a thin rubber obstacle and a fluid flowing over it. The sequence shows that as the flow rate increases, the obstacle starts to bend in the direction of the flow. Eventually an eddy forms on the obstacle's back side, and that eddy increases the pressure on the obstacle, causing it to bounce back slightly forward before it reaches a steady position. This dynamic behavior is difficult to resolve accurately unless the structural, fluid-flow, and mesh-displacement equations are solved in a fully coupled scheme.

The FSI modeling interface

In COMSOL Multiphysics, the modeling interface for an FSI simulation consists of three parts: a solid structure, a fluid domain, and a set of equations that generates a smooth extension of the mesh deformation from the solid into the fluid domain. In the solid part, the mesh follows the material, and the nonlinear structural equations are written with respect to the nondeformed shape. Inside the fluid domain, mesh displacements are smoothed by the Winslow equations, which are designed to keep element quality as high as possible.

The technology that enables this in COMSOL Multiphysics is based on a set of frames. Each frame essentially defines a set of coordinates. Except for the default reference frame, which is based on the original mesh, different frames represent different sets of displaced coordinates. These can be determined through the deformation of a solid, with a smoothing equation in the fluid, or as user-defined expressions. The FSI modeling interface uses a combination of the first two alternatives.

All dependent variables must be tied to a frame, and the software evaluates their spatial derivatives in that frame. In an FSI model, the structural equations



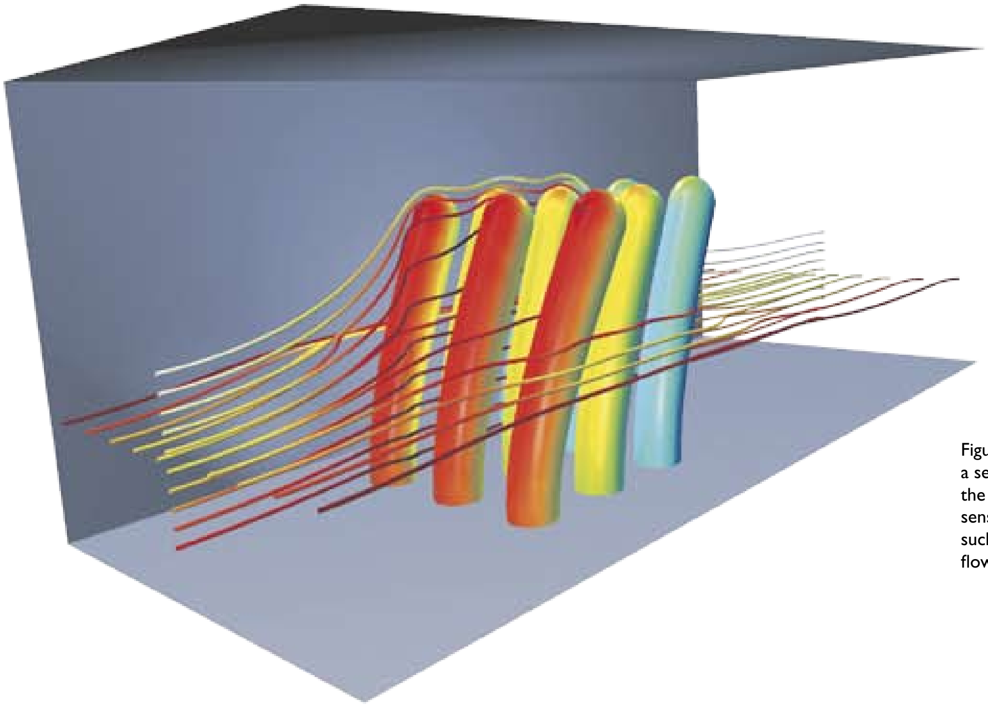
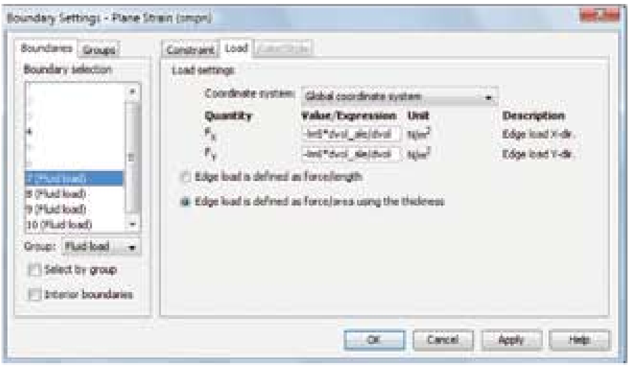


Figure 2: This image shows the steady flow around a set of pillar-shaped structures used to increase the sensitivity of surface acoustic wave (SAW) sensors. These typically detect adsorbing species such as proteins. The pillars are 5 μm long and the flow is of the scale of 100 μm/s.

Figure 3: The modeling interface lets you select the interface between the solid and fluid domains. The model equations and boundary conditions are then automatically defined in COMSOL Multiphysics.



Boundary Settings - Plane Strain (smpn)

Boundary selection: 7 (Fluid load), 8 (Fluid load), 9 (Fluid load), 10 (Fluid load)

Group: Fluid load

☐ Select by group

☐ Interior boundaries

Load settings

Coordinate system: Global coordinate system

Quantity	Value/Expression	Unit	Description
F_x	-lm1*dvol_ale/dvol	N/m^2	Edge load x-dir.
F_y	-lm2*dvol_ale/dvol	N/m^2	Edge load y-dir.

○ Edge load is defined as force/length

● Edge load is defined as force/area using the thickness

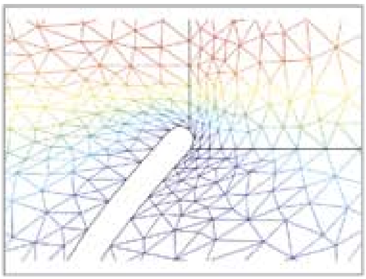
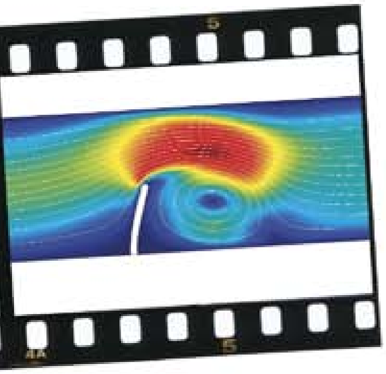


Figure 4: Deformation of the mesh from an original vertical position of the obstacle. In this case, a master-slave mesh node approach achieves maximum deformation without remeshing.

Figure 1: The displacement and flow field around an obstacle subjected to a flow after 0.2 s, 0.4 s, 0.6 s, 0.8 s, and 1 s after injection of a flow at the left vertical boundary.



are written with respect to the reference frame whereas the fluid dynamics equations are defined on the deforming spatial frame. Any equation originally written in spatial (Eulerian) coordinates can be applied without modification in a moving frame. Likewise, you can set up equations in reference (Lagrangian) coordinates in a fixed reference frame. The combination of these formulations forms the arbitrary Lagrangian-Eulerian (ALE) method. The ALE method is automatically adopted by the application mode, but you can also access it as a standalone application mode.

The same code for all physics

In an FSI model, mesh deformation is a part of the solution (see Figure 4). What sets COMSOL Multiphysics apart is that when using a fully coupled solution strategy, it calculates a complete Jacobian—also with respect to the mesh movements. Accuracy is further improved by the fact that no interpolation is needed at the fluid-solid interface because the same code solves both types of physics (structural and fluid). Therefore, the continuity of velocity and conservation of mass can be guaranteed. At the same time, an integral formulation of the boundary condition can ensure a very accurate force balance at the interface, as well as accurate postprocessing of drag and lift.

Yet, a true strength of COMSOL Multiphysics is that you can take the approach it uses for FSI modeling and extend it to any other type of multiphysics couplings, involving moving meshes, directly in the user interface. ■

Argonne investigates alternate hydrogen-production technique

BY DR. S. A. LOTTES AND R. W. LYCZKOWSKI, ARGONNE NATIONAL LAB, ARGONNE, IL

BMW's Hydrogen 7 is among the first hydrogen-drive luxury performance automobiles for everyday use. Being built in a limited series, it is equipped with a 260-hp internal combustion engine capable of running either on hydrogen or on gasoline and is based on the BMW 7 Series. The car's hydrogen storage tank holds approximately 17.6 lb of liquid hydrogen. Engine power and torque remain identical regardless of the fuel used. *(photo courtesy of BMW)*

The "hydrogen economy" aims to reduce the USA's reliance on imported fossil fuels along with the emission of greenhouse gases. Simulation is helping find the most effective path towards that goal.

A major US-based research initiative is looking at ways to make hydrogen a major transportation fuel that could largely replace fossil fuels. A first step is to find the most cost-efficient way to generate this hydrogen from domestic feedstocks without creating unnecessary greenhouse gases and yet be economically viable. Thus the US Department of Energy is investigating the use of nuclear energy for hydrogen production through the Nuclear Hydrogen Initiative. Although hundreds of possible thermochemical cycles have been identified, only a few seem to promise technical feasibility.

A team at Argonne is examining the potential of the calcium-bromine (Ca-Br) water-splitting cycle, where that material reacts endothermically with water to create calcium oxide (CaO) and hydrogen bromide (HBr). The latter is then converted through electrolysis or through a plasma decomposing process into bromine (Br_2) and hydrogen (H_2).

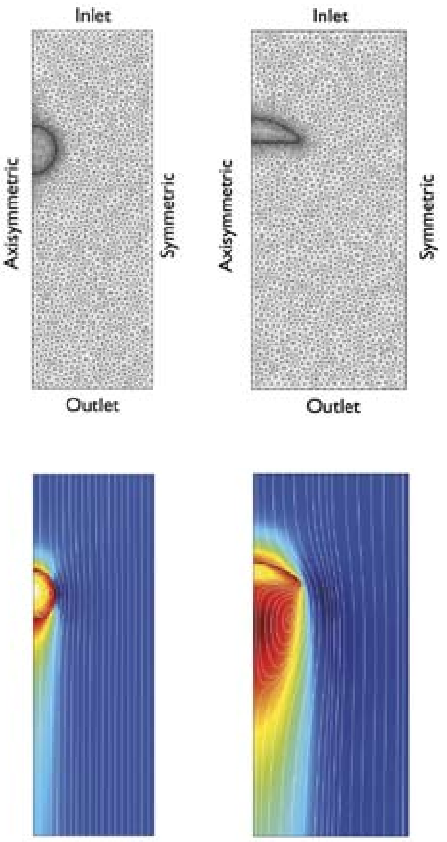


Figure 1. Mesh plot and results from the cases of a steam spherical bubble and steam spherical-cap bubble flowing through molten $CaBr_2$. The results show the velocity magnitude in the vertical direction (color plots), and vector (streamline plots) in both the bubbles and fluid flowing around the bubbles. The spherical bubble exhibits no recirculation in its wake, whereas the spherical-cap bubble does.

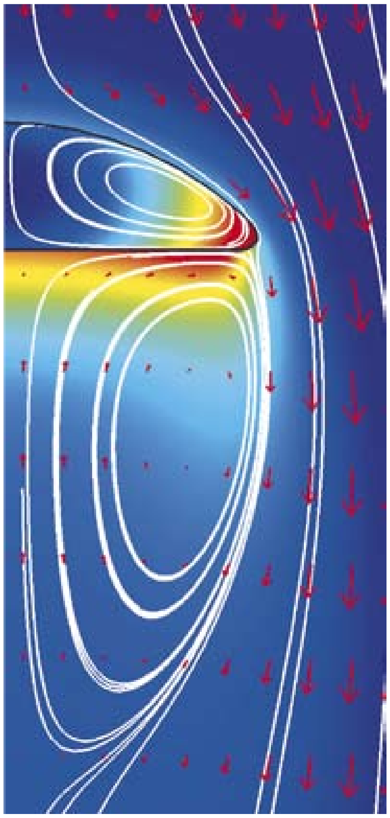


Figure 2: Concentration of the product, HBr, in the bubble and the product, CaO, in the molten $CaBr_2$. Here you can see the extent that CaO accumulates in the recirculation zone in the wake of the spherical cap bubble.

This cycle is particularly attractive because although it is highly endothermic, nearly half of the required thermodynamic energy for water splitting is delivered as nuclear heat.

Methods of $CaBr_2$ hydrolysis

Two options are under consideration for bringing the $CaBr_2$ (which carries much of the heat required for reaction) and steam together in a continuous process: either spraying molten $CaBr_2$ into a steam environment, or sparging bubbles of steam through a pool of molten $CaBr_2$. The COMSOL Chemical Engineering Module provides an environment wherein models for these complex interacting phenomena can be built and studied.

For the spraying method, the researchers ran simulations with droplet diameters and steam inflow velocities over two orders of magnitude. They found that for larger Reynolds numbers, a recirculation zone develops in the droplet wake into which reaction products tend to be swept rather than moving efficiently away from the region of reaction. They also discovered that the latent heat from solidifying $CaBr_2$ droplets supplies only a small fraction of the heat required for reaction of the entire droplet.

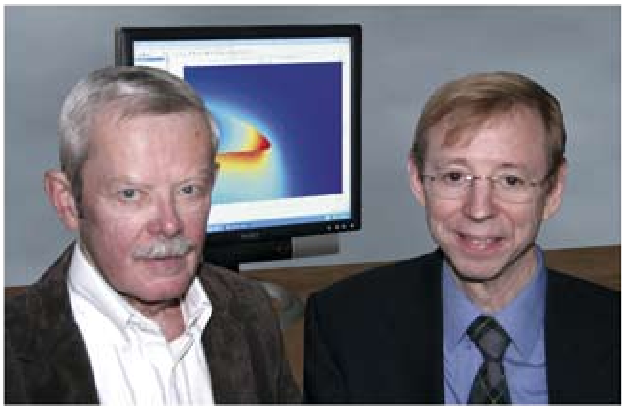
Can sparging steam do better?

What about the molten-pool method? The low viscosity of molten $CaBr_2$ opens up the possibility of using it as a heat reservoir, sparging steam into the pool as a bubble column. The modeling first studied the two limiting cases—the spherical and spherical-cap bubble regimes. With the former, the ratio of the reacting surface to volume is quite large, but producing small bubbles in a high-temperature molten salt in the laboratory is challenging. In contrast, the faster flow with spherical-cap bubbles induces turbulence and a wake where chemical reaction product species might accumulate and slow down the reaction at the interface behind the bubble (Figure 1).

Simulation results showed that only negligible amounts of the product, CaO, are drawn into the wake of the spherical-cap bubble, precluding any possible reverse reaction and reduction of conversion (Figure 2). Furthermore, steam diffusion and induced recirculation within the bubble itself bring steam to the bubble surface at a rate sufficient to keep up with the reaction.

Funding for alternative cycles is limited, so modeling identifies designs that are not likely to be successful. With COMSOL we are able to quickly get rough answers to many questions that helped our decision-making. ■

READ THE RESEARCH PAPER AT:
www.comsol.com/academic/papers/1643



The authors: Robert W. Lyczkowski (left) and Steven A. Lottes (right), both of Argonne National Laboratory

Modeling metamaterials leads to major scientific breakthrough

In their efforts to use metamaterials to construct the world´s first working prototype of an **invisibility cloak**, researchers relied on COMSOL Multiphysics to lead them to the materials and designs that would make this sci-fi dream a reality. This work was acknowledged by *Science* magazine as being among the scientific breakthroughs of 2006.

BY STEVEN A. CUMMER, DUKE UNIVERSITY, DURHAM, NC


PHOTO: LES TODD, DUKE PHOTOGRAPHY

Steve Cummer (left) and David Schurig adjust some equipment in their experimental set-up for measuring the effects of metamaterials.

Modeling software is generally used to make the invisible visible—to show the fields and flows in a product or process that are impossible to see with the eye or instruments. A group at Duke University, however, has done just the opposite: With the help of COMSOL Multiphysics, we ran simulations that showed it should be possible to fabricate the metamaterials necessary to make objects invisible. Based on the special properties of those materials, we created a computer simulation of an "invisibility cloak" that makes an object invisible to certain frequencies. We then successfully built and tested it.

Modeling every step of the way

Mathematical modeling has accompanied us most of the way down this trail. Our first simulation followed the publication of a paper in which Prof. Sir John Pendry of the Imperial College London and two of my Duke colleagues, David Schurig and David Smith, described the theoretical properties of a material shell that could bend electromagnetic

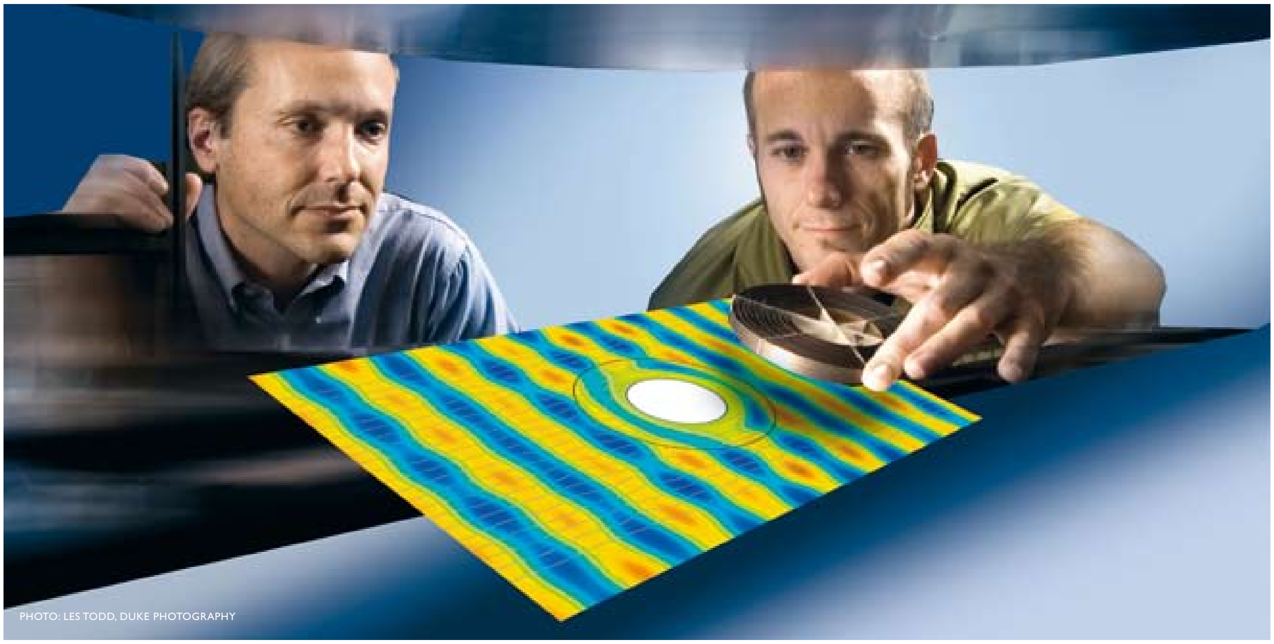


PHOTO: LES TODD, DUKE PHOTOGRAPHY

The author, Steve Cummer (left), and his colleague, David Schurig (right), both from Duke University, Durham, NC.

waves such that the shell and any object placed in the interior would be effectively invisible. The required electromagnetic properties of the shell are not of the sort found in natural materials, and as recently as a decade ago it would not have been feasible to make such a material. But our knowledge of how to engineer materials with specific and complex electromagnetic properties has increased dramatically in that time. We now understand how to create “metamaterials” composed of metallic structures that behave as if they were continuous materials with permittivity, ε, and permeability, μ, that can vary with direction and position and can even be negative.

We chose COMSOL because it is likely the only commercial simulation tool that enables the user to specify the shell’s unusual electromagnetic properties.

Early efforts at creating these materials, however, were unsuccessful because of the delicate sensitivities involved. If a process did not create a material with exactly the correct properties with almost no variation from the ideal, that material was not useful at all. We started asking ourselves if our approach was similar to “trying to balance on the head of a pin” or was it a bit more forgiving? How difficult is it to actually build the desired material successfully? And finally, if we could not meet specifications for the material in software, was this idea really practical?

Numerical simulations are an excellent tool for exploring these questions because material imperfections, like those that are unavoidable in any real experiment, can easily be included. If we could simulate the ideal and non-ideal conditions successfully in COMSOL Multiphysics, then we would have some hope of being able to demonstrate cloaking in an experiment.

The geometry of the COMSOL Multiphysics simulation is simple (Figure 1). Using the RF Module, we solved the 2D cylindrical problem in which a perfect electrical conductor (PEC) infinite circular cylinder is wrapped by a cloaking shell. The PEC shell is a strong reflector of electromagnetic energy, and we wish to mask this scattering in all directions. On the left and right sides are regions of perfectly matched layers (PMLs), which simulate the infinite domain in which the system resides. A uniform plane wave is launched by a sheet of uniform current density near the left edge of the domain. The top and bottom boundaries are perfect magnetic conductors (PMCs) so that a uniform plane wave with its electric field pointed out of the page can terminate without reflection on these edges. The model uses the RF Module’s In Plane Hybrid-Mode Waves application mode so that all possible reflected fields are accounted for.

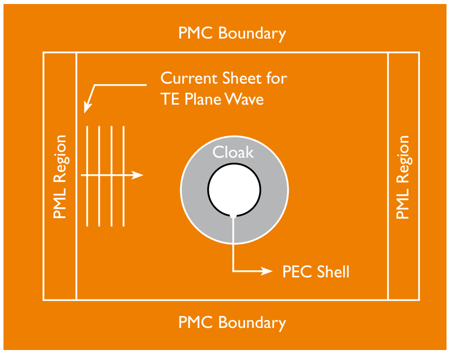


Figure 1: Computational domain and boundary conditions for the full-wave cloaking simulation. The PEC (perfect electrical conductor) has a diameter of 0.2 m, which is 1.33 wavelengths of the incident 2-GHz transverse electric (TE) polarized time-harmonic uniform plane wave.

Note that this model does not simulate the metamaterial’s fine structure. Instead we simulate

AUTHOR’S BIOGRAPHY

Steve Cummer is an Associate Professor in the Department of Electrical and Computer Engineering at Duke University’s Pratt School of Engineering. His research focuses on electromagnetic wave propagation in complex materials and presently includes design and measurement of engineered electromagnetic materials and geophysical remote sensing with low-frequency radio waves.

continuous materials that for this application are anisotropic and smoothly inhomogeneous. The next step is determining how to design the structures like SRRs (split-ring resonators) that approximate the desired continuous material properties. Once we get the desired properties from one unit cell, we fabricate many of them and hopefully get the right bulk properties.

Figure 2a shows the resulting fields for the ideal cloaking shell that has continuously variable permittivity and permeability prescribed by the original theory as modeled in COMSOL Multiphysics. As it travels from left to right, the plane wave is smoothly deformed by the cloaking shell much like river water flowing around a rock. The wave exits the shell looking exactly as it would if there were no object at all. An observer on the right side would thus see only the undisturbed wave, rendering the scattering object transparent and effectively invisible.

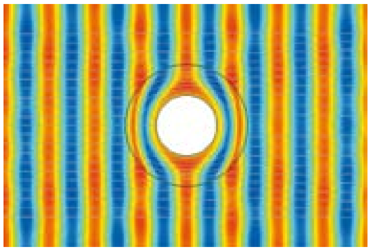


Figure 2a: Ideal parameters

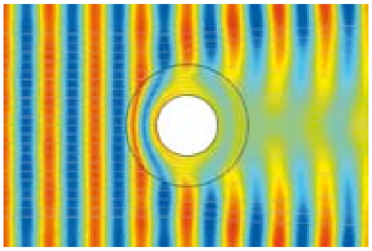


Figure 2b: Ideal parameters with loss

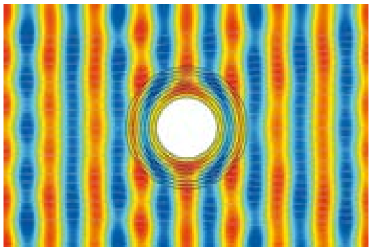


Figure 2c: 8-layer stepwise approximation

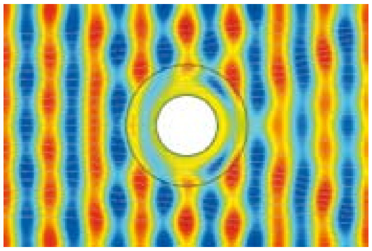


Figure 2d: Reduced material parameters

A continuous anisotropic material

For this simulation we chose COMSOL because it is likely the only commercial simulation tool that enables the user to specify the unusual electromagnetic properties of the shell. Specifically, the shell in our theoretical electromagnetic cloak has highly anisotropic properties that vary smoothly and continuously. Implementing this was straightforward using COMSOL, and to our knowledge, no other commercial products offer this flexibility in specifying a material.

A first simulation (Figure 2a) confirmed that an ideal material would work, so our next step was to see the effects of adding energy absorption as is expected in real-world materials. The use of such absorption had made previous attempts to simulate or realize other metamaterial applications fail. We added substantial energy absorption to the shell's permittivity and permeability, and the resulting simulation (Figure 2b) shows that the cloaking effect does not fall apart in the face of losses. The object would now cast a shadow because the incident electromagnetic power is partially absorbed before it can exit the shell, but the wave is otherwise undisturbed and thus the object does not reflect in any other direction.

Figure 3: The 2D cloaking structure where the electromagnetic radiation is limited to the x-y plane. An object located in the center of this structure is almost invisible to microwave radiation in a narrow range of frequencies. (photo: Smith, Schurig, Pendry, and Cummer, *Science*)

Our next challenge addresses our present inability to build continuously variable metamaterials. Instead, we must approximate one with discrete layers. What happens if we approximate the material with eight discrete homogeneous cylindrical layers? A simulation (Figure 2c) shows that the cloaking effect, while not perfect, is still evident. Finally, it is difficult to control all three of the key electromagnetic parameters in a fabricated metamaterial at one time. Would it be possible to hold one or two constant, vary only one, and still get reasonable results? Figure 2d shows the field distribution when the cloaking shell is composed of a simplified material in which only the radial component of permeability is spatially varying. Although there is considerable scattering, the smooth deformation of the wave fronts still shows the cloaking principle at work.

We next fabricated an 8-layer metamaterial structure with the simplified cloaking shell parameters described earlier (Figure 3). We simulated exactly what we built, and the experimentally measured fields were in almost exact agreement with the COMSOL-simulated fields. ■

VISIT THE RESEARCH WEBSITE AT:
www.ee.duke.edu/~drsmith

To find out more about metamaterials and the emerging field of plasmonics read:
"The Promise of Plasmonics", by Harry A. Atwater; Scientific American, April 2007

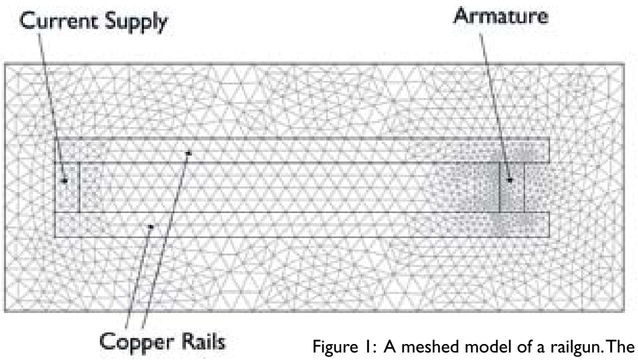


Figure 1: A meshed model of a railgun. The power supply on the left provides a current pulse to the parallel rails, and the armature (projectile) completes the circuit.

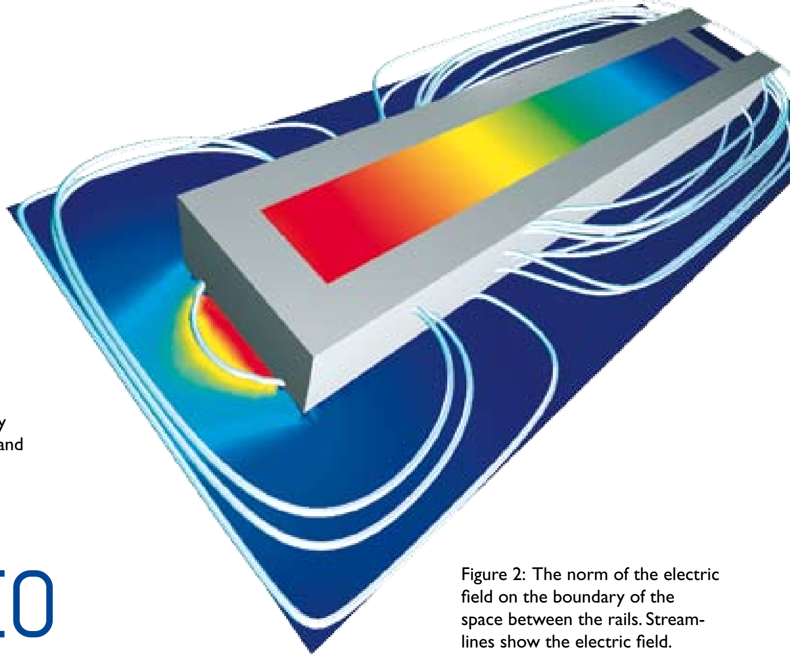


Figure 2: The norm of the electric field on the boundary of the space between the rails. Streamlines show the electric field.

A new approach to railgun operation

A DISCUSSION WITH DR. PAUL J. COTE, BENET LABORATORIES, US ARMY RESEARCH

Railguns—which propel a projectile using electromagnetic forces instead of chemical explosions—promise to revolutionize projectile launchers. Compared to conventional guns, they can double muzzle velocities and thus increase firing ranges with less drift. Such guns have been built and operated successfully on a test basis, but several problems are holding them back from usage in the field. To solve these problems, researchers must understand the inner workings of these weapons, and a group at the US Army Research Engineering and Development Command, Watervliet, NY, is using COMSOL Multiphysics to do so.

In a railgun, a power supply creates a voltage across two parallel conductive rails, and a conductive projectile, called the armature, touches each rail to complete the circuit path (Figure 1). A voltage pulse creates a very high current, and the resulting magnetic field accelerates the projectile along the rails and then out the muzzle. Typical peak currents in large systems can exceed 1000 kA.

This current, however, creates problems, especially along the rails, which are prone to considerable erosion due to the high heat generated by the current and also the propulsion of the armature. Another source of rail damage is the transition of the armature conductive interface from a molten layer to a high temperature plasma-brush interface. Railguns today require that the rails be replaced frequently, which limits their effective use as standard weapons.

How are the EM fields generated?

Considerable research is required to find the best materials and design for effective railguns. But how, exactly, are the electromagnetic fields generated, and what is their distribution? A new approach to railgun analysis proposes local flux creation as the source of the EMF associated with armature motion. As the armature moves, the space behind it is continually filled with new flux, so the induced EMF exists in the immediate vicinity of the armature so that potentially damaging high fields exist along most of the length of the railgun. The design team turned to COMSOL Multiphysics to get some insight into the problem, and they found that the modeling results offer an understanding of previously unexplained phenomena (Figure 2).

With these multiphysics models the research team made two discoveries. First, they demonstrated that the transmission-line equation applies to railguns. Second, with the model they also showed that local flux creation can have a profound effect on current distribution in and around the armature. ■

READ THE RESEARCH PAPER AT:
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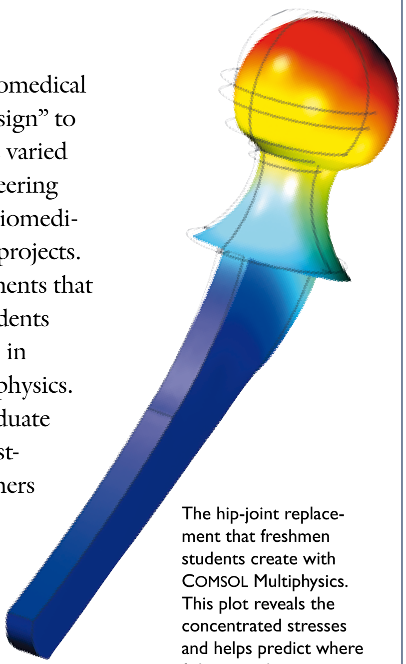
From left to right, Drs. Krystyna Truszkowska, Paul Cote, and Mark Johnson inspect the damage on the armature after a test firing of the subscale launcher.

Biomedical Engineering and Multiphysics: Joined at the Hip

"Traditional" engineering curricula teach foundational principles based on either technical or thematic disciplines, but newer fields such as biomedical engineering are interdisciplinary. Students must become familiar with basic principles in many topics. In this sense, biomedical engineering is an excellent example of a multiphysics application, and innovative educators are turning to software such as COMSOL Multiphysics for everything from entry-level courses to post-doctoral research

A striking example comes from Dr. Richard T. Hart, the Edgar C. Hendrickson Chair of the Biomedical Engineering Department at Ohio State University. Previously, when at Tulane University in New Orleans, he had taught freshmen "Elements of Biomedical Engineering Design" to introduce all the varied aspects of engineering that enter into biomedical-engineering projects. He gave assignments that required the students to create models in COMSOL Multiphysics. In addition, graduate students and post-doctoral researchers working under Dr. Hart used the software to find new knowledge about how bones react to physical stress and other stimuli.

"I discovered COMSOL Multiphysics just a few years ago, and I was struck by how cool it would be to have a biomedical finite element course that could incorporate not only structural aspects but also thermal, electromagnetic, and other physics. I've never known a program that is so powerful and intuitive at the same time," which made it a perfect candidate for classroom use as well as for research assignments. ■



The hip-joint replacement that freshmen students create with COMSOL Multiphysics. This plot reveals the concentrated stresses and helps predict where failures might appear.

Professor Richard Hart (middle) discusses the simulation of a hip replacement with two undergrad members of the "BoneHead Lab," Apu Borcar (left) and Katie Nobes (right).

READ THE RESEARCH PAPER AT: www.comsol.com/academic/papers/1028

International Congress on Industrial and Applied Mathematics

Considered the most important event in its field worldwide, the International Congress on Industrial and Applied Mathematics (ICIAM) is held every four years. It covers new developments and applications of mathematics in industry and science. It brings together several thousand attendees from around the globe including those who will shape the development of this discipline in coming years.

ICIAM 2007 takes place in Zurich, Switzerland from July 16 to 20, 2007. The program consists of 27 invited lectures; 300 mini-symposia with 1700 talks; an additional 1150 contributed talks; and 130 posters. Accompanying this is a commercial exhibition including COMSOL, which will conduct a week of workshops and sessions dedicated to multiphysics modeling. ■

For additional information about this conference, go to www.iciam07.ch.

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Dahlquist Research Fellowship makes its debut

The first winner of the Dahlquist Research Fellowship is Raul Tempone, an assistant professor at the School of Computational Science at Florida State University.

The award recognizes "his important contributions to the field of numerical approximation of deterministic and stochastic differential equations. In particular his innovative results on a posteriori error estimates and adaptive techniques for stochastic differential equations are leading the international development." The prize consists of a year of full-time research at the department of Numerical Analysis, The Royal Institute of Technology (KTH) in Stockholm.

This fellowship is named in honor of professor Germund Dahlquist (1925–2005), an internationally recognized mathematician and numerical analyst who spent most of his career at KTH. There he founded the Department of Numerical Analysis and Computer Science (NADA), built a broad scientific research and educational program, and wrote the textbook *Numerical Methods*, which was the standard reference for many years. The fellowship is financed by KTH and COMSOL, which has a special connection with Dahlquist, who encouraged a couple of his students to start the company. ■

Continued from page 32

develop all sorts of better high-tech products, such as making cars more fuel efficient and safer.

All this would be impossible without the speedy implementation of novel algorithms. One good example is the PARDISO solver for shared-memory multiprocessors, developed in a PhD project at ETH Zurich just a few years ago. Today it is an integral part of COMSOL Multiphysics. In the near future even laptop PCs will have multiple processors, and so that engineers can take advantage of them, many new algorithms will appear or have to be rewritten.

Meanwhile, fundamental research is tackling even more complex problems. For instance, my colleagues are investigating simulations for high-current arc plasmas. On the algorithm front we are studying better finite-element methods, meshing, linear algebra, and stochastic differential equations. In particular, with algorithms we are focusing on "breaking the curse of dimensionality" such as in sparse tensor product methods for radiative transfer. In order to solve ever more demanding problems, a key feature seems to be the development of algorithms focusing on the reduction of complexity. We have seen enormous progress here recently, but it will not be simple to put them into practice for 3D engineering problems.

Going after the big problems

With large memory, high computational speeds, and new algorithms we can approach problems much larger and more complex than ever before. It's even possible today to model the world's climate with a crude model. Yet there is a long way to bring such models to perfection. As for other fields, we have started modeling in nanotechnology, biology, and medicine. Biomolecular simulations still need an increase in computer power, memory, and algorithm speed. In engineering, new algorithms must be developed; for instance, for high-current switches where there is still no off-the-shelf software and in fact even the physical model is not quite clear.

All these application areas are so complex that mathematicians can no longer prove convergence and we need techniques to convince ourselves of the validity of the calculations. In our project on magnetohydrodynamic (MHD) solvers in real 3D geometries we are trying to test the quality of methods, such as Riemann solvers, and programs through the development of multidimensional test examples.

I look forward with fascination to the new problems that challenge us on the research front. To get a taste of where research in algorithms and numerics is heading, I invite you to attend ICIAM 07, being held from July 16-20 in Zurich, Switzerland. We meet only every four years, and I promise that this year's event will have plenty of excitement and stimulating discussions. ■

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COMSOL NEWS

GUEST EDITORIAL

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Simulations tackle ever more complex problems

In 1949, Professor Stiefel—my "academic grandfather" and founder of the Seminar for Applied Mathematics—rented the Zuse Z4 for complex calculations. It used 2200 relays and a mechanical memory of 64 words. He first used this machine to solve a 4th-order partial differential equation related to the damming of a water reservoir and to solve a system of eight ordinary differential equations to calculate rocket flight. But it was also this machine for which Stiefel developed the conjugate gradient method, and Rutishauser was led through numerical experiments for stability analysis of linear multistep methods.

Computers developed quickly, and research has meanwhile concentrated on developing fast, reliable algorithms for basic numerical problems such as solving systems of ODEs along with quadrature, linear system, and eigenvalue problems. Those early days saw the creation of perfectly coded algorithms. They were originally written in Algol, but in the 70s they were converted into FORTRAN and extended to become EISPACK and LINPACK.

Enter: easy-to-use software

The 90s saw the emergence of easy-to-use software such as COMSOL Multiphysics, which could be used in standard situations by engineers at least for problems that could be mathematically well described.

In the meantime, computers have increased their speed dramatically. While the Z4 needed 0.5 s for an addition operation and 6 s for a division operation, the fastest computer today produces 367 teraFLOPS, which is $2*10^{12}$ faster. As for memory, when I asked for 4 GB in 1990, the device that ETH installed was a 1.20 meter cube in an air-conditioned room—and today memory sticks have the same capacity.

These developments have brought the ability to solve engineering problems of high complexity. You are no longer limited to computing just a simple flow, but a simulation today can deal with, for instance, chemical reactions in combustion. With tools such as COMSOL Multiphysics, engineers can

Continued on page 31

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