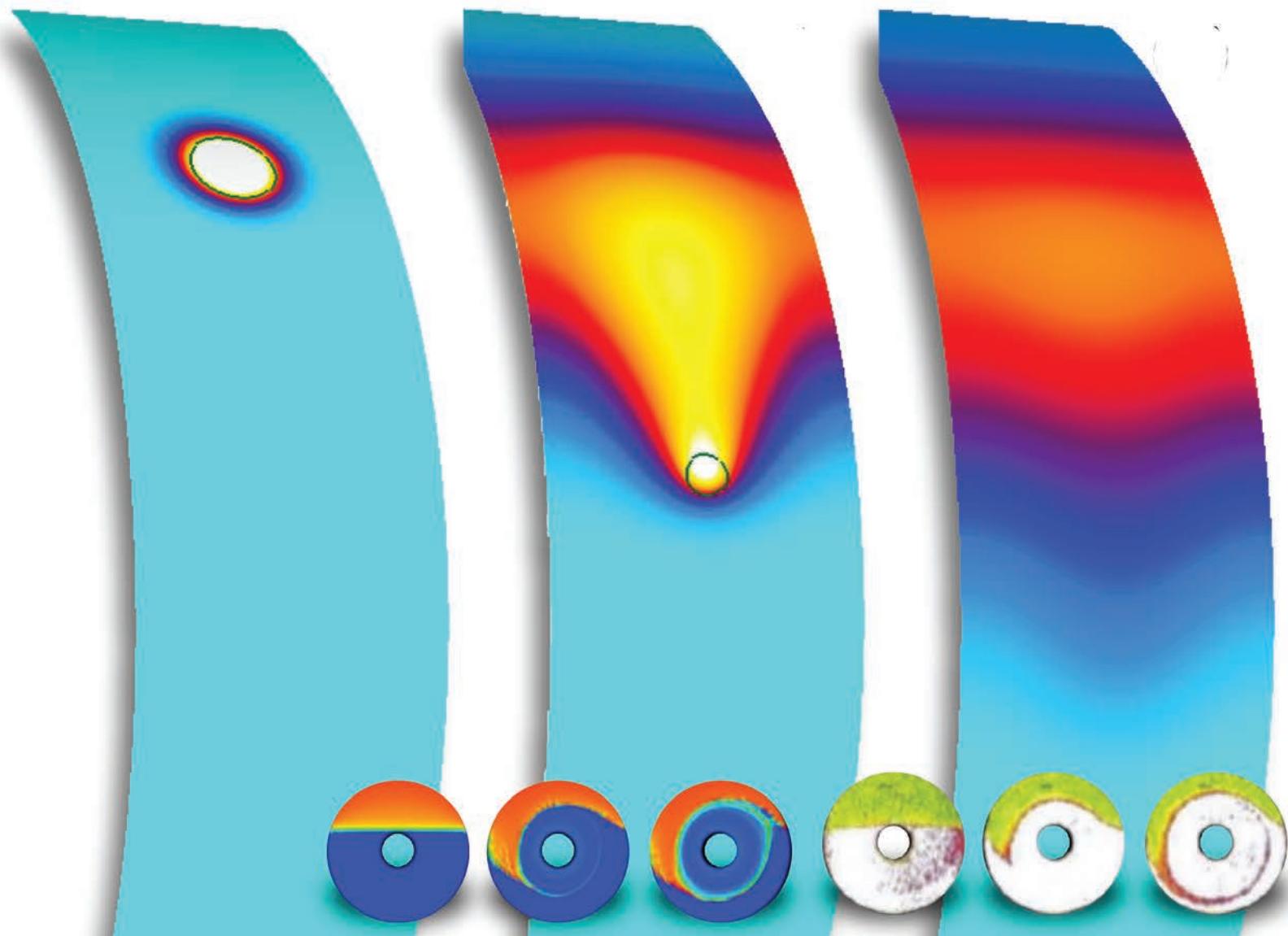


# GOMA

An Open-Source Multiphysics Software Package



*Exceptional service in the national interest*





**Cover Art:**  
**Top:** The Goma logo created from a multiphysics simulation of fluid flow past heated letters.

**Middle:** The flow of a droplet down a thin porous substrate modeled as a curved shell.

**Bottom:** Goma 6.0 simulation of viscous resuspension of particles in a couette geometry compared to NMR data.

For associated video,  
[CLICK HERE](#)

## 1. General Entry Information

### A. Product Name

GOMA 6.0

### Name of Submitting Organization:

Sandia National Laboratories (SNL), Albuquerque, NM 87185

### B. Short Description of the Product

Goma 6.0 is an open-source, parallel, and scalable multiphysics software package for modeling and simulation of real-life physical processes, with a basis in computational fluid dynamics for problems with evolving geometry. It solves problems in all branches of mechanics, including fluids, solids, and thermal analysis. Goma 6.0 uses advanced numerical methods, focusing on the low-speed flow regime with coupled phenomena for manufacturing and performance applications. It also provides a flexible software development environment for specialty physics. Goma 6.0 is being used to reduce process-development time, understand fundamental processes, and to educate the next generation of computational mechanics experts.

### C. Product Photo

The screenshot shows the Eclipse IDE interface with three main panes:

- Left pane:** Shows the source code for `mm_lll_shell.c`. The code is a C program containing various meshing and simulation logic, including loops for element types and material properties.
- Middle pane:** Shows the terminal output of the code execution. It includes error messages like "No search results available. Start a search from the search dialog.", command-line arguments, and numerical results such as "Number of unknowns = 9610" and "Number of matrix nonzeros = 62956".
- Right pane:** Shows the Project Explorer view, listing various source files for the Goma 6.0 project, including `mm_lll_shell.c`, `mm_input_bc.c`, `mm_input_bc.h`, `mm_input_mp.c`, `mm_input_mp.h`, `mm_input_particles.c`, `mm_input_particles.h`, `mm_input_ud.c`, `mm_input_ud.h`, and `mm_interface.c`.

Figure 1. A screen shot of Goma 6.0 showing the listing of source files, output from running the code, and details of the C code for the parser.

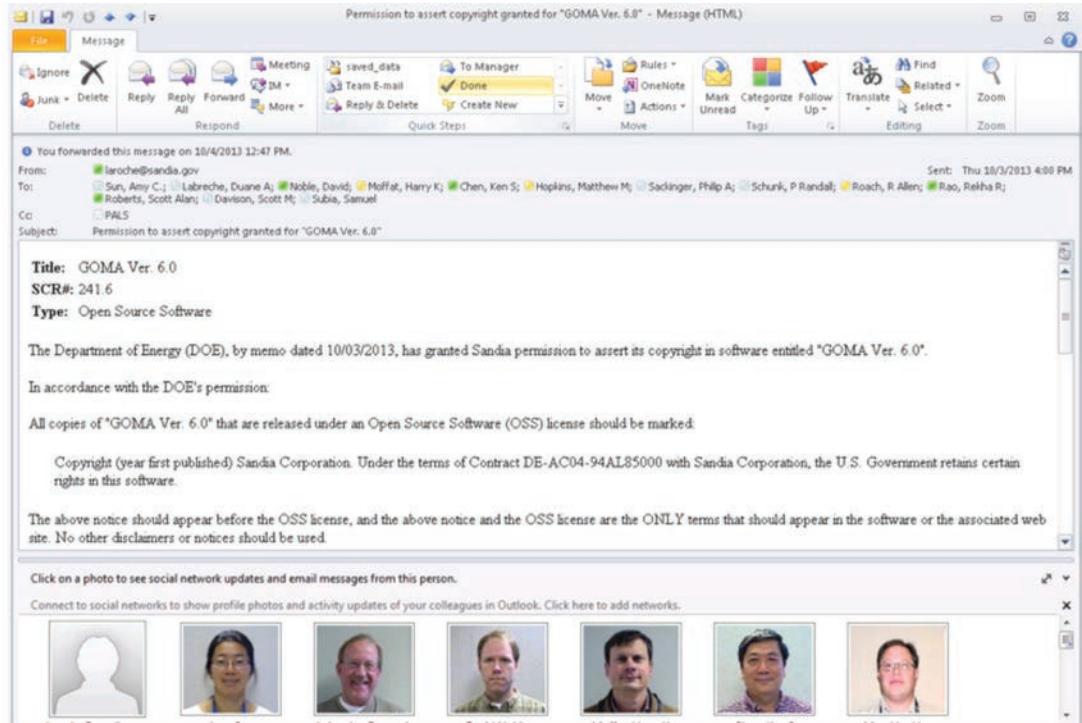
*Goma 6.0 solves the fundamental equations of mass, momentum, energy, and chemical species transport using the finite-element method.*

## D. Price in U.S. Dollars

Goma 6.0 is freely available as open-source software to interested parties. The open-source website address is <https://goma.github.io/>.

## E. Release date for Goma 6.0

The email image below provides evidence that Goma 6.0 was released as open-source software on October 13, 2013.



## 2. Product Description

### A. What does Goma 6.0 do? What are Goma's principal applications?

Goma 6.0 is software for numerical simulation of multiphysics continuum processes, including moving geometry, phase-change, fluid-structural interactions, complex rheology, and chemical reactions. It solves the fundamental equations of mass, momentum, energy, and chemical species transport using the finite-element method.

Goma 6.0 has been applied to manufacturing process design and device-performance within the national laboratory system and in industry. Specific examples include flat-panel glass processing at Corning, composites such as 3M® Aluminum Conductor Composite Reinforced materials for power lines, and porous-adsorbent media applications at Procter & Gamble. At SNL, applications range from coating and drying, to polymer processing and joining processes.

## B. How Goma 6.0 benefits the market it serves

Goma combines the merits of a production-level modeling and simulation tool including extensive documentation, training materials, and software quality control, with the flexibility of a highly adaptable software package ideal for physics/capability prototyping, research, and education.

Though commercial and open source codes are available,

The partnership with Sandia and access to their world-class modeling and simulation tools, in particular Goma 6.0, have been a great resource; helping us tackle multiple technical challenges across our business.

– Dr. Ken Comer, Senior Engineer, Procter & Gamble, Research and Development

Goma 6.0 offers greater ease and agility for adding new features and physics. Goma brings many novel, currently unavailable capabilities to the market. This is particularly the case in manufacturing, where guidance and development from industry partners has contributed to unique strengths in Goma's algorithms. Most importantly, Goma 6.0 possesses special advanced capabilities that aid the analyst in predicting product quality and process operability, which can significantly reduce time-to-market for a new product or decrease operating costs for a new process.

Because of Goma's great extensibility and source code availability, it is an ideal platform for graduate students to learn numerical methods and the benefits of code development for research. Because the source code can be modified, Goma 6.0 will help create the next generation of computational fluid dynamics (CFD) experts through this hands-on development process. Writing Goma software and analyzing it for a new application gives real-world experience and grows CFD expertise.

### *3. Technology Description*

#### A. How does Goma 6.0 operate?

Goma 6.0 solves problems from all branches of mechanics, including fluid mechanics, solid mechanics, chemical reactions and mass transport, and energy transport. The conservation principles for momentum, mass, species, and energy, together with material constitutive relations, can be described by partial differential equations. The equations are made discrete for solution on a digital computer with the finite element method in space and the finite difference method in time. The resulting nonlinear, time-dependent, algebraic equations are solved with a full Newton-Raphson method. The linearized equations are solved with direct or Krylov-based iterative solvers. The simulations can be run on a single processor or on multiple processors in parallel using domain decomposition, which can greatly speed up engineering analysis.

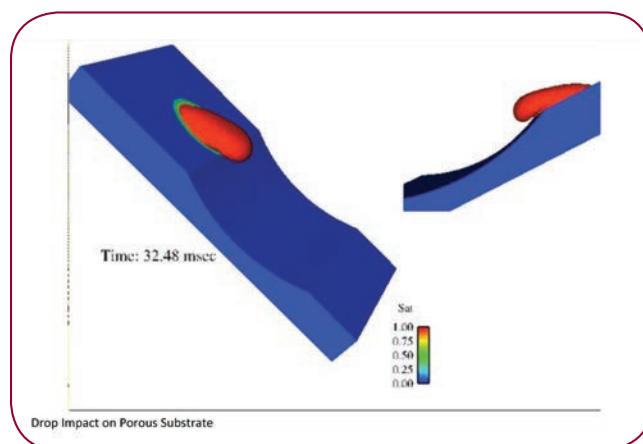
*A novel algorithm for mesh motion is at the heart of Goma, where boundary motion is accommodated by allowing mesh nodes to move as if they were a pseudo-solid rubbery material. This is where Goma gets its name, which means “rubber elasticity” in Spanish.*

Goma is designed as a general mechanics code, with no features that tie it to any particular application. Applications, or problems to be solved, are specified completely in input files, which include code and material properties specifications. The multitude of differential equations, material constitutive equations, and boundary conditions has evolved with the applications, but they are all from theories fully published in the open literature and Goma's theory manual.

Although many of Goma's applications involve fixed boundaries, Goma really stands out when applied to problems with dynamic geometries, i.e. free and moving boundaries. A novel algorithm for mesh motion is at the heart of Goma, where boundary motion is accommodated by allowing mesh nodes to move as if they were a pseudo-solid rubbery material. This is where Goma gets its name, which means “rubber elasticity” in Spanish. From the principles of kinematics, this algorithm can be applied to either fluid- or solid-material regions or to problems of fluid-structure interactions. The problem can be Lagrangian, meaning that the mesh moves with the material, or Arbitrary Lagrangian Eulerian, meaning that in some places the mesh moves with the material and in others it does not. Goma 6.0 also includes purely Eulerian boundary tracking methods on stationary meshes, using either the level set or the overset-grid methods.

Making better plastic wrap is a multiphysics application involving a complex interplay between energy, fluid flow, melting and unknown free surface location for which Goma 6.0 is perfectly suited. An analyst would begin the problem by

creating a mesh representing the extruder for plastic wrap production. The material melts downstream and is pushed through a thin die into the open air, forming a sheet. The sheet is pulled out of the extruder, much like plastic wrap is pulled from a box. If pulled too fast, the sheet can break; too slow and the sheet could be too thick or it could



*Drop impacting porous substrate (e.g. Ink drop on paper)*

fold over itself. The thickness of the sheet is determined by a nonlinear interaction between the temperature-dependent plastic properties, the die shape and the

tensioning of the sheet. Goma could be used to predict the sheet thickness as a function of the die shape, system temperatures, plastic viscosity, and sheet tension. A successful product must be transparent and not suffer from crystallization. It needs to be the same thickness everywhere, without lumps and bumps. It needs to be strong, but not so strong that it cannot be cut. Goma 6.0 can be used to predict the final properties of the plastic wrap, given the operating conditions. It can also be used to optimize the process by determining the right temperature, flow rate, die design and web tension to make clear, perfect, plastic wrap with a constant thickness. An example of mesh motion in Goma is shown in Figure 2 where the initial mesh is undeformed and shown in the top figure. The bottom figure give the result from a Goma 6.0 simulation, showing the thinning of the free surface as it leaves the extruder.

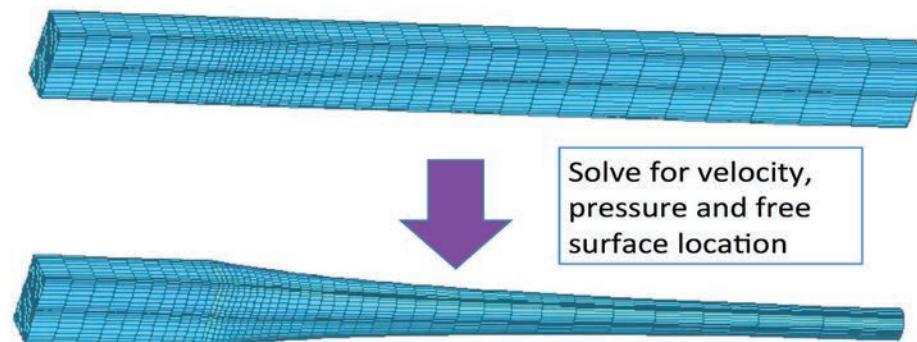
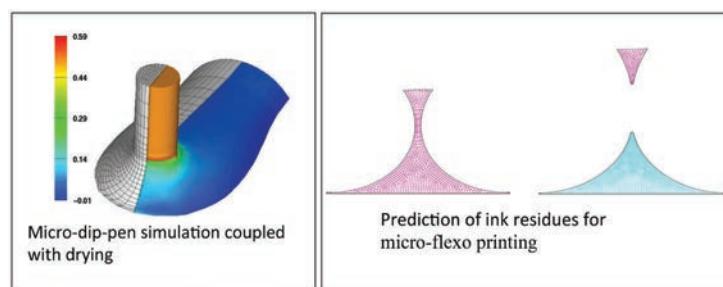


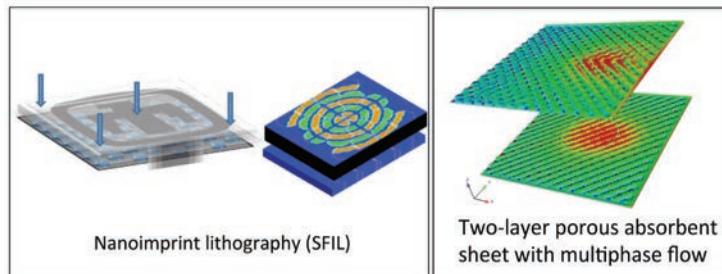
Figure 2: Mesh motion for an extrusion flow similar to plastic wrap formation. The top image is the undeformed mesh and the bottom image is the solution to the extrusion problem.

Goma's significant capabilities include:

- Unprecedented flexibility for mixing and matching physics and physical-chemical interactions between material domains. Prototypical Goma 6.0 applications are direct-numerical simulation of a liquid drop impacting a porous substrate or deposition and drying of polymeric and sol-gel coating solutions. These are processes common in the ink-jet printing and adhesive/decorative coating technologies.

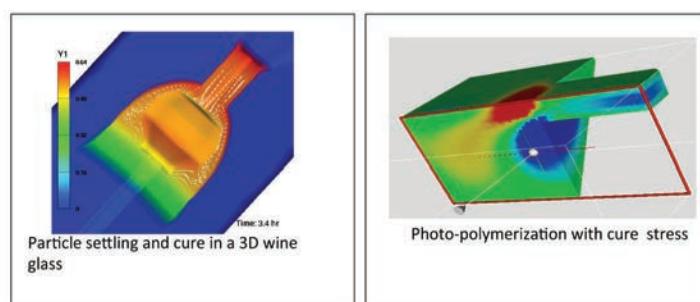


- Fully-coupled thin-region shell-element capability for fluids, structures (beam, bar, membrane elements), and other surface mechanics and transport (heat transport, surface species). Applications include machine lubrication design, thin film wiping flows (painting, doctoring), and laser-surface processing and

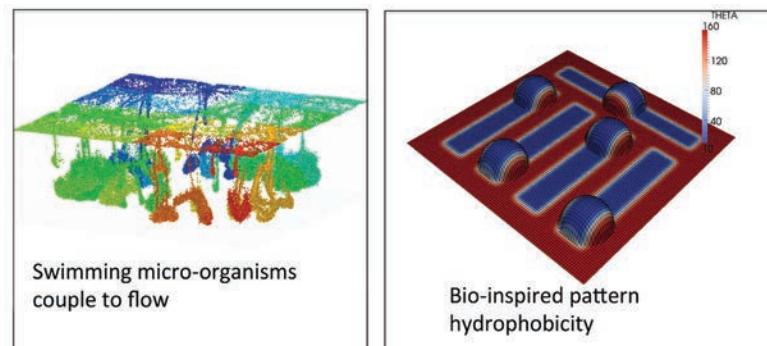


heat treatment.

- Fully-coupled porous-media transport capability, with multi-region porous-continuum compatibility.
- Complex rheology including yield stress, shear thinning, and viscoelastic fluids with thermal or chemical-dependent properties. Modeling the rheology of particle-filled polymers is one of Goma's strengths.



- Solid material models for complex behavior including elasto-viscoplasticity and nonlinear Hookean response.
- Extensive diffusion/reaction models for electrochemical processes (corrosion, battery performance, electroplating, etc.).
- Bio-inspired applications for particle-phase including independent motion from the bulk fluid to hydrophobicity similar to lily pads.



Pattern-to-mesh capability to incorporate microstructure

*Goma has been identified as the only viable option to simulate nanoimprint lithography, which involves multiphase flow, fluid-solid interactions, strong capillary forces and disparate length and time scales.*

- Advanced capabilities allowing for easy implementation of design constraints (augmenting conditions based on any combination of fluxes, forces, primitive variables), sensitivity analysis, operating window calculation (linear stability analysis and automated multi-parameter continuation), and pixel/voxel-to-mesh translators.

All these and more capabilities are integrated in Goma's fully coupled finite element framework. This gives rise to a sparse matrix, which must be inverted at each time-step or Newton iteration. Goma relies on the solver packages Trilinos 10.0, UMFPACK 5.0 or Sparse 3.1 to solve the matrix equations. The format of the mesh and unknowns is stored in the Sandia National Laboratories Exodus II format. Mesh generators compatible with Exodus II include CUBIT, Patran and Solidworks. Visualization packages compatible with Goma 6.0 and Exodus II include SEAMS (Sandia Engineering Analysis Mechanics System) Blot, Ensight 10, VisIt, Tecplot, and ParaView.

Goma 6.0 is primarily developed in Red Hat 6.0 Linux but can be readily ported to other Unix environments. A Mac OS 10 port also exists, and although Goma 6.0 has not been ported to Windows, it can be run on Windows via a Unix emulator. The source code for Goma 6.0 is written in C, but has some C++ and FORTRAN dependencies. It can be run in serial or parallel modes, with OpenMPI used for parallel computation. Compilation involves a simple “makefile” with dependencies on required open-source third-party libraries.

- Exodus II V2
- NetCDF
- Trilinos 10.0
- UMFPACK 3.2
- Sparse 1.3
- BLAS, ARPACK – Eigensolver, an optional package, can be added for solving Eigenvalue problems

## B. Describe the key innovations of Goma 6.0 and the supporting scientific theories.

### Key innovations:

Goma 6.0's key innovations lie in its flexibility and extensibility to add specialty physics models quickly and efficiently. This allows the user community to conduct research or address novel processes or application areas with a short turnaround time. It has a rare combination of features for an open source multiphysics modeling platform; it is an agile development platform with readable code, while still retaining production features. For instance, Goma has been identified

*Through open sourcing Goma 6.0 we plan to help create the next generation of computational fluid dynamics experts using a hands-on development process.*

as the only viable option to simulate nanoimprint lithography, which involves multiphase flow, fluid-solid interactions, strong capillary forces and disparate length and time scales. Describing any two of these aspects is computationally challenging and provides a testament to the flexibility and robustness of Goma in handling all four of them accurately and efficiently. At Procter & Gamble, Goma 6.0 has been used to “shorten development time, increase process stability, and drive fundamental understanding of complex interacting phenomena.” Additional state-of-the-art algorithms include porous shell equations for reduced order models, hysteresis for unsaturated porous media, suspension models with shear-induced motion and buoyancy, etc.

Goma can solve many generic steady or time-dependent partial differential equations, but primarily focuses on those derived from applied mechanics fields, specifically incompressible flow, nonlinear elasticity, energy transport, and convection-diffusion-reaction equations. Goma has a unique capability of solving all of these equations in a Lagrangian, Eulerian, or combined frame of reference, and hence is able to track free and moving boundaries readily. An extensive documentation system includes input, theory and advanced capability manuals in addition to tutorials, reports, and journal articles. Many of Goma’s algorithms, available in the literature or source code, have been adopted by other research and commercial codes, demonstrating the power of the methods developed here. Through open sourcing Goma 6.0 we plan to help create the next generation of computational fluid dynamics (CFD) experts using a hands-on development process.

#### 4. Product Comparison

##### A. List your product’s competitors by manufacturer, brand name, and model number.

As of 2014, over 30 codes were being marketed in the broad category of computational fluid dynamics (CFD) multiphysics software. In this category, the following commercial codes are industry leaders that cover a significant portion of problem types best suited for Goma 6.0 and use similar foundational methods: COMSOL Multiphysics®, FLOW-3D®, and ANSYS® Fluent. COMSOL is most similar to Goma, because it is also of the finite-element type and focuses on low-speed flows and coupled physics.

Of the more than 10 codes in the open source category, OpenFOAM® is the closest competitor. The demand for these codes is extensive and worldwide, which testifies to the demand for Goma 6.0’s technology.

**B. Supply a matrix or table showing how the key features of your product compare to existing products or technologies. Use numerical figures to represent performance metrics. For price, and capital and operating costs, use actual dollar amounts or a relative scale (\$\$, \$\$\$) to show a comparison.**

Feature	COMSOL	OpenFOAM	GOMA 6.0
Availability/cost	\$10k-\$20k per seat, annually depending on modules selected: <ul style="list-style-type: none"> <li>• COMSOL Multiphysics \$9,000 new/\$1,800 renewal</li> <li>• ChemE Module \$4,000new/\$800 renewal</li> <li>• ChemE Module \$4,000new/\$800 renewal</li> <li>• Heat Transfer Module \$4,000new/\$800 renewal</li> <li>• CAD Import Module \$2500new/\$500 renewal</li> </ul>	Open source	Open source
Numerical method	Finite element	Finite volume	Finite element
Massively parallel	No	Yes	Yes
Ease of use	COMSOL is easy to use	OpenFoam takes some CFD expertise to use	Goma takes some CFD expertise to use
Ease of adding new physics	Yes, if the changes fit within the COMSOL framework	Yes, if you don't plan to do the work yourself	Yes
Ease of adding new algorithms	No	No	Yes, Goma is very easy to program in and debug. We expose all of the major algorithm details and how to modify or interoperate with them in a freely available developer's and theory/usage manuals
Teaching tool for training CFD graduate students and researchers	No. New features can be added, but only in the context of the existing framework. Since the source code is not available, it is hard to debug the new feature.	No. Difficult to add a new model or algorithm. Open Foam has a group of people that you can hire to add new capabilities.	Yes. Easy to add new features such as equations and material models. The code is well-documented and includes a developer's manual. Standard software development debugging tools can be used.
Graphic user interface	Yes	No	Yes, but not integrated
Extensive documentation	Yes, but may have to purchase additional licenses.	No	Yes, user's manual, developer's manual, advance capability manual, and tutorial memos and templates.

*Goma is the first general-purpose, finite element, multiphysics mechanics code with production capabilities to be open sourced and freely available.*

### C. Describe how Goma 6.0 improves upon competitive software products.

Goma is the first general-purpose, finite element, multiphysics mechanics code with production capabilities to be open sourced. Because of Goma's use and improvement by more than 10 industrial partners and numerous internal developers, it has achieved high standards of verification, validation, and quality assurance. Goma is a versatile simulation code for free and moving boundary problems, but still possesses the simplicity of a well-documented research code, allowing its use at many universities. Goma has numerous unique capabilities including reduced order modeling, shell-element technology for all branches of mechanics, free surface methods, porous media technology, multimode viscoelasticity, electrochemistry coupling, and more. Several useful capabilities not found in commercial codes include sensitivity analysis, inverse engineering capability, automated continuation, and stability analysis. These capabilities, which accelerate analysis, are not readily available elsewhere.

Currently, Goma is the go-to platform for rapid response modeling activities for a variety of internal and external customers because of its extremely flexible and simple structure. This flexibility makes it ideal for testing and prototyping new algorithms and material models, allowing users to solve unique problems that require rapid development. Goma serves a niche market of those who need to add new physics, equations, and material models to evaluate their process or product. This is not the market served by commercial codes, where the source code is unavailable and is difficult to verify. Every commercial code is missing one or more advanced capabilities that would make them amenable to geometrical or engineering analysis challenges. In addition, Goma takes advantage of parallel processing architectures without extra licensing fees assessed per processor that is often standard practice in commercial codes.

Goma has extensively benefitted manufacturing process design in thin-film coating and related manufacturing industries. Use of Goma has saved Sandia and their Cooperative Research and Development Agreement partners significant costs by decreasing the scope of experiments and has facilitated process improvements unavailable by any other means. Even as a "research class" code, Goma's documentation and tutorial suite is by far its biggest asset, with over 4,000 pages of indexed and cross-referenced documentation including user manuals, tutorials, validation reports, and usage memos.

***Goma 6.0 serves a niche market for those who need to add new physics, equations, and material models to evaluate their process or product. Unlike commercial codes, Goma's source code is available allowing easy exploration of new algorithms, physics, and verification.***

#### D. Describe limitations of your product. What criticisms would your competitors offer?

- Goma 6.0 does not have a graphical user interface (GUI). Though Goma 6.0 is a powerful computational fluid dynamics (CFD) tool and development platform for multiphysics applications, it may not be for everyone. Many users prefer commercial codes with a GUI and built-in pre- and post-processing tools. Meshing and visualization is available through compatible packages, many of which are available for no cost, but no integrated GUI is available.
- Goma 6.0 is a research platform that requires expertise in CFD and numerical methods to use successfully. Our user and developer base is the CFD community that has expertise in transport phenomena and numerical methods, though extensive tutorials and templates exist for new users to get started.
- Goma 6.0 is only available on Linux and Mac platforms. No Windows port is available. Goma 6.0 is being marketed to researchers who are familiar with “makefiles” and Unix software development environments. Goma may not be the best code for users who do not have computer experience.

#### 5. Summary

Goma 6.0 has just been released under an open source license and is the first finite-element code with multiphysics mechanics and production capabilities to be freely available. Goma has been used both as a production modeling tool to improve manufacturing processes and as a research platform to better understand the physical world. Moreover, Goma enjoys two decades of novel-algorithm design, use, and improvement by more than 10 industrial and university partners, helping it achieve high standards of verification, validation, and quality assurance. Goma is a versatile simulation code for free and moving boundary problems peculiar to thin-film manufacturing and polymer processing, but still possesses the simplicity of a well-documented research code with a user/theory and developer’s manual.

Goma 6.0 serves a niche market for those who need to add new physics, equations, and material models to evaluate their process or product. Unlike commercial codes, Goma's source code is available allowing easy exploration of new algorithms, physics, and verification. Additionally, Goma takes advantage of parallel processing architectures without extra licensing fees assessed per processor, which is often standard practice in commercial codes. Through open sourcing Goma, we plan to help create the next-generation of CFD experts through a hands-on development process.

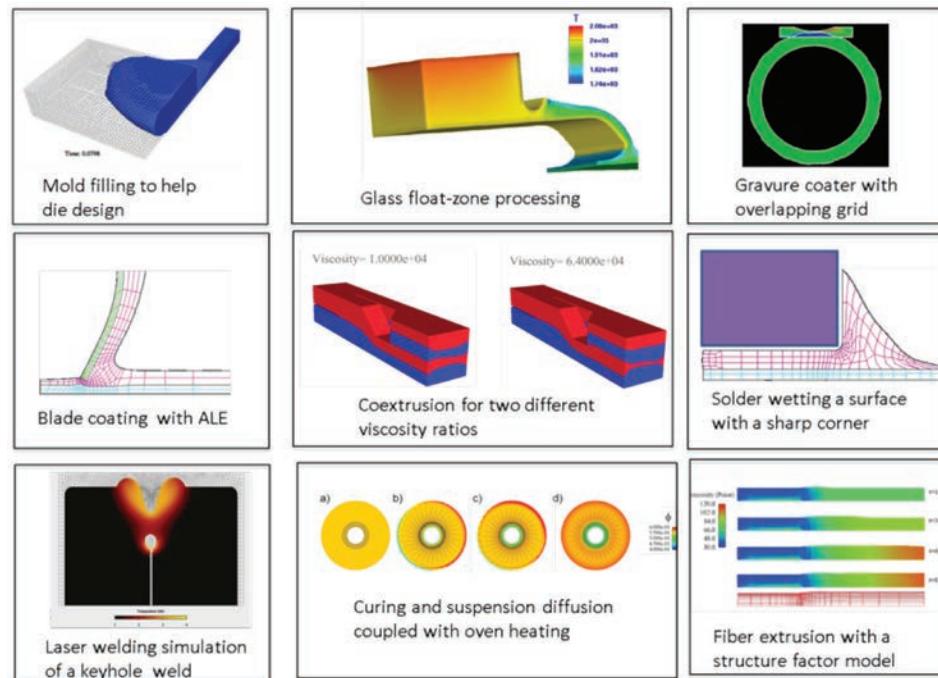


Figure 3. A montage of some Goma 6.0 applications and capabilities.

## 6. Contact Information

Please provide names and contact information (title, organization, phone number, email) for each of the following individual associated with the entry submission:

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For associated video,  
**CLICK HERE**

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### *7. Affirmation*



This entry is a fair and accurate representation of this Goma 6.0

### *8. Acknowledgement*

Many thanks to experimentalist Lisa Mondy (Sandia National Laboratories) and Steve Altobelli (New Mexico Resonance) for their nuclear magnetic resonance imaging of the suspension flow in the couette.

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**Phone:** (505) 272-7551  
**Email:** tjiptowi@unm.edu

**Team Member:** Ed Wilkes  
**Title:** Scientific Computing Consultant  
**Organization:** Prism Software  
**Address:** 24 McKinley Ave, Suite 205, Endicott, NY 13760  
**Phone:** (505) 604-2174  
**Email:** ew86@juno.com

## Appendix B: Letters of Support

**3M General Offices**

3M Center  
St. Paul, MN 55144-1000  
651 733 1110



To: 2013 R&D 100 Award committee

From: Robert B. Secor

Date: March 23, 2014

It is my pleasure to write a letter in support of the R&D 100 Award nomination for Goma 6.0 software. We've been using Goma as an integral tool for advancing manufacturing process technology in precision coating, drying, replication, and other areas for over a decade. Particularly noteworthy is Goma's straightforward customization for emerging physical models and novel conditions which has enabled a greater understanding of ultrasonic, electrostatic, and photo-polymerization processes. Goma also has unique multiphysics capabilities for fluid-structural interactions and valuable methods for representing capillarity in mobile systems and component migration during solidification. The documentation and training provided with the software and the expertise of the developers has been indispensable in equipping analysts with the skills to effectively utilize the software platform.

In summary, the Goma 6.0 software has been a critical component of our computational suite leading to process knowledge creation and we look forward to future collaborations with the open source Goma community.

Sincerely,

Robert B. Secor

Staff Scientist, Modeling & Simulation Group leader  
Precision Coating and Web-Handling Cluster  
Corporate Research Process Laboratory

*Appendix B: Letters of Support (cont.)***CORNING**

**Dr. Gautam Meda**  
Research Director,  
Modeling & Simulation  
Science & Technology

**Corning Incorporated**  
One Riverfront Plaza  
SP-TD-01-01  
Corning NY 14831

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f 607-974-3405  
medag@corning.com  
www.corning.com

February 25, 2014

To: R&D 100 Award Committee  
Re: Nomination of GOMA 6.0 for R&D 100 Award

About 15 years ago, we wanted the capability to accurately simulate flows with large free surfaces. After looking at various options, including the major commercial computational fluid dynamics codes, we decided that GOMA is the most promising option. To gain access to GOMA, we joined a consortium organized by SANDIA. We found GOMA to be top-quality code, with robust numerical algorithms that converge well. We made careful comparisons to experimental results, and found the results from GOMA to be highly accurate. We have used GOMA simulations to gain deeper insight into the physics of precision glass forming, and imbibition-induced distortion of porous ceramics. This insight saved us considerable time and effort in advancing our process technology.

The developers of GOMA were very helpful when we were getting started with GOMA. They supplied several example problems, and made themselves available for consulting about all manner of issues, ranging from trivial questions about input file format to technically deep questions. We were so impressed with GOMA, and with the committed engagement from the developers, that when the original consortium ended, we promptly signed up to join another consortium involving GOMA in a different technical area of interest to Corning. We expect to continue our partnership with SANDIA's GOMA developers for a long time.

Even today, we find that for the most demanding simulations, commercial codes rarely match GOMA in accuracy, robust convergence, or parallel performance. GOMA lets users have full access to its capabilities – and like all truly powerful tools, it requires users to know what they are doing. GOMA's program-drivable interface, which is well-documented and accessible, enables us to automate parametric studies. The interface also allows us to build models like code, so that we can use standard methods for version control of models. We welcome the release of GOMA 6.0 under the GPL. Our past experience with GOMA developers shows that they have the commitment needed to provide the core for forming a vigorous user/developer community.

The performance of GOMA demonstrates that its developers have world-class scholarship in applied mechanics and mathematics. They devised the key numerical algorithms that give GOMA its power and differentiate it from other codes. They set high standards for themselves in implementing and testing the numerical algorithms. To us, GOMA represents the best in class for the complicated multi-physics simulations it is designed for. We strongly support the nomination of GOMA for the prestigious R&D 100 Award.

Dr. Olus Boratav, Research Associate  
Dr. Amy Rovelstad, Research Manager, Materials Modeling  
Dr. Gautam Meda, Research Director, Modeling & Simulation

*Appendix B: Letters of Support (cont.)*

The Procter & Gamble Company  
8611 Beckett Road  
West Chester, Ohio 45069

To: 2013 R&D 100 Award committee

Date: February 21, 2014

From: Tom Lange, Director

It is our pleasure to support the R&D 100 submission for the Goma 6.0 software from Sandia National Labs. As a past winner with Los Alamos National Labs for Reliability Engineering (2003) we believe Sandia has put forward a strong submission. The new open-source Goma 6.0 software provides a unique set of multi-physics capabilities not available in any other package open-source or commercial. The combination of fully coupled fluid/solid solvers for momentum, energy, mass, and chemical species transport with a free-and-moving boundary are well suited to solving complex product and process challenges. The recent public release of Goma along with its extensive documentation and training material will enable broader access both domestically and worldwide and will allow researchers/students/industry to take advantage of a state-of-the-art Multi-Physics computational platform. This broad based access will insure continued advancement and development in future versions of Goma by harnessing the energies of the open source community.

The Goma software has been used at P&G for well over a decade. It has impacted products & manufacturing processes across multiple P&G Business units from Baby Feminine & Family to Personal Grooming and Personal Power. Its strength in the area of thin film mechanics, coating, and absorbency coupled with its flexible/extensible design has allowed us to tackle a number of complex process & product design challenges which require both a robust multi-physics solver and complex material properties. The impact has been to shorten development time, increase process stability and drive fundamental understanding of complex interacting phenomena. With the new Goma 6.0 public release we expect this impact to increase as we can more seamlessly incorporate Goma globally across P&G.

In summary, having been on the Sandia advisory board for 10 years I was able to see the value of Sandia capabilities and development from the Columbia LOM to the Sierra Computational Framework for massively parallel computations, and I believe Goma 6.0 is another example of high quality technical service to the US and broader community.

Sincerely,

Thomas J. Lange

The Procter & Gamble Company  
P&G Modeling and Simulation



The power to transform.

Thomas J. Lange  
Director, R&D, Modeling & Simulation, Global Capability Organization (M&S GCO)

## Appendix B: Letters of Support (cont.)



### COCKRELL SCHOOL OF ENGINEERING Department of Petroleum and Geosystems Engineering

200 E. Dean Keeton, Stop C0300 • Austin, Texas 78712-1585  
CPE 2.502 • 512-471-3161 • FAX 512-471-9605

March 21, 2014

Dr. Rekha Rao and Dr. Randy Schunk  
Engineering Sciences  
Sandia National Laboratories  
Albuquerque, NM 87185-0836

Dear Dr. Rao and Dr. Schunk,

I wanted to offer my enthusiastic support for the nomination of GOMA 6.0 for an R&D 100 award. Since GOMA 6.0 was open-sourced last year, it has made it very easy to collaborate, especially when the collaboration involves foreign national graduate students and post-doctoral appointees. I have been working with Randy and you in conjunction with Professor Roger Bonnecaze for some time. In addition, my student, Ali Afsharpoor, and postdoc, Dr. Peixi Zhu, attended a technical training session on GOMA last year. GOMA has a unique combination of capabilities; it can model steady and time-dependent free-surface flow in very complex geometries, in both two (2D) and three dimensions (3D), together with non-Newtonian rheological models. These rheological models can range in complexity from shear thinning, to yield stress, to fully multi-mode viscoelasticity. It also has excellent training material and documentation for the new user, while being a platform for research.

We recently started using GOMA 6.0 to look at the deformation of a drop of oil embedded in a non-Newtonian fluid traveling through a constriction. We have also chosen to use GOMA 6.0 to perform the CFD simulations in support of an NSF proposal entitled “Pore-Scale Modeling and Microfluidic Experiments of Viscoelastic Flow in Porous Media” that we recently submitted, since GOMA gives us more flexibility to add our specialty models than commercial codes.

Because of GOMA’s parallel capabilities, we are able to utilize our TACC clusters at UT-Austin to make 3D simulations more manageable. Since GOMA is open-source, there is no licensing fee, we do not have a per processor charge on the code usage, and we have access to the source code so that we can customize the code for our problems of interest. Direct Gaussian elimination methods are needed to invert the matrices arising from finite element discretization of viscoelastic flow, but only scale to 6-10 processors. Stabilization methods allowing for matrix inversion using Krylov-based iterative solution of the matrix system, and thus massively parallel simulations, are still an active research issue. We are very interested in collaborating with you on developing advanced numerical methods for speeding up the 3D VE free-surface problems and enabling massively parallel solution methods.

In summary, I think GOMA 6.0 is an exceptional multiphysics software product and I highly recommend that it be considered for an R&D 100 Award.

Sincerely,

Matthew T. Balhoff  
Assistant Professor, Department of Petroleum and Geosystems Engineering  
Anadarko Petroleum Corporation Centennial Fellowship #1 Petroleum Engin  
The University of Texas at Austin  
CPE 4.168A, 200 E. Dean Keaton

*Appendix B: Letters of Support (cont.)***Yale Department of Chemical  
& Environmental Engineering**

PO Box 208286  
New Haven CT 06520-8286  
T 203 432-2222  
F 203 432-4387  
[www.yale.edu](http://www.yale.edu)

*courier*  
Mason Laboratory  
9 Hillhouse Avenue  
New Haven CT 06511

April 9, 2014

Dr. Rekha Rao  
Fluid Sciences and Engineering  
Sandia National Laboratories  
Albuquerque, NM 87108-0836

Dear Rekha,

I wanted to write to strongly support your R&D 100 nomination for Goma 6.0. First, congratulations on the open source release of Goma 6.0. The fact that a multiphysics finite element code like Goma, with its breadth and depth, including advance methods for fluid dynamics and capillary hydrodynamics, is now freely available for collaboration and fundamental research is an impressive accomplishment. As a researcher, I prefer to write my own software rather than using commercial products, because I like to know the details of the algorithms and often wish to include specialty physics models that I have developed myself.

I chose to use Goma 6.0 for my proposed NSF project entitled: “A new coarse grained model for drop breakup.” This work has the goal of developing new, more accurate models for understanding drop-size distribution in immiscible two-phase flows. Emulsions are formed through the application of shear and the evolving drop size distribution is formed by a complex interplay of breakup and coalescence events, both of which are complex and poorly understood. Detailed analyses are available but they are ill suited for simulations of large populations of drops thus coarse grained models are needed. Reliable coarse-grained models for breakup are unavailable. The current models assume that the daughter drops produced by a breakup event scale with the size of the parent drop. Although reasonable sounding, this very basic assumption appears to be incorrect, based on the results of boundary integral simulations that we have performed for drop dynamics in creeping flows. Our simulations indicate that daughter drops actually scale with a critical drop size that is determined by the local flow conditions and the properties of the fluids. The volume of the parent drop determines the number of daughter drop fragments but not their sizes.

The capability of Goma 6.0 to describe drop breakup at arbitrary Reynolds numbers makes it a key tool for our research by extending the range of its applicability beyond the creeping flow regime. “Numerical experiments” with Goma will be carried out on inertial flows of single

## Appendix B: Letters of Support (cont.)

droplets breaking up in fluctuating flow field to determine the daughter drop distribution. This will generate statistics to test the new model, and elucidate any missing physics.

We also plan to advance the computational models of droplet breakup in Goma using three-dimensional arbitrary-Lagrangian Eulerian formulation to predict motion of the droplet interface. Because we use a moving mesh algorithm, with a meshed free surface, we can follow the shape change to the stage of necking that occurs just before breakup. As part of the project, we plan to add an automated approach to handle topology changes for droplet break up. Using Goma 6.0, we will also be able to extend our work to non-Newtonian fluids.

Goma will provide an ideal platform for collaboration since the software can be installed at Yale and I will have access to the source code repository, input files, and extensive documentation and tutorials. I feel that Goma 6.0 will be a valuable teaching tool, giving students the opportunity to learn about software development, the finite element method, and computational mechanics all while carrying out fundamental research. In this way, we hope to develop the next generation of engineers proficient in computational mechanics.

I enthusiastically support Goma 6.0 for an R&D100 award. I believe it to be an essential software product for research such as ours and therefore very deserving of this recognition.

Sincerely,



Michael Loewenberg  
Professor, Chemical Engineering

*Appendix B: Letters of Support (cont.)***Sandia National Laboratories**Operated for the U.S. Department of Energy's  
National Nuclear Security Administration  
by **Sandia Corporation**P.O. Box 5800  
Albuquerque, NM 87185-0836Phone: (505) 844-1994  
Fax: (505) 844-2415  
Internet: [jejohan@sandia.gov](mailto:jejohan@sandia.gov)**Dr. Justine Johannes**  
Director  
Engineering Sciences Center

8 March 2014

**RE: Letter of Support for *Goma* 6.0 for R&D 100 Award**

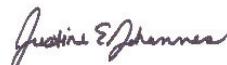
Dear R&amp;D 100 Award Selection Committee:

It is with great enthusiasm that I lend my support for *Goma* 6.0 for a 2014 R&D 100 award. As a former staff member, manager, senior manager and now director of the Engineering Sciences Center I have seen *Goma* evolve to set the standard for computational mechanics software in the area of manufacturing, with particular strengths in free and moving boundary tracking. In my current position, I have responsibility for the majority of Sandia's computational mechanics software platforms and codes, ranging from structural mechanics, structural dynamics, heat transfer, chemically reacting flows, incompressible flows, radiation transport, and more. Our investments in software of this nature are extensive, with over 60 developers (full or part-time) and more than 10 mechanics applications. The novel algorithms and mechanics integration in *Goma* 6.0 developed through a highly motivated and creative research team has laid the foundation for many of these current software platforms. *Goma* 6.0 has also greatly benefited from industrial customer "pull", as I have been personally involved in partnerships with Procter and Gamble, 3M, and Corning which centered around advancing and innovating numerical algorithms for manufacturing.

I am particularly excited that *Goma* 6.0 is now publically available through the GNU public license. One aspect of the underlying strategy of this public release is to foster external collaborations and partnerships with those in the broader computational mechanics community. *Goma* is accompanied by extensive documentation and training materials often not available with open-source software. Its readily adaptable design I am sure will be of great value to the broader community and lead to continued fruitful collaborations with industrial and academic partners.

The numerous open-literature publications and strong, sustained customer pull attest to the novel and unique nature of *Goma* 6.0 and its production quality. I urge the committee to give it strong consideration for the prestigious R&D 100 awards this year, as I am certain *Goma* is worthy.

Sincerely,

Justine Johannes  
Director, Engineering Sciences Center*Exceptional Service in the National Interest*

*Appendix B: Letters of Support (cont.)*

**UNITED STATES DEPARTMENT OF COMMERCE**  
National Institute of Standards and Technology  
Gaithersburg, Maryland 20899

February 27, 2014

Dr. Rekha Rao  
Fluid Sciences and Engineering, 1513  
Sandia National Laboratories  
Albuquerque, NM 87185-0836

Dear Rekha:

It is a great pleasure to write a letter of support for Goma 6.0, the multiphysics finite element software package developed at Sandia National Laboratories which you have now released as open source. I was very excited to hear of this development, the finite element community has long waited something like this!

Truly, the range of problems which Goma can handle is remarkable: complex flows with non-newtonian rheology; free and moving boundary problems; non-isothermal systems; fluid-structure interaction problems; multiphase and multi-component systems; welding/soldering; electrochemical processes. As it exists now, the public is receiving a remarkable tool which will undoubtedly find use in both commercial and research applications. However, the ability to modify code and/or add code in the open source paradigm sets this effort apart from commercial codes. Among many capabilities, I cite in particular Goma's ability to simulate viscoelastic flows which is poorly represented in the commercial sector and for which a stable research platform to build on will be a significant development. Another great thing is that Goma is fully and extensively documented. This is vital, and will speed adaption by both users and developers.

As an example, in our own group as you know interfacial rheology is an important measurement effort. Efforts to model these complex systems using commercial codes have met with limited success for Newtonian interfaces, and none of the codes we have licensed can handle the complex viscoelastic interface that arises in protein therapeutics, which is our most important application at present. A collaborative effort on this problem using Goma would be of immediate and great benefit to our group.

In summary, I believe that Goma deserves serious consideration for an R&D 100 award in 2014. I am fully convinced that this project can have incredible impact and that Goma can become the "LAMMPS of the finite element community" – a stable, state of the art, worldwide platform for developing solutions



*Appendix B: Letters of Support (cont.)*

UNITED STATES DEPARTMENT OF COMMERCE  
National Institute of Standards and Technology  
Gaithersburg, Maryland 20899

to the toughest, coupled multiphysics problems which we are facing the need to tackle in this emerging age of functional materials.

Sincerely,

Frederick R. Phelan Jr., Ph.D.  
Polymers & Complex Fluids Group  
Materials Science and Engineering Division  
National Institute of Standards and Technology  
100 Bureau Drive, STOP 8542  
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✉ [frederick.phelan@nist.gov](mailto:frederick.phelan@nist.gov)  
🌐 [http://www.nist.gov/mml/msed/complex\\_fluids/fred-phelan.cfm](http://www.nist.gov/mml/msed/complex_fluids/fred-phelan.cfm)

*Appendix B: Letters of Support (cont.)***Center for Nanomanufacturing Systems for Mobile Computing and Energy Technologies (NASCENT)****THE UNIVERSITY OF TEXAS AT AUSTIN**MER 1.206, Mail Code R8800 • 10100 Burnet Road • Austin, Texas 78758 [www.nascent-erc.org](http://www.nascent-erc.org)

7 February 2014

**RE: Letter of Support for *Goma* 6.0 for R&D 100 Award**

Dear R&amp;D 100 Award Selection Committee:

I write to strongly endorse *Goma* 6.0 for a 2014 R&D 100 Award. My successful past and present collaborations with researchers at Sandia National Laboratories and the University of New Mexico were and are enabled by this flexible and robust modeling and simulation tool. We have applied and validated models built with *Goma* to understand fluid mechanics in immersion lithography and elastohydrodynamics in nanoimprint lithography. These problems demand computationally efficient software with the unique combination of accurate free and moving boundary tracking capabilities with a wide-variety of wetting models. These are simply not available in commercial software, in part because they are VERY challenging to implement. Our need to solve this class of problems led us to *Goma* as the only viable tool to simulate these important applications. Two PhD student dissertations and highly cited papers from my group have resulted due to *Goma*. In addition to nanomanufacturing, we are also applying *Goma* to understand viscoelastic flow in porous media, taking advantage of its ability to simulate a wide range of non-Newtonian fluids with strong interfacial effects.

We are developing a core set of computational simulations of the nanomanufacturing processes and systems created at the National Science Foundation Engineering Research Center for Nanomanufacturing Systems for Mobile Computing and Energy Technologies (NASCENT). *Goma* has been identified as the only viable option to simulate these systems, which involve multiphase flow, fluid-solid interactions, strong capillary forces and disparate length and time scales. Describing any two of these aspects is computationally challenging. It is a testament to the flexibility and robustness of *Goma* that it can handle all them accurately and efficiently.

The open-source release of *Goma* 6.0 in 2013 is especially valuable to the academic research community in a number of ways. The source code is well-organized and flexible, making it easily modified and enabling novel research endeavors. Despite the open-source release, many production-level qualities are available to the academic community, including extensive training, documentation, and help-networks. *Goma* developers recently ran a valuable three-day training course at UT Austin aimed at educating graduate students on the capabilities of finite element modeling and more specifically the capabilities of *Goma*. Many of these students are using it today for their research. Finally, without export control *Goma* will be embraced by the larger international community, expanding its impact.

*Goma* 6.0 is a superb simulation tool. It has already enabled an enormous amount of valuable research and its open-source release in 2014 will greatly expand its impact. It is most deserving of a 2014 R&D 100 Award.

Sincerely,

A handwritten signature in black ink that reads "Roger T. Bonnecaze".

Roger T. Bonnecaze

William and Bettye Nowlin Chair in Engineering  
Director, NASCENT NSF Engineering Research Center

*Appendix C: Publications***SANDIA REPORT**

SAND2013-1844  
Unlimited Release  
Printed July 2013

# **GOMA 6.0 - A Full-Newton Finite Element Program for Free and Moving Boundary Problems with Coupled Fluid/Solid Momentum, Energy, Mass, and Chemical Species Transport: User's Guide**

P. R. Schunk, P. A. Sackinger, R. R. Rao, K. S. Chen, T.A. Baer, D. A. Labreche, A. C. Sun, M. M. Hopkins, S. R. Subia, H. K. Moffat, R. B. Secor, R. A. Roach, E. D. Wilkes, D. R. Noble, P. L. Hopkins and P. K. Notz, S. A. Roberts

Prepared by  
Sandia National Laboratories  
Albuquerque, New Mexico 87185 and Livermore, California 94550

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Approved for public release; further dissemination unlimited.



**Sandia National Laboratories**

*Appendix C: Publications (cont.)*

Journal of Non-Newtonian Fluid Mechanics 166 (2011) 1100–1115



Contents lists available at ScienceDirect

## Journal of Non-Newtonian Fluid Mechanics

journal homepage: <http://www.elsevier.com/locate/jnnfm>**Numerical simulations of mounding and submerging flows of shear-thinning jets impinging in a container<sup>☆</sup>**Scott A. Roberts <sup>\*</sup>, Rekha R. Rao

Thermal and Fluid Processes Department, Sandia National Laboratories, Albuquerque, NM 87185, United States

**ARTICLE INFO****Article history:**

Received 7 October 2010

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CFD

Finite element method

Free surface flow

Jet

Non-Newtonian

Shear-thinning

**ABSTRACT**

Continuous jets of non-Newtonian fluids impinging on a fluid surface exhibit instabilities from jet buckling and coiling at low Reynolds numbers to delayed die swell, mounding, and air entrainment at higher Reynolds numbers. Filling containers with complex fluids is an important process for many industries, where the need for high throughput requires operating at high Reynolds numbers. In this regime, air entrainment can produce a visually unappealing product, causing a major quality control issue. Just prior to the onset of air entrainment, however, there exists an ideal filling regime which we term "planar filling," as it is characterized by a relatively flat free surface that maintains its shape over time. In this paper, we create a steady-state, 2-D axisymmetric finite element model to study the transition from planar filling to the onset of air entrainment in a container filling process with generalized-Newtonian fluids. We use this model to explore the operating window for Newtonian and shear-thinning (or, more generally, deformation-rate-thinning) fluids, demonstrating that the flow behavior is characterized by a balance between inertial, viscous, and gravitational forces, as characterized by the Reynolds and Froude numbers. A scaling analysis suggests that the relevant parameters for calculating these dimensionless numbers are located where the jet impacts the liquid surface, and simulations show that the transition from planar filling to air entrainment often occurs when  $Re \sim O(10)$ . We found that the bottom and side surfaces of the container drastically influence this transition to entrainment, stabilizing the flow.

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**1. Introduction**

A jet of a rheologically complex fluid impinging onto a liquid surface can exhibit a variety of flow regimes, including jet dripping and pinch-off [1–4], hydraulic jumps [5,6], buckling, coiling, and mounding [7–16], and submerging flow and unstable air entrainment [17–21]. This range of behavior has implications in many industrial applications, such as the filling of bottles and containers. Understanding this behavior is especially important in industry, where the fluids filling containers are often highly non-Newtonian, exhibiting some combination of viscoelastic, shear-thinning, and yield-stress properties. Overall product appearance, such as the absence of air bubbles in a transparent product, is highly important.

The production capacity of industrial plants is often limited by the speed at which containers can be filled. Containers often have labels applied before filling, and in some cases containers are already loaded in cardboard boxes, leading to a low tolerance of container over-fill or of product splashing out of the container. Regulations in some regions limit the amount of void space at

the tops of container, requiring a precise fill process [22]. Precise filling also allows the use of smaller containers, saving container and transportation costs. Sales of some products also rely on their clarity, and any entrained air bubbles can detract from their appearance. For these and other reasons, it is of great interest to understand the operating conditions that lead to the various flow profiles seen in container filling processes, especially for complex fluids. This understanding will allow an increase in throughput while meeting product quality constraints.

Fig. 1 shows four experimental flow regimes found in container-filling processes. The two regimes of most interest are mounding and air entrainment. While a mounding flow can be seen in Fig. 1b, the air entrainment regime is inherently unsteady and a snapshot is not shown in Fig. 1. At relatively low jet velocities, complex fluids often exhibit mounding behavior, where the jet diameter greatly increases as it nears the liquid pool. These mounds can be stable or unstable, forming ripples, coils, or buckles, all of which may entrain air. These mounds may also grow very tall, reaching the top of the container before the sides completely fill. Taylor [24] discovered this phenomenon in experiments from the late 1960s. Over a decade later, [7,8] performed an extensive experimental investigation into this behavior for Newtonian, viscous jets, finding the jet length-to-diameter ratio,  $H/D$ , to be a key physical parameter in determining buckling behavior. Surface tension was found to play a significant

<sup>☆</sup> This paper was submitted as part of the special issue of JNNFM from the XVIth International Workshop on Numerical Methods for Non-Newtonian Flows.

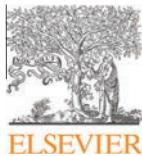
\* Corresponding author. Tel.: +1 505 844 7957; fax: +1 505 844 4507.

E-mail address: [srober@sandia.gov](mailto:srober@sandia.gov) (S.A. Roberts).



## Appendix C: Publications (cont.)

Computers & Fluids 87 (2013) 12–25



Contents lists available at SciVerse ScienceDirect

### Computers & Fluids

journal homepage: [www.elsevier.com/locate/compfluid](http://www.elsevier.com/locate/compfluid)



## Multiphase hydrodynamic lubrication flow using a three-dimensional shell finite element model



Scott A. Roberts <sup>a,\*</sup>, David R. Noble <sup>a</sup>, Eric M. Benner <sup>b,1</sup>, P. Randall Schunk <sup>b</sup>

<sup>a</sup> Thermal and Fluid Processes Department, Sandia National Laboratories, PO Box 5800, MS-0836, Albuquerque, NM 87185-0836, United States

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#### ARTICLE INFO

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Finite-element method

Shell elements

Level-set method

Multiphase flow

#### ABSTRACT

Reynolds' lubrication theory has been widely used to study thin-region fluid flows for a variety of scientific and manufacturing applications. In this work, we set forth an extension of this theory to model the effect of free fluid interfaces and fluid–structural interactions in lubrication films. This model is implemented using curvilinear shell elements in a general three-dimensional finite element code, allowing the study of lubrication flows in arbitrarily complex geometries. This implementation also allows coupling with continuum mechanics, such as solid body deformation, through lubrication-based and fluid–structural interactions. Simulations using this model are compared to analytical solutions and experimental results for a number of model problems.

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### 1. Introduction

The theory of lubrication flow has been in use for well over a century, beginning with Tower's 1883 experiments of a rolling bearing [1] and the landmark mathematical formulation of Reynolds in 1886 [2]. Since then, countless studies have used Reynolds' theory to analyze lubricating flows for numerous scientific and practical manufacturing applications, including journal bearings, coating beads, and hard-drive read heads [3–13]. Many extensions of this basic theory exist, including elastohydrodynamic lubrication [14–21], thermohydrodynamic lubrication [22–26], turbulent hydrodynamic lubrication [27,28], and lubrication of non-Newtonian fluids [29–35], among others [36–42]. Recent books by Hori [12] and Szeri [13] thoroughly review the history and applications of lubrication theory and derive the governing equations.

In practice, lubrication theory is commonly used to study problems where the geometry is either simple, such as in slider bearings, or regular, as in journal bearings. These types of problems often lend themselves to elegant analytical solutions [2,39,43] or simple numerical solutions involving finite difference or finite element techniques [3,5,44]. When these numerical techniques are

used, the equation is often specifically adapted to the given geometry, and a custom computer code is written for solving the specific problem.

Flows in complex geometries are typically studied using full three-dimensional (3-D) simulations in a large-scale, unstructured finite element code, such as GOMA [45]. Yet, problems involving thin fluid layers, such as coating flows with tensioned webs [46,47] and imprint lithography [43,48–50], may benefit significantly from the mathematical order reduction provided by lubrication theory using shell-type elements within a larger 3-D code. Shell elements have been used for decades in the solid mechanics community for modeling thin materials [51–53], but their use in fluid dynamics has been relatively rare [9]. However, the coupling of curvilinear shell elements for fluid flows with 3-D elements for solid deformations would allow the study of elastohydrodynamic lubrication in complex geometries via a direct coupling with continuum solid element regions. Few studies have used these fluid–structure interactions (FSIs) to couple lubrication shell elements with 3-D solid deformation [21,34].

In all of the previously cited studies, the lubrication layer was a single liquid phase confined between two substrates, either rigid or deformable. While there has been considerable work on unconfined or multilayer lubrication flows, modeled by the thin film equations [54], there have been very few computational treatments of confined multiphase lubrication flows together with a free interface across the thin film. One of the few examples of existing work is by Reddy and Bonnecaze [44], who used a finite difference method to solve liquid flow between two plates and a

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*Appendix C: Publications (cont.)*

## Modeling Coupled Migration and Settling of Particulates in Curing Filled Epoxies

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**ABSTRACT:** Epoxy resins filled to a high solids loading (40–60% by volume) with noncolloidal particles are used to mitigate stress and vibration in electronic components. We perform continuum-level finite element method (Schunk et al., A Full-Newton Finite Element Program for Free and Moving Boundary Problems with Coupled Fluid/Solid Momentum, Energy, Mass, and Chemical Species Transport User's Guide, Sandia National Laboratories) simulations of filler particle redistribution during the nonisothermal cure of the epoxy under both quiescent and bulk flow conditions. An extent of reaction is used to track the degree of cure. To determine the particle migration, we couple a diffusive flux suspension model (Zhang

and Acrivos, *Int J Multiphase Flow* 1994, 20, 579.) with the curing model. The heat transfer, including the exothermic polymerization reaction, is also modeled. The result is a generalized Newtonian model that has viscosity as a function of temperature, cure and particle volume fraction. With x-ray computed tomography, we examine settling of the particulate phase in both flowing and quiescent curing systems and compare the experimental results to the model predictions. The model is also validated with temperature measurements. © 2011 Wiley Periodicals, Inc. *J Appl Polym Sci* 122: 1587–1598, 2011

**Key words:** simulation; polymerization; sedimentation

### INTRODUCTION

Filled polymers are found in manufacturing applications ranging from encapsulation of microelectronics to injection molding of composite parts. We specifically address epoxy composites, which are used to prevent corona discharges or catastrophic electrical arcs in high voltage electrical devices.<sup>1</sup> Similar filled epoxies are found in liquid molding technologies for the aerospace industry<sup>2</sup> and emerging technologies to develop functionally graded materials.<sup>3</sup> Developing predictive models of these manufacturing processes requires knowledge of time- and temperature-dependent rheology of the polymer.<sup>2,4,5</sup> The rheology of filled polymers is not only highly dependent on the extent of reaction of the polymerization or cure, but also on the particle volume fraction.<sup>6,7</sup> Furthermore, the local particle volume fraction can change due to gravity, convection, and shear-induced migration.<sup>8–10</sup> Even under quiescent

conditions, gravity-driven particle settling in simple geometries with sharp features leads to instabilities and chaotic flow.<sup>8</sup> Shear induced migration during the mold fill and gravity-driven instabilities during the quiescent curing stage can lead to detrimental inhomogeneities in the final filler particle density. Although others have modeled simultaneous settling and curing,<sup>7,11,12</sup> these models are generally one-dimensional and do not take into account convective or shear-induced migration of particles. In this article, we couple continuum-level finite element method (FEM) simulations of filler particle redistribution during the nonisothermal cure of the epoxy under both bulk flow and quiescent conditions.

Systems of interest are epoxy resins filled with a high loading (40–60% by volume) of solid noncolloidal particles. Particle volume fraction gradients in such suspensions have been shown to develop in flows in which a shear gradient occurs, as particles are driven away from the high-shear-rate regions.<sup>9</sup> This particle migration occurs even in creeping flow and in the absence of significant nonhydrodynamic effects. Phillips et al.<sup>13</sup> distilled Leighton and Acrivos's<sup>9</sup> scaling arguments to develop a set of continuum constitutive equations based on three major causes of particle migration, which are gradients in shear-rate, particle volume fraction and relative viscosity. The Phillips model, also called the diffusive-flux model, uses a particle-volume fraction-

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## Appendix C: Publications (cont.)

Metting Technologies

Research Summary

## The Macroscale Simulation of Remelting Processes

L.A. Bertram, P.R. Schunk, S.N. Kempka, F. Spadafora, and R. Minisandram

Vacuum arc remelting and electroslag remelting processes are used to produce large (five tonne) ingots of nickel-based superalloys, titanium alloys, and other high-value-added alloys. The remelting processes provide controlled solidification conditions capable of producing extremely uniform chemistry and microstructure; however, the consequences of a single defect are potentially so great, that process improvements are being vigorously pursued by the Specialty Metals Processing Consortium. The ultimate modeling goal is the realistic description of the liquid-solid mixed-phase region of the ingot ("mushy zone"), so that solidification defects such as freckles, macrosegregation, and solidification white spots can be avoided. Reaching this goal requires a numerical strategy capable of yielding not only accurate temperatures at the macroscale, but also accurate temperature gradients. The numerical procedure also requires thermophysical-property data for the alloy and some furnace data (such as contact resistance at ingot-crucible interfaces) as well as characterization of the heat sources.

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When cylindrical ingots (rounds) are prepared by vacuum arc remelting (VAR) or electroslag remelting (ESR), many potential deviations from ideal conditions can lead to defects. For descriptions of the melting practice, see Chowdhury,<sup>1</sup> Hoyle,<sup>2</sup> Medovar et al.,<sup>3</sup> Maurer et al.,<sup>4</sup> or Bertram et al.<sup>5</sup> for discussions of VAR defects. In order to minimize the likelihood of such defects in shipped alloy, the Specialty Metals Processing Consortium (SMPC) is integrating simulation capability with production-scale experimental work to avoid less-than-ideal solidification conditions in practice. The first stage of this effort is aimed at characterizing the macroscale ingot heat transfer in furnaces to assess the effect of changes in furnace-control settings (e.g., melt current, feed rate of the electrode, size of ingot, and enhancements of ingot cooling) on solidification processes.

In both VAR and ESR, a readily appreciated benchmark for simulation is the pool shape, as determined from macrographs of sectioned ingots.<sup>6,7</sup> The actual calibration procedure involves careful consideration of many other variables and extensive instrumentation of industrial furnaces. Defining experimental conditions to capture sufficient data to ensure consistency is now possible,<sup>7,8</sup> although continuing effort is needed to bring all of the necessary parts of the picture fully into focus.

### ELECTROSLAG REMELTING

To start the process characterization, a study combining industrial, academic, and Sandia Liquid Metals Processing Laboratory research was carried out.<sup>17,18,19</sup> One of the full-scale industrial tests is described here.

### Experiment

This experiment was designed to benchmark the ESR simulation capability and correlate metallurgical structure with melting parameters. A 0.56 m diameter round of alloy 625, which has a melting range of 1,562–1,622 K, was produced under highly controlled conditions in a Consarc ESR furnace at Inco Alloys International in October 1994. Slag composition was 33CaF<sub>3</sub>-33CaO-33Al<sub>2</sub>O<sub>3</sub>. At five equally spaced time intervals, the melt rate was changed (0.063–0.126 kg/s, as determined from a load cell) with a combination of techniques that amounted to controller-scheme changes and hence, included voltage and immersion-depth variations. Conditions for the simulation were 7.3 kA of constant root mean square (rms) current and nominal electrode immersion depth of 0.0127 m. The resulting voltage was 43 V.

The ingots were sectioned and etched to reveal the pool shape, grain structure, and presence of defects. Only the general shape of the pool could be determined from these measurements and not the outright depth, due to the omnipresent molten-metal head in ESR melting. The results are indicated schematically in Figure 1 (cf. Brooks et al.).<sup>17</sup>

### Simulation

The discrete equations of momentum, energy, and electromagnetics over the domain (illustrated in Figure 1) were solved using the finite-element code GOMA2.0.<sup>10</sup> The solutions in electrode, slag, and ingot were obtained simultaneously because of the complex coupling among these elements (i.e., the coupling between the electromagnetics and the fluid and heat transfer occurs through several mechanisms). First, there is the Joule heating effect, through which the current generates heat resistively (mainly in the slag). Second, there is the flow that the combined current flux and the magnetic field can drive through the Lorentz force. The thermal field affects the electric potential at any point through the dependence of electrical conductivity on temperature. The current distribution and, hence, the Lorentz force and Joule heating are also influenced by the extent and degree of electrical contact between the slag and molten metal with the crucible.

The boundary conditions on the governing equations were fairly standard. The electromagnetic solutions were obtained as described by Gartling.<sup>20</sup> The slag skin between ingot and crucible was expected to have a significantly different electrical resistivity than the bulk slag, complicating the electrical and thermal boundary conditions. Because the slag skin was not resolved in these calculations, we were forced to speculate the effect of the slag skin on the current flux distribution; we chose

## Appendix C: Publications (cont.)

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### Hydrophilicity and the Viscosity of Interfacial Water

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We measure the viscosity of nanometer-thick water films at the interface with an amorphous silica surface. We obtain viscosity values from three different measurements: friction force in a water meniscus formed between an oxide-terminated W tip and the silica surface under ambient conditions; similar measurements for these interfaces under water; and the repulsive “drainage” force as the two surfaces approach at various speeds in water. In all three cases, we obtain effective viscosities that are  $\sim 10^6$  times greater than that of bulk water for nanometer-scale interfacial separations. This enhanced viscosity is not observed when we degrade the hydrophilicity of the surface by terminating it with  $-H$  or  $-CH_3$ . In view of recent results from other interfaces, we conclude that the criterion for the formation of a viscous interphase is the degree of hydrophilicity of the interfacial pair.

#### Introduction

Interfacial water is important in a wide range of surface processes such as protein folding,<sup>1–3</sup> stability of colloid suspensions,<sup>2,4</sup> enzyme activity,<sup>5,6</sup> swelling in clays,<sup>7,8</sup> stiction in microelectromechanical systems (MEMS),<sup>9</sup> and scanning probe microscopy.<sup>10,11</sup> The ordering of water molecules on the nanometer scale next to hydrophilic surfaces has been studied extensively through vibrational spectroscopy,<sup>12–14</sup> scattering techniques,<sup>7,15</sup> atomic force microscopy (AFM) imaging,<sup>16,17</sup> and computer simulations.<sup>18,19</sup> Experiments on the surface of  $SiO_2$ , one of the most abundant materials on earth,<sup>20</sup> have revealed a change in the intermolecular bonding of interfacial water that is attributed to an increase in the ordering of water molecules near the surface.<sup>11–13</sup> Although these results indicated that the interfacial water was structured, it was unable to solidify to an ice-like structure at room temperature and neutral pH. Previous studies concluded that, at intermediate pH values above the

isoelectric point of silica ( $\sim 2$  to 3), there is competition between water molecules hydrogen bonding to protonated silanol ( $Si-OH$ ) groups with their dipoles pointing away from the surface and water molecules aligning in the electric field of deprotonated silanol anions on the surface with their dipoles pointing into the surface.<sup>12</sup>

Although thin water films adsorbed on silica and other hydrophilic surfaces do not usually solidify at room temperature, they do possess physical properties that are distinctly different from those of bulk liquid water. It is well known that there is a repulsive force between hydrated surfaces in close proximity at 1–3 nm.<sup>21</sup> Examples include oxides (silica, alumina, mica, and clay) and molecules (lipids, DNA, surfactants, etc.). This interfacial repulsion, termed hydration forces or hydration repulsion, has been attributed to the energetic requirement of disturbing the hydration structure near the surface. Force measurements by a number of techniques, including the surface force apparatus (SFA), AFM, and osmotic stress, have established an exponentially decaying repulsive force between hydrated surfaces, with the decay length in the range of 0.2–1.4 nm. Unlike the long-range electrostatic double-layer force, which depends strongly on ionic strength, the short-range hydration force is independent of ionic strength. Whereas theoretical models, such as the DLVO (Derjaguin, Landau, Verwey, and Overbeek) theory,<sup>22,23</sup> are well established for the electrostatic repulsion, no quantitative theory yet exists for the hydration force.

Shear force measurements have also shown distinctly different mechanical properties of adsorbed water on hydrophilic surfaces. However, experimental results are more varied as compared to those dealing with the hydration force. An earlier measurement by Israelachvili using the SFA technique showed bulklike viscosity of water confined between two mica surfaces with an interfacial separation of  $< 2$  nm.<sup>24</sup> Klein and co-workers carried out SFA measurements and reported no appreciable change<sup>25,26</sup> over the viscosity of bulk values for water confined between two

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## Appendix C: Publications (cont.)

PHYSICS OF FLUIDS 17, 122104 (2005)

### Dynamics of low capillary number interfaces moving through sharp features

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The success of any nanoimprint process depends upon its ability to exactly reproduce the template pattern. Thus, complete filling of recessed features in the template is an important issue that is controlled by the dynamics of the flow through these sharp structures. At these small scales, capillary forces are large and must be included in the fluid flow model. The mechanism of interface advancement at low capillary number through sharp rectangular features is useful for understanding how and why features fill or trap air. In this study we present a two-dimensional simulation of this feature filling to capture the details of the process, including the viscous and capillary effects. Fluid is injected into the channel between the template and substrate, where the fluid-air interface soon encounters a rectangular feature with some height greater than the channel gap. As the fluid advances through the channel, the shape of the interface is a circular arc due to the strong capillary forces. The interface maintains this circular arc as it negotiates the first sharp corner of the feature; the upper contact line effectively pins to the initial corner of the feature as it moves around this corner, during which time the lower contact line continues to advance forward along the substrate surface, causing the interface to stretch. For sufficiently wide or shallow features, once the upper contact line has negotiated the first corner and has moved vertically up the inner wall of the feature, it must move through the top corner of the feature. At this point the interface undergoes a rapid reconfiguration from a high surface area circular arc to a lower surface area circular arc inside the feature. Alternatively, for narrow or high features, the stretched interface can catch on the far, final corner of the feature, trapping air inside the feature and preventing filling. The conditions for filling are studied parametrically for a variety of wetting contact angles and feature dimensions with both the simulation and a simpler, successful geometric model. The dynamics of the feature filling suggest an effective boundary condition for a macroscopic lubrication model of the imprint lithography process in which a critical pressure is required to move fluid through a feature. © 2005 American Institute of Physics. [DOI: 10.1063/1.2140691]

#### I. INTRODUCTION

The Step and Flash Imprint Lithography (SFIL) process offers a high-throughput, low-cost alternative to modern methods of lithography. The process makes use of the liquid monomer form of the etch barrier. The monomer drops, which are typically acrylate-based formulations, are pressed into the desired shape by bringing a template, typically a quartz mask, down with a given speed or applied force, making the best use of the capillary and viscous force interaction to minimize the imprint time.<sup>1</sup> The imprint area is one square inch with a final base layer of approximately 50 nm; the template velocity begins on the order of a micron per second and drops to just a few nanometers per second at the end of

the process. The SFIL technique has allowed the production of features as small as 30 nm, after imprint and etch.<sup>2</sup> Typical capillary numbers for these flows are very small due to the small feature size and relatively low flow rates. Given a monomer with typical density,  $O(1 \text{ g cm}^{-3})$ , interfacial tension  $O(30 \text{ dyn cm}^{-1})$ , and viscosity  $O(1 \text{ cP})$ , the capillary number is as small as  $10^{-3}$ . The Reynolds number is, at the largest, on the order of  $10^{-3}$ .

Clearly, capillary wetting is an important part of the filling process, and is particularly important for the filling of features in the template. If features do not fill appropriately, instead trapping an air bubble inside, the resulting photore sist image is untrue to the original mask, and the failed pattern transfer can lead to a nonfunctional circuit on the wafer. A fundamental understanding of this nanoscale filling process is useful for predicting which types of features will fill or trap air; the goal of this study is to obtain this fundamental

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*Appendix C: Publications (cont.)*

INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS  
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## A numerical and experimental study of batch sedimentation and viscous resuspension

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### SUMMARY

A suspension of non-neutrally buoyant, large, nearly monodisperse spheres is studied both in batch sedimentation and in shear between concentric rotating cylinders. We apply a continuum constitutive equation based on the diffusive flux model augmented with buoyancy terms derived by Acrivos and coworkers and discretize the resulting equation set with the finite element method. We simulate batch sedimentation using this method and obtain a reasonable match with experiment. Next used two-dimensional NMR imaging to measure the evolution of solid fraction profiles in the same suspension undergoing flow between rotating concentric cylinders with two different initial conditions. Here, both gravity-induced and shear-induced particle migration are significant. Under these conditions, we have found that simulating the correct initial condition is critical to matching the experimental results. When this is done, the model results compare well with the experiments. Copyright © 2002 John Wiley & Sons, Ltd.

KEY WORDS: shear flows; batch sedimentation; viscous resuspension, Couette flow

### INTRODUCTION

Particle-laden shear flows are important in a wide variety of applications in oil and gas production and in the mineral, chemical and food processing industries. These include such application as batch sedimentation, hydraulic fracturing technology and slurry transport. Particle separation due to density differences occurs in many non-colloidal mixtures of particles and liquids, and many processing activities can benefit from knowledge of the physics of systems undergoing sedimentation or flotation. For this reason, we are trying to develop a modeling capability that allows us to predict the flow and particle transport properties of arbitrary buoyant suspensions in complex geometries.

It is now well known that flowing suspensions of particles in a liquid have been known to exhibit particle migration even in creeping flow and in the absence of significant nonhydrodynamic or gravitational effects [1–3]. In particular, Leighton and Acrivos [2] proposed scaling arguments that identified three causes of particle migration, namely, gradients in shear rate,

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*Appendix C: Publications (cont.)*

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ARTICLE NO. 0081

## A Newton–Raphson Pseudo-Solid Domain Mapping Technique for Free and Moving Boundary Problems: A Finite Element Implementation\*

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An implicit, pseudo-solid domain mapping technique is described that facilitates finite element analysis of free and moving boundary problems. The technique is based on an implicit, full-Newton strategy, free of restrictions on mesh structure; this leads to many advantages over existing domain mapping techniques. The fully coupled approach using Newton's method is particularly effective for problems with strong coupling between the internal bulk physics and the governing physics at unknown free boundary locations. It is also useful when the distinguishing conditions which constrain the free boundary shape provide only an implicit dependence on the boundary location. Unstructured meshes allow for efficient resolution of internal and boundary layers and other regions of strong local variations in the solution and they also reduce the amount of user interaction required to define a problem since the meshes may be generated automatically. The technique is readily applied to steady or transient problems in complex geometries of two and three dimensions. Examples are shown that include free and moving boundary problems from solidification and capillary hydrodynamics. © 1996 Academic Press, Inc.

### 1. INTRODUCTION

Free and moving boundary problems in fluid dynamics, heat transfer, and other disciplines pose a challenge to computational techniques because the computational domain, or boundary shape, must be determined, together with any field variables internal to the domain. From an industrial perspective, many materials processing issues involve free boundary (FB) or moving boundary (MB) problems; solidification and capillary hydrodynamics, the focus of two of the example applications presented here, are important to the production and quality control of metals, semiconductors, and various coatings. Robust, accurate, and efficient computational methods for locating free and moving boundaries, together with the internal physics, are essential for analysis and design of these processes. This is a particular challenge in the face of the

nonlinear nature of many of the conservation equations and of the coupling between the boundary or interface shapes and the internal field variables.

Among the several computational approaches available for FB or MB problems, the best choice depends on the particular set of field equations, boundary conditions, parameter ranges of interest, and the range of domain topologies that need to be simulated. Each computational technique offers its own balance between efficiency, accuracy, and robustness, all of which are desirable objectives for any computational approach to analyzing FB or MB problems [1, 2].

The most *accurate* techniques parameterize the free or moving boundary as a mathematical curve (two dimensions) or surface (three dimensions) in space, i.e., *boundary parameterization* techniques, so that the boundary conditions may be applied precisely at an interface with a well-represented location, orientation, and curvature. Moreover, exact boundary parameterization makes possible the solution of distinctly different field equations, according to the governing physics in each region of the computational domain. Clearly, if accuracy of the boundary shape representation is an overriding concern, this precludes the use of interface-tracking schemes based on representing unknown FB or MB boundary shapes with partially filled cells of finite thickness. Included in the latter approach are techniques employing a “concentration function,” such as the volume of fluid (VOF) approach [3], and schemes relying on material marker particles, such as the marker-and-cell (MAC) technique [4]. These approaches trade a less accurate boundary shape representation for a faster speed of solution, especially for certain problems with discontinuous evolution of domain topology.

The purpose of this research is to make a boundary-conforming *domain* mapping technique as robust as possible. Here the term *robust* implies a technique that will most often succeed in converging to the solution, if a solution exists. If there are circumstances where coaxing convergence requires an analyst to modify the approach, then

\* This work was performed at Sandia National Laboratories for the U.S. Department of Energy under Contract DE-AC04-94AL85000.

*Appendix C: Publications (cont.)*

INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS  
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## A finite element method for free surface flows of incompressible fluids in three dimensions. Part I. Boundary fitted mesh motion

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### SUMMARY

Computational fluid mechanics techniques for examining free surface problems in two-dimensional form are now well established. Extending these methods to three dimensions requires a reconsideration of some of the difficult issues from two-dimensional problems as well as developing new formulations to handle added geometric complexity. This paper presents a new finite element formulation for handling three-dimensional free surface problems with a boundary-fitted mesh and full Newton iteration, which solves for velocity, pressure, and mesh variables simultaneously. A boundary-fitted, pseudo-solid approach is used for moving the mesh, which treats the interior of the mesh as a fictitious elastic solid that deforms in response to boundary motion. To minimize mesh distortion near free boundary under large deformations, the mesh motion equations are rotated into normal and tangential components prior to applying boundary conditions. The Navier-Stokes equations are discretized using a Galerkin-least square/pressure stabilization formulation, which provides good convergence properties with iterative solvers. The result is a method that can track large deformations and rotations of free surface boundaries in three dimensions. The method is applied to two sample problems: solid body rotation of a fluid and extrusion from a nozzle with a rectangular cross-section. The extrusion example exhibits a variety of free surface shapes that arise from changing processing conditions. Copyright © 2000 John Wiley & Sons, Ltd.

**KEY WORDS:** capillarity; extrusion; finite element method; free surface; pseudo-solid mesh motion; three dimensional

### 1. INTRODUCTION

More and more researchers and practitioners in the field of computational mechanics, heat transfer, and mass transfer are now solving three-dimensional models. Until recently, however,

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## Appendix C: Publications (cont.)

### Computational Modeling of the Pattern Formation of Swimming Microorganisms in 3D

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Similar to the 2D models in [1], a collection of  $O(10^5)$  discrete computational representative (or notional) microorganisms are coupled to the incompressible Navier-Stokes equations, viz.,

$$\rho_f \left[ \frac{\partial \underline{u}}{\partial t} + (\underline{u} \cdot \nabla) \underline{u} \right] = -\nabla p + \nabla \cdot (\mu \nabla \underline{u}) + N(\rho_m - \rho_f) v_m g \sum_i \delta(\underline{x} - \underline{x}_i)$$

$$\nabla \cdot \underline{u} = 0$$

$$\frac{d \underline{x}_i}{dt} = \underline{u}(\underline{x}_i) + \underline{s} + \underline{\hat{s}}$$

Where  $\underline{u}$  is suspension velocity,  $p$  is pressure,  $\mu$  is viscosity,  $N$  is the ratio of real microorganisms to computational microorganisms,  $\rho_f$  is fluid density,  $\rho_m$  is microorganism density,  $g$  is gravity,  $v_m$  is microorganism volume,  $\underline{x}_i$  is the location of the  $i^{\text{th}}$  computational microorganism,  $\underline{s}$  is the base swimming velocity and  $\underline{\hat{s}}$  is a stochastic swimming adjustment to microorganism  $i$ .

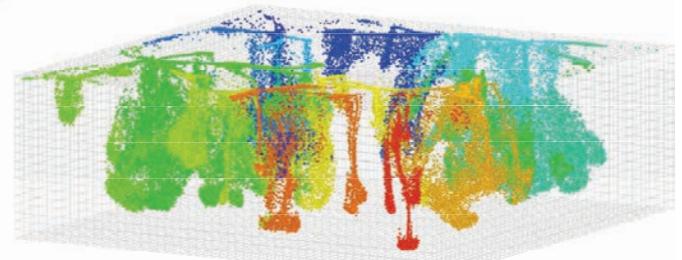
The fluid equations are solved with a full Newton-based FEM. Linear interpolation functions are used for velocity and pressure (with pressure stabilization). All aspects of the algorithm are parallelized, including matrix assembly, linear solver, microorganism trajectories, and ghost microorganisms.

The model microorganisms are based on *Chlamydomonas nivalis* algal cells, with model parameters based on [2]. A real population density of  $10^6$  cells/cm<sup>3</sup> is assumed, resulting in  $N = 160$ . Microorganism locomotion is assumed to be pure geotaxis (negative gravitaxis) with swimming vector  $\underline{s} = (0, 0, 100)\mu\text{m/s}$  and  $\underline{\hat{s}}$  is constructed to give a distribution of  $N(0, 50)\mu\text{m/s}$  over 1s.

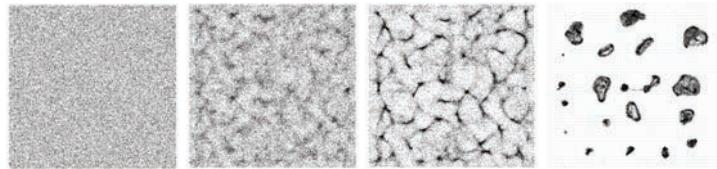
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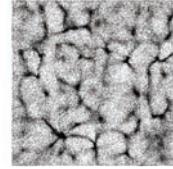
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.



4cm x 4cm x 1.4cm box with 140,000 computational microorganisms at time 636s.  
Color indicates processor number.



Top views of 4cm x 4cm x 0.6cm box with 60,000 computational particles at times (left to right) 0s, 213s, 373s, and 1973s.



Top view of 1.4cm tall box at time 193s.



1.4cm tall box and 0.6cm tall box at "final" times of 897s and 1973s, respectively.



*Appendix C: Publications*

P.R. Schunk, P.A. Sackinger, R.R. Rao, K.S. Chen, A.C. Sun, M.M. Hopkins, S.R. Subia, P.L. Hopkins, H.K. Moffat, R.A. Roach, D.R. Noble, P.K. Notz, S.A. Roberts, D.A. Labreche, R.B. Secor, and E.D. Wilkes, "GOMA 6.0 - A Full-Newton Finite Element Program for Free and Moving Boundary Problems with Coupled Fluid/Solid Momentum, Energy, Mass, and Chemical Species Transport: User's Guide," SAND2013-1844, June 2013.

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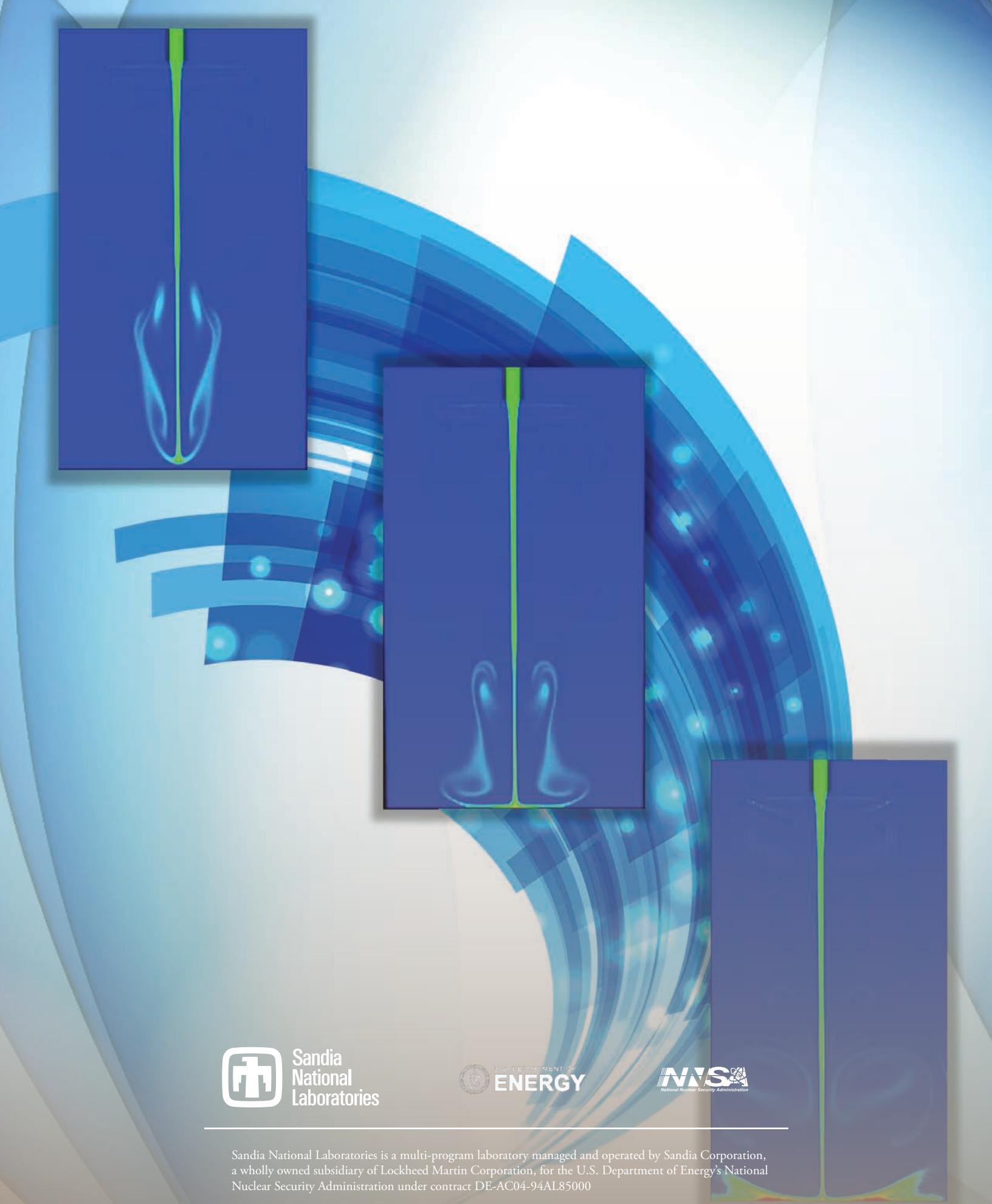
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