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Towards Enhancing Sandia's Capabilities in Multiscale Materials Modeling and Simulation

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Towards Enhancing Sandia's Capabilities in Multiscale Materials Modeling and Simulation

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Abstract:

We report our conclusions in support of the FY 2003 Science and Technology Milestone ST03-3.5. The goal of the milestone was to develop a research plan for expanding Sandia's capabilities in materials modeling and simulation. From inquiries and discussion with technical staff during FY 2003 we conclude that it is premature to formulate the envisioned coordinated research plan. The more appropriate goal is to develop a set of computational tools for making scale transitions and accumulate experience with applying these tools to real test cases so as to enable us to attack each new problem with higher confidence of success.

Acknowledgment

The authors thank all the technical staff who participated in the seminar series and engaged us in discussions. JBA thanks Timothy Trucano for repeated, insightful contributions and encouragement. JBA also thanks Peter Schultz, Mark Stevens, Veena Tikare and Jon Zimmerman for providing extended comments.

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Sandia's Capabilities in Multiscale Materials Modeling and Simulation

Introduction

The authors' preliminary inquiries with the technical staff in FY '02 into the need and status of capabilities at Sandia for multiple scale materials modeling and simulation led to our being invited to pursue the following Science and Technology (S&T) milestone on the topic in FY '03:

> Develop a coordinated research plan, including required partnerships, for developing computational and theoretical methods to link quantum electronic and atomistic simulations to discrete or continuum mesoscale systems, in order to expand and strengthen Sandia's capabilities in materials modeling and simulation. This milestone will constitute a major step toward the longer range goal to link quantum, atomistic, and coarse-grained mesoscale simulations to continuum constitutive models.

The overarching conclusion from our inquiries and discussions with technical staff during the past year is that it is premature to attempt to formulate the 'coordinated research plan' envisioned in the milestone. Owing to the complex and ill-defined nature of the problem there is no single solution for making any particular transition between two scales. The more appropriate goal is to develop a set of tools for making scale transitions and experience with applying these tools to real test cases so as to enable us to attack each new problem with higher confidence of success. Below, under "Future Directions," we list several elements that can contribute to and promote the desired capability in multiscale material modeling and simulation (M&S). The aim of these is for Sandia to acquire capabilities for accomplishments with material simulation that we cannot now make. Such multiscale material M&S will be new, technically desirable, and deserving of greater visibility internally and externally.

Overview

Multiple length and time scale ("multiscale") numerical simulation for science and engineering is an idea whose time has come . . . and gone. Over the past decade it has been widely discussed and attempted in many ways by many research groups, but with limited fundamental progress. About ten years ago the Division of Materials Research at NSF and the Office of Basic Energy Sciences at DOE funded programs that emphasized linking length scales. Owing to the difficulty and broad scope of the problem, the research community inadvertently oversold the prospects for making progress on developing multiscale material modeling and simulation (MM&S) methods. One upshot of this is that it is now a disadvantage to discuss MM&S when interacting with this segment of NSF or BES.

Though in some regards multiscale material modeling is already passé, there are many indications that MM&S is important, that it has captured the imagination of the research community, and that it will continue to be actively pursued: One or more versions of MM&S is regularly the topic of sessions at current technical meetings on physics, chemistry, materi-

als science, or engineering of materials (see Appendix A); two new journals devoted to MM&S have come out in the past year (see Appendix B); research universities are actively pursuing, on a departmental or institutional basis, different approaches to MM&S.

Three examples of the latter are U. Wisconsin – Madison's College of Engineering recruitment for three new faculty to fill out a Materials By Design "Cluster", RPI's nearly successful (and still potentially so) creation of an NSF-funded Engineering Research Center (ERC) for multiscale simulation methods development, and Caltech's highly successful Center for Simulation of Dynamic Response of Materials. UW Madison is launching an interdisciplinary group of faculty in Materials by Design to design materials from first principles using theory, modeling, and computation at the atomic, molecular, nano, and meso-scales. RPI's goal for the Multiscale Systems Engineering Research Center (MSERC) is to advance integrated engineering design of systems at the macro scale, microscale, and nanoscale to enable the development of new products and industries. While not funding the MSERC outright, the NSF Engineering Directorate does want to see a demonstration of the value of multiscale systems engineering. For this reason, NSF is providing RPI a 3-year grant with which to begin to develop multiscale systems engineering and demonstrate its concepts on the chosen application of nanocomposites. Finally, Caltech's Center constructed a Virtual shock physics Test Facility (VTF) under their ASCI Alliance program project. This integrated research project coordinates research activities across several departments to facilitate multiscale simulation of dynamic materials response. The project focuses on five areas: compressible turbulence; computational and computer science; solid dynamics; materials properties; validation (http://csdrm.caltech.edu/mission.html).

During FY '03 the authors extended their preliminary discussions and information gathering activities begun in FY '02 with the aim of developing a plan for linking from quantum calculations to simulating mesoscale systems. Based on our observations of developments in the external research community, discussion with technical staff and managers, and our in-house seminar series at which several project leaders reported on their respective multiscale materials project underway at SNL (see Appendix C), we reached the following conclusions, which we discuss in the sequel of this report:

1. There is an increasing need for MM&S for materials as we seek to understand and control the behavior of increasingly complex materials. It is attractive for enabling the higher fidelity, integrated engineering simulations that are needed in many Sandia programs but are not currently possible.
2. There is no single solution or approach for bridging between all scales of length and time, nor even for bridging between any pair of neighboring scales. The solutions are material- and application-specific.
3. Sandia, and the materials research community in general, will need to develop a collection of tools, and experience using them, to attack different classes of multiscale problems.
4. Tool development for multiscale material M&S is best pursued in the context of ongoing problem-driven work.
5. The fundamental issues are physics problems, not computer science

6. It is currently feasible to bridge between only two "neighboring" length or time scales in a given multiscale method, but even this can be highly advantageous.
7. A formal visiting scientist program, as drafted, is not appealing. But some form of visitors' program would be welcome and beneficial to advancing MM&S capabilities at SNL.
8. Sixteen Federal agencies or departments now have active nanoscience and/or nanotechnology programs that are all part of the National Nanoscience Initiative (http://www.nano.gov/start.htm). These are a strong driver for development of multiscale material M&S capabilities.

Discussion

Here we expand on the conclusions given above.

1. There is an increasing need for MM&S for materials as we seek to understand and control the behavior of increasingly complex materials. It is attractive for enabling the higher fidelity, integrated engineering simulations that are needed in many Sandia programs but are not currently possible.

Material behavior is determined by the collective, coordinated action of the phenomena associated with each scale of material heterogeneity. Common material heterogeneities include atomistic discreteness, lattice defects or other structural variation, subgrain domains, grain boundaries, multiple phases, micro-cracks, and surfaces and interfaces (a.k.a. "boundaries"). When phenomena are coupled it is usually necessary to resort to some method of direct numerical simulation (DNS) to investigate and understand the response. When the coupled phenomena proceed with different response times or on different length scales, DNS requires a multiscale method. Even for uncoupled or loosely coupled phenomena, with increasing number of types of heterogeneity it becomes increasingly difficult to predict the overall response of a material without using a multiscale method of DNS.

Extreme engineering, which is the hallmark of Sandia's work, requires understanding and controlling the properties and behavior of materials. Taken in its full generality, the goal is, in effect, to be able to design the key materials in each application. Controlling material properties, in turn, requires understanding and controlling processing, which determines many aspects of material performance. MM&S is attractive for enabling high fidelity, integrated simulations that are needed and being pursued in ASCI Materials and Physics Models (M&PM) projects like: corrosion; shock-activated power generation with ferroelectrics; radiation effects in ICs; competitive adsorption in zeolite sorbants; grain boundary evolution of micro parts; thermo-mechanical fatigue of solder joints. It is also attractive for S&T projects using numerical modeling and simulation to investigate biomolecule structure and function, biological cell function, integrated nanotechnology, and nanofluidics.

Indeed, MM&S is attractive for understanding complex materials, and for the increasingly precise control of "common" materials, *e.g.* metal alloys or silica glass. Achieving detailed control over material behavior forces us to consider common materials in greater detail and in new response regimes with the result that even common materials begin looking more and more complex.

There are three general types of applications for which MM&S offers to enable substantially greater capability: understanding complex material behavior; capturing sub-grid scale physics in continuum simulations; guiding design and interpretation of accelerated aging tests.

2. There is no single solution or approach for bridging between all scales of length and time, nor even for bridging between any pair of neighboring scales. The solutions are material- and application-specific.

The essential challenge of simulating coupled material phenomena is making the transitions between scales. A transition to a coarser scale must capture the dominant aspects of the physical processes, but not more. Doing this is not an engineering or algorithms issue. It is a science issue: What averaging can we do to remove the many unimportant degrees of freedom – the uninteresting details – to be left with just the important degrees of freedom at a coarser scale? Hence, MM&S projects need to focus on developing the science of making the links. Capabilities are needed to treat a variety of types of transitions, including (i) discrete (atomistic) to *thermomechanical* continuum; (ii) quantum to classical; (iii) deterministic to statistical.

3. Sandia, and the materials research community in general, will need to develop a collection of tools, and experience using them, to attack different classes of multiscale problems.

Multiscale materials M&S entails multi-physics modeling in an essential way. Successful scale bridging methods are likely to be multi-disciplinary approaches that cross organizational boundaries. The viability of a coupling method is highly context specific, depending on the details of the material phenomena involved (intrinsic factors) and on the goals of the intended application (extrinsic factors). This requires that we develop a set of methods for making transitions in material simulations and sufficient know-how so that we can be confident of being able to treat our future materials engineering problems with high confidence of success.

4. Tool development for multiscale material M&S is best pursued in the context of on-going problem-driven work.

Development of coupling methods can be best fit into on-going applied research programs at Sandia if it is done in the course of problem-driven work, rather than as separate projects focused on development of computational tools. A close coupling of tool development with application and problem solving also is advantageous for producing the most robust and relevant simulation methods. In pursuing this course we recognize the importance of maintaining the vital interchange between multiscale modeling and experiment. Indeed, it is through an iterative exchange between experiment, theory, and modeling that we can hope to identify and implement a practical treatment of the necessary physics.

5. The fundamental issues are physics problems, not computer science.

Simulating a mole of atoms would be of some additional use over current capabilities, but it would not fulfill the goal of being able to design materials. The approach needed to

simulate a variety of coupled physical phenomena is to implement intelligent communication between models that act at neighboring scales.

Even with MM&S capabilities in hand, every investigation will continue to need to address basic questions, which are also problem specific: In what regimes is single-scale physics dominant? When are boundaries important? When do you make operational approximations in order to get the job done? When must you be attentive to the fundamental physics? What ensures credibility of the simulations?

6. It is currently feasible to bridge between only two "neighboring" length or time scales in a given multiscale method, but even this can be highly advantageous.

The performance of a given material in a specific application is determined by the material phenomena that contribute most greatly to the material's overall response. We will call this set of influential material processes the "dominant phenomena." These phenomena can be put in a sequence ordered by the magnitude of the characteristic sizes and times of their operation. By "neighboring scales" we mean coupled phenomena that are adjacent in the sequence of dominant phenomena for the given material and application. The characteristic size of a material process usually corresponds to the characteristic size of a type of heterogeneity. There is not a corresponding relation between the characteristic time of a fundamental material process and that of the associated heterogeneity since the process may evolve at electronic, acoustic, or chemical/diffusional speeds.

By way of illustration, in infinite homogeneous systems, like a uniform fluid or an ideal perfect single crystals, atomic motions and continuum elastic response are at neighboring scales. For such systems statistical mechanics theory is successful for analytically making the transition between the phenomenon at the atomistic scale and the macroscopic continuum scale. However, addition of any heterogeneity to a system in this class, which necessarily will be of intermediate scale, completely changes the situation. The intermediate scale heterogeneity greatly complicates relating atomistic processes to the macroscopic behavior. It requires that perhaps several additional phenomena associated with the added heterogeneity be treated. And it necessitates successively linking between the macroscopic behaviors and the intermediate scale phenomena, and then between the latter and atomistic scale phenomena.

A characteristic of current capabilities for MM&S, both within and outside Sandia, is that little is gained by bridging between more than two scales; the shortest response time is usually so much smaller than the response time two scales up that the processes occurring at the second coarser scale do not evolve during the attainable duration of a multiscale simulation. Though this situation should be taken as a caution as to the challenges of developing MM&S methods, it is not a fundamental limitation. There is much to be gained by coupling material simulations pair-wise across adjacent scales, but ultimately the driver for MM&S development is what is needed for the application, not what can we manage to do.

Coupling simulations of material processes across neighboring scales can serve at least one of several purposes. Spatially embedding a fine scale simulation within a coarser scale simulation can provide a desirable boundary condition for the finer scale simulation. For example, a properly contrived coarse surrounding region might be used to absorb all acoustic

vibrations incident on it from the central finer scale simulation so that the central region evolves as though it were part of a very large sample. Testing the validity of boundary conditions is one situation in which a strong interchange between modeling and experiment is important for evaluating the adequacy of the physics of the model. Another purpose for a coupled simulation can be to use a finer scale simulation to evolve the material characteristics locally in a coarse scale simulation as changes take place at the coarse scale. A third purpose can be to provide a way to render a sufficiently accurate treatment of collective, coupled phenomena for material having a rich set of response modes.

7. A formal visiting scientist program, as drafted, is not appealing. But some form of visitors' program would be welcome and beneficial to advancing MM&S capabilities at SNL.

It appears that the program, as outlined (see Appendix D), was too busy at this time. It would perturb the technical staffs' research efforts but not necessarily achieve the intended goal of fostering communication and interaction among the in-house teams developing multiscale materials M&S methods, as well as between Sandia and external researchers. Nonetheless, staff members appeared interested in trying a less structured visitors' program and expect that the desired interaction between the project teams and the visitors, and consequently among the project teams, would develop naturally. Hence, it remains of interest to use available support through existing visitors programs in the Computational Sciences Research Institute (CSRI) and the MESA Institute, and, potentially, one in the Center for Integrated Nano Technology (CINT), to bring graduate students and professors to visit Sandia to pursue collaborations in MM&S with Sandia staff. A recurring, productive visitors' program to advance MM&S capabilities at SNL will need to develop in phases over time and it continually needs to demonstrate its benefit to ongoing project work.

8. Sixteen Federal agencies or departments now have active nanoscience and/or nanotechnology programs that are all part of the National Nanoscience Initiative (http://www.nano.gov/ start.htm). These are a strong driver for development of multiscale material M&S capabilities.

The rapid advance of experimental investigations at the nanoscale is creating an urgent need for quantitative understanding of matter at the nanoscale. The absence of accurate models of newly observed phenomena limits progress. New, robust computational tools and models for quantitatively describing structure and dynamics at the nanoscale are needed to enable rapid progress in nanoscience.[1,2] MM&S to bridge electronic through macroscopic length and time scales is prominent among the modeling and simulation challenges faced in nanoscience. Particular areas of research that require MM&S capabilities include: understanding transport mechanisms at the nanoscale; investigating nano-interfaces, which are complex and heterogeneous, and dominate nanoscale systems; modeling nanoscale opto-electronic devices; simulating nano-interfaces between hard and soft matter. These nano-systems are complex and, though small, most are too large to be simulated directly with quantum density functional theory (DFT). MM&S methods will be needed linking quantum to classical molecular dynamics and, perhaps, to some type of meso-scale simulation to perform the simulations of interest in nanoscience.

The DOE Center for Integrated Nanotechnology (CINT), administered jointly by Sandia and LANL, appropriately has Theory & Simulation as one of its five technical thrusts.[3] The thrust leaders recognize the computational challenge arising because overall material properties and function in nanosystems are often controlled by the coupling of structure and dynamics across many length and time scales. Soft and biomaterials present particular challenges as their responses are governed by complex phenomena, including polyelectrolyte interactions, phase behavior, pattern and structure formation on multiple length scales, and non-equilibrium processes. Similarly, understanding the mechanical responses of nanostructured materials can require spanning from atomic to macroscopic scales.

Hence, the intensity of research and development in nanoscience, the dependence on improved coupled material simulation methods for continued rapid progress, and Sandia's emerging role as a leader in nanoscience research, in combination, make it strategic to focus MM&S method development on particular needs of nanoscience. This will support Sandia's nanoscience R&D and it will give the materials M&S community at Sandia an opportunity to demonstrate the potential of multiscale material simulation in a high visibility field.

Future Directions

The overarching conclusion from our inquiries and discussions with technical staff during the past year is that it is premature to attempt to formulate the 'coordinated research plan' envisioned in the milestone. Owing to the complex and ill-defined nature of the problem, as captured in Conclusions 2 and 3, there is no single solution for making any particular transition between two scales. The more appropriate goal is to develop a set of tools for making scale transitions and experience with applying these tools to real test cases so as to enable us to attack each new problem with higher confidence of success.

This said, here we list several elements that can contribute to and promote the desired capability in multiscale material M&S. The aim of these is for Sandia to acquire capabilities for accomplishments with material simulation that we cannot now make. Such multiscale material M&S will be new, technically desirable, and deserving of greater visibility internally and externally.

1. Continue the Computational Complex Materials Forum (CMF) to foster communication and interaction among staff working on MM&S methods development projects.
2. Develop a web site resource for multiscale material M&S efforts:
    a. list multiscale projects; PIs; project team members; project description; archive of presentation slides;
    b. list technical staff working in materials M&S; their interests; their expertise;
    c. list available materials M&S tools/programs; points of contact; help pages.
3. Capitalize on opportunities to bring in collaborators in MM&S through programs run by the CSRI, MESA Institute, and, possibly, CINT.
4. Maintain a Sandia presence at major technical meetings with sessions on MM&S.

5. Launch a coordinated, broadly based M&S materials project, possibly an LDRD funded project, aimed at promoting further development of MM&S methods and that has strong interchange with experiment.
    a. It would be strategic to chose a nanoscience focus for the test application;
    b. The need is to establish credibility of MM&S by solving a problem that could not be done before. Then this kind of success needs to be used to gain visibility within Sandia for these pursuits.
6. Establish a recurring workshop to advance understanding of a focus area of Sandia interest that is inherently multiscale and reliant on simulation.

A few additional remarks can be made concerning launching a coordinated demonstration project. From discussions with technical staff the idea emerged that there are some canonical problems that demand a multiscale treatment. As conceived, each canonical problem is representative of a class of application problems and captures the essential physics of the class in the simplest, most abstract form. When a canonical problem can be identified it provides the possibility of developing a MM&S method that is suitable for treating at least the basic aspects of an entire class of application problems.

The canonical problem of broadest interest among the Sandia technical staff who participated is that of *interactions of a hydrated ion at a solid surface*. This is the entry problem to simulating surface reactivity in aqueous environments. It is intrinsically multiscale, requiring quantum accuracy near the ion and solid surface, but also needing account made of the essential contributions of the bulk fluid and solid.

That this problem captured the broadest interest is, in part, due to our focusing initially on computational and theoretic methods to bridge the time and length scales from discrete quantum electronic up to discrete or continuum mesoscale, and, hence, preferentially attracting those technical staff with expertise and interest in these areas to our seminar series. We confined ourselves to this scale range to help ensure sufficient commonality of interest and issues among the different projects to make it feasible to promote interactions and coordination among them. Also, though bridging from atomistic to continuum time and length scales is a widely shared, long-term goal, it is a daunting challenge that we did not propose to pursue in its entirety at this time.

Nonetheless, there is a second, well known canonical multiscale problem that drives development, at Sandia and elsewhere, of methods to bridge from atomistics to continuum. It is the problem of material fracture, in which macroscopically applied loads transfer stress to a crack tip, yet the atomic scale events near the crack tip, in the "process zone," govern the evolution of the fracture process. World wide, this problem drives much of multiscale methods development related to mechanics, as illustrated by the upcoming workshop.[4] Sandia's long standing, on-going efforts in understanding fracture, of necessity, include development of multiscale capabilities. The investigators include E.P. (Tony) Chen and his staff in Dept. 8763, E.D. Reedy and R.S. Chambers in Dept. 9123, and E.A. Holm and M.J. Stevens in Dept. 1834.

These two canonical problems differ in two interesting key respects. First, fracture entails *all* length scales while the length scales of interest for ion hydration extend only to meso-scale cooperative phenomena that may occur in the solvent. The important time scales

for the two problems are not necessarily very different. Second, though fracture can involve chemical reaction, it is typically treated as a purely mechanical or thermo-mechanical problem. In contrast, ion hydration is a physico-chemical problem.

It is desirable to identify additional canonical problems for other classes of application like material mechanics, thermal behavior, surface physics, or electrical modeling. For instance, is there one or a few prototypical versions of the multiscale problem of informing internal state variable models used in continuum mechanics calculations with sub-grid scale information on the material state? Perhaps one is to be found in the role of grain boundary behavior and microstructure in determining material constitutive properties.

A capability to treat the hydrated ion problem efficiently and with high accuracy would promote progress in several applications of interest to Sandia: the geochemistry problem of heavy atom adsorption at a mineral surface; metal corrosion; catalysis; technologies for desalination; the electric double layer in batteries and fuel cells; ligand binding with application to sensor design, biological signally, and pathways of infection ; nano-scale interfaces and functionalized surfaces. When coupled with capabilities to determine transition states, this problem also relates to the role of collective phenomena in chemical reactions, which becomes more critical in confined spaces as occur in micro- and nano-fluidics, zeolites and catalysts, active sites of proteins, and ion channels in biological cell membranes.

Sandia has world-class expertise in modeling hydrated systems among staff in Centers 1100, 6100, and 9200 and simulation capabilities in these Centers and Centers 1800 and 8700 in quantum Monte Carlo, quantum DFT, classical Monte Carlo, molecular dynamics, and molecular theory (a.k.a. classical DFT). The broad impact of a capability to accurately treat a hydrated ion at a surface combined with the interest of about a dozen staff having a variety of expertise in computational and experimental materials research are the ingredients needed for creating an exciting project.

REFERENCES

1. Theory and Modeling in Nanoscience, *Report of the May 10-11, 2002 Workshop. Conducted by DOE Basic Energy Sciences and Advanced Scientific Computing.* *http://www.er.doe.gov/production/bes/Theory_and_Modeling_in_Nanoscience.pdf*
2. Nanoscale Science, Engineering and Technology Research Directions, *http://www.sc.doe.gov/production/bes/nanoscale.html*

   Also see: http://www.er.doe.gov/production/bes/NNI.htm
3. *http://cint.lanl.gov/theory.html*
4. "Multiscale Modeling of Strength and Fracture: Linking through the Mesoscale," *http://www-cms.llnl.gov/multiscale/*

Of related interest:

5. R.E. Miller, "Direct coupling of atomistic and continuum mechanics in computational material science," J. Multiscale Comput. Eng., 1, pp. 57-72 (2003).

6. W.A. Curtin and R.E. Miller, "Atomistic/continuum coupling in computational materials science," Modeling and Simul. Mater. Sci. Eng, 11, pp R33-R68 (2003).

APPENDIX A - A sampling of Technical Meetings and Symposia on Material Multiscale M&S

- Symposium on Recent Advances in Microstructural Mechanics and Damage Mechanics of Materials. ASME International Mechanical Engineering Congress (November 14-19, 2004, Anaheim, CA) http://www.asmeconferences.org/Congress04/index.cfm
- Symposium on Nanomechanics and Multi-Scale Simulation of Multi-Physics, the 6th World Congress on Computational Mechanics (September 5-10, 2004, Beijing, China) http://www.wccm6-apcom04.org.cn/minisym/23.htm
- 2nd International Workshop. Multiscale Modeling of Strength and Fracture: Linking through the Mesoscale (January 7 – 9, 2004, Berekeley CA. Sponsored by LLNL). *http://www-cms.llnl.gov/multiscale/*
- Symposium on Predictive Material Modeling and Computational Strategy for Creep and Fatigue Damages. ASME International Mechanical Engineering Congress (November 15-20, 2003, Washington DC)
- Fifth Biennial Tri-Laboratory Engineering Conference (October 21–23, 2003, Santa Fe, NM. Sponsored by LANL) http://www.lanl.gov/projects/ncsd/Tri-Labs/CONFERENCE_SCHEDULE.doc
- The 7th U.S. National Congress on Computational Mechanics (July 27-31, 2003, Albuquerque, NM.):
    - Symposium on Recent Developments in Multiscale Modeling. http://usnccm.sandia.gov/mslist/msDetail.lasso?RecID=fi1160.52
    - Symposium on Multiscale Modeling and Simulation of Material Behavior. http://usnccm.sandia.gov/mslist/msDetail.lasso?RecID=cs920.28
    - Symposium on Multiple-scale analysis of nanoscale mechanics and materials. http://usnccm.sandia.gov/mslist/msDetail.lasso?RecID=Dc1170.53
    - Symposium on Stabilized and Multiscale Finite Element Methods. http://usnccm.sandia.gov/mslist/msDetail.lasso?RecID=ac1220.58
    - Symposium on Mechanism-based approaches to fracture and fatigue. http://usnccm.sandia.gov/mslist/msDetail.lasso?RecID=pa1190.55
- Symposium on Multiscale Material Modeling and Simulation. The 2nd MIT Conference on Computational Fluid and Solid Mechanics (June 17-20, 2003, Cambridge, MA). http://www.secondmitconference.org/
- Multiscale Computational Mechanics for Material and Structures (September18-20, 2002, Cachan, France). http://www.lmt.ens-cachan.fr/mcm2002/

- CECAM Workshop -- Upscaling from *ab initio* to Molecular Dynamics: Interatomic potentials and hybrid methods (July 8-12, 2002, Lyon France). http://www.wag.caltech.edu/home/strachan/cecam_upscale_home.html
- Symposium on Modeling and Simulation of Micro and Nano Systems. The 6th U.S. National Congress on Computational Mechanics (August 1-4, 2001, Dearborn, MI)
- Symposium on Multiscale Material Modeling and Simulation. The 1st MIT Conference on Computational Fluid and Solid Mechanics (June 12-15, 2001 in Cambridge, MA)

Recent Materials Research Society (MRS) symposia:

- MRS Spring 2004 Symposium P: Nanoscale Materials and Modeling Relations Among Processing, Microstructure, and Mechanical Properties. http://www.mrs.org/meetings/spring2004/symp_p.html
- MRS Fall 2003 Symposium KK: Atomic Scale Materials Design-Modeling and Simulation.
- MRS Spring 2003 Symposium W: Multiscale Phenomena in Materials - Experiments and Modeling Related to Mechanical Behavior.
- MRS Spring 2002 Symposium W: Modeling and Numerical Simulation of Materials Behavior and Evolution.
- MRS Fall 2001 Symposium T: Statistical Mechanical Modeling in Materials Research.
- MRS Spring 2001 Symposium AA: Advances in Materials Theory and Modeling-Bridging Over Multiple-Length and Time Scales.
- MRS Fall 2000 Symposium Z: Multiscale Materials Modeling. http://www.mrs.org/meetings/fall2000/program/pdf/ProgramBookZ.pdf
- MRS Spring 2000 Symposium P: Multiscale Modeling of Organic Materials.
- MRS Fall 1999 Symposium A: Multiscale Phenomena in Materials - Experiments and Modeling. http://www.mrs.org/meetings/fall99/progbook/ProgramBookA.html
- MRS Fall 1998 Symposium J: Multiscale Modeling of Materials.
- MRS Spring 1998 Symposium BB: Computational and Mathematical Models of Microstructural Evolution. http://www.mrs.org/meetings/spring98/progbook/ProgramBookBB.html
- MRS Fall 1997 Symposium P: Modeling Across Length Scales for Materials Development. http://www.mrs.org/meetings/fall97/program_book/p.html

APPENDIX B - New Technical journals devoted to Multiscale M&S

Multiscale Modeling and Simulation (SIAM), Editor: T.Y. Hou, Caltech.

International Journal for Multiscale Computational Engineering (Begell House, Inc.), Editor: J. Fish, RPI.

Of related interest:

Modelling and Simulation in Materials Science and Engineering (IOP), Editor: M. Baskes, LANL.

Challenges in Molecular Simulations – A program of the European Science Foundation aimed at building cooperation across Europe in the field of computational physics and chemistry of condensed matter, with emphasis on the development of tools to perform multiscale molecular simulations. http://simu.ulb.ac.be/home.html

APPENDIX C - Complex Materials Forum (CMF) seminars on Sandia projects concerned with multiscale materials M&S methods development

December 12, 2002
Kevin Leung, Nanostructure and Semiconductor Physics (1112)
Title: VASP-QM/MM

I will give an informal talk on my implementation of quantum mechanics/molecular mechanics (QM/MM) capability to the Vienna DFT code (VASP) – an example of the multiscale modeling effort at Sandia. QM/MM methods treat localized regions with ab initio accuracy and apply classical force field boundary conditions. They are potentially useful for addressing problems including solvation of ions/molecules/biological species, water-material interfaces, and electrochemical systems. After a survey of the literature, I will describe my plane wave implementation of QM/MM, the effect of classical force field "pseudo potentials," and the nature of those force fields. Preliminary results will be presented. The main objective of the talk is to promote discussion about this important and growing modeling method.

February 6, 2003
ANNOUNCING: A CMF Seminar Series

Status Reports on Current Multiscale Material Modeling and Simulation Projects
Hosted by: John Aidun, Charles Barbour, Tony Chen, Eliot Fang, and Hank Westrich

Please join us for a series of works-in-progress status reports by the PIs of current Sandia projects that are concerned with various aspects of multiscale materials simulation (the "multiscale projects").

These presentations will be held Thursday afternoons, at 3PM, through the spring. Different from the standard CMF format, 90 minutes will be reserved to allow time for questions and discussion during and after the PI's 30 to 50 minute presentation.

The sessions will be video-conferenced to SNL/CA. Refreshments will be provided.

The target audience is the team members of the set of multiscale projects and other staff interested in multiscale materials modeling and simulation. The aim is to share information, generate discussion, and promote communication among the multiscale projects. Being in-

formal, works-in-progress presentations, these should be "warts and all" discussions of the challenges to achieving the particular multiscale capabilities targeted by each project.

First talk (no abstract):

Jon Zimmerman, Science Based Materials Modeling (8721) will be our next speaker in the series.
Jon's presentation will be next Thursday, Feb 13th at 3PM:
"A Robust, Coupled Approach for Atomistic-Continuum Simulation"

March 20, 2003
John B. Aidun, Mngr., Computational Materials & Molecular Biology (9235)
Title: (Impaired) Vision of the Future of Multiscale Material Simulation at Sandia
Coauthors: J. Charles Barbour, Mngr., 1112 (Nanostructure and Semiconductor Physics); E.P. Tony Chen, Mngr 8726 (Science Based Materials Modeling); H. Eliot Fang, Mngr 1834 (Materials and Process Modeling); Henry R. Westrich, Mngr 6118 emeritus (Geochemistry)

As managers of computational materials departments, we believe that our departments can best continue to increase their impact upon Sandia's missions by developing simulation methods that can treat the set of coupled phenomena that occur over a substantial range of length and time scales in any particular heterogeneous (including reacting) material – in application, all materials are heterogeneous. We are attempting to support and accelerate efforts among the technical staff to achieve such multiscale material simulation capabilities by facilitating information exchange, promoting coordination, and providing visibility. This presentation will begin with a review of the preliminary steps we've taken in these directions.

An early "success" of our efforts was being invited to sign up for a corporate Science and Technology milestone in FY03. In short, the task is to develop a research plan for developing theory, models, and computational methods to link quantum and atomistic scale phenomena to mesoscale (discrete or continuum) system behavior in order to strengthen Sandia's capabilities in materials modeling and simulation. This milestone is intended to move us much closer to the longer term goal of linking quantum, atomistic, and coarse-grained mesoscale simulations to continuum constitutive models, which are essential for the finite element method calculations that are the workhorse computational method contributing to Sandia's mission. The major portion of this presentation will outline apparent constraints and practicalities that the desired research plan will need to accommodate and engage the participants in discussing what they will require to be able to develop the desired multiscale material modeling and simulation capabilities, and your ideas for how to approach the technical challenges.

April 17, 2003
Randy Cygan and Louise Criscenti, Geochemistry (6118)
Title: Multiscale Investigations of Mineral-Water Interactions

The fate of chemical and radioactive contaminants in the environment is related to the ability of natural phases like oxide and clay minerals to attenuate them through chemical sorption. Our ability to understand these processes is provided by bulk experimental data on the partitioning of contaminant species between aqueous solution and a solid phase, and molecular-level data provided by analytical methods such as X-ray absorption, vibrational, and NMR spectroscopies. However, due to complexities in the structure and composition of clay-like minerals, and analytical difficulties in examining mineral surfaces in aqueous solution, it is important to apply theoretical approaches to gain a fundamental understanding and interpretation of these phenomena. In this effort, we use ab initio cluster calculations, classical force field methods, and thermodynamic surface complexation models to examine mineral-water interactions at different length scales.

A general force field suitable for the simulation of hydrated and multicomponent mineral systems has been developed to study the ability of clay-like minerals to sorb contaminants. Interatomic potentials were derived from parameterizations incorporating structural and spectroscopic data from a variety of simple hydrated compounds. A flexible water model is used to describe the water and hydroxyl behavior. Bulk structures, relaxed surface structures, and intercalation processes are compared to experimental and spectroscopic findings for validation. Simulations of clay, hydroxide, oxyhydroxide, and layered double hydroxide phases combine energy minimization and molecular dynamics methods to describe the structure and behavior of water, hydroxyl, surface species, and intercalates in these systems. The dynamics of the water-clay interlayer can be determined with atomic density profiles and surface maps derived from molecular dynamics trajectories. We have successfully simulated the swelling behavior of various clays and the complex structure of antigorite. We have also used these methods to extract partition coefficients for the sorption of radionuclides onto the basal surfaces of clays, that can be incorporated into larger-scale continuum models for risk assessment purposes.

To investigate the efficiency of oxide and hydroxide minerals to attenuate divalent metal contaminants, we first developed a continuum surface complexation model. Thermodynamic parameters were extracted by fitting bulk metal adsorption data with this model. The results suggest that transition and heavy metals adsorb to oxide surfaces in combination with the electrolyte anion. To date, analytical techniques available to investigate this possibility are still under development. Therefore, two other approaches to investigate the potential role of metal-anion complexation at oxide surfaces are underway. The first, is to use ab initio cluster calculations to investigate how metal speciation varies as a function of changing water properties from the mineral surface into bulk solution. The second, is to extend the general force field for clay-like minerals to other metal oxides and hydroxides and examine the distribution of aqueous metal species as a function of distance from the oxide surface into bulk solution. Information from these studies will then be incorporated into surface complexation models for use in field-scale continuum reactive-transport models.

May 1, 2003
Peter Schultz, CMMB (9235) with Aidan Thompson (9235) and Mary Roehrig, Distributed Information Systems (6545)

Title: Quantum-derived empirical simulations for chalcogenide and silica - OR - The dirty, grubby side of a "multiscale" atomistic approach to studying complex materials systems

We describe our efforts to define the methods and develop the simulation tools necessary to study two complex materials systems: chalcogenide phase change material as a candidate for non-volatile radiation-hard memory elements, and silica for examining radiation effects in electronic devices. The crucial phenomena in these materials involve chemical processes - diffusion, phase changes, reactivity - that require dynamical simulations with quantum accuracy or better. The challenge is a familiar one: quantum chemistry is much too slow for adequate dynamics, force-field simulations are too inaccurate to adequately describe the chemistry, and, moreover, mastering and tailoring all the necessary methods to tackle a particular materials system is a major undertaking. We will describe the particular challenges posed by chalcogenides and silica, our roadmap for tackling these challenges, and give progress reports on two software efforts arising from the need to overcome these challenges. Aidan will give an overview of the development of his code GRASP to perform MD simulations with reactive force fields. Mary will describe development of MAUI interfaces to coordinate materials codes, and demonstrate a working interface for Quest, a quantum code.

May 15, 2003
Susan Rempe, Computational Biology (9212) and Mark Sears, CMMB (9235)
Title: Modeling interfacial fluid effects: What it takes to make quantitative predictions

When theorists predict the properties of materials at fluid interfaces, the common complaint is that better implicit solvation models are needed. We will describe our efforts to evaluate quantitatively different approaches, including different implicit solvation models, for predicting the properties of charged and neutral species in liquid water.

May 29, 2003
Edward S. Piekos, Microscale Science and Noncontinuum Transport (9113)
Title: Scale Effects in Energy Transport: We've Got You Surrounded

The trend of producing ever-smaller devices with ever-increasing functionality is pushing thermal management up the list of obstacles that must be negotiated on the road to a successful microsystem design. Compounding this problem, noncontinuum effects appear at short length and time scales, degrading the accuracy of commonly-used design tools, sometimes producing order-of-magnitude differences between predicted and observed behavior.

In response to this situation, Sandia has established a multi-pronged research program in microscale thermal transport. This program combines experiment with modeling at a range of scales in order to provide improved understanding of the relevant processes and, subsequently, predictive models for microsystem designers.

In this talk, I will outline our approach and show results from our work to date. For obvious reasons, I will provide the highest level of detail on my aspect of the program: Monte Carlo simulation of phonon transport. This technique, in terms of where it is most beneficial, lies between atomistic and continuum simulations. Similarities to (and key differences from) di-

rect-simulation Monte Carlo (DSMC) for noncontinuum gas dynamics will be highlighted and insights gained from these simulations will be discussed.

June 26, 2003
N. A. Modine, Nanostructure and Semiconductor Physics (1112) M. Chandross and E. Jaramillo, Materials and Process Modeling (1834)
Title: Modeling Local Chemistry in the Presence of Collective Phenomena

Confinement within the nanoscale pores of a zeolite strongly modifies the physical and chemical behavior of small molecules such as water, ammonia, and carbon dioxide. Realistic modeling of such phenomena requires simultaneously capturing the detailed behavior of chemical bonds and the possibility of collective dynamics occurring in a complex unit cell (672 atoms in the case of Zeolite-4A). This interplay between local chemistry and collective phenomena is characteristic of many important materials science problems. Classical simulations alone cannot reliably model the breaking and formation of chemical bonds, while quantum methods alone are incapable of treating the extended length and time scales characteristic of complex dynamics. Therefore, we have taken a mixed quantum/classical approach. We report our progress in embedding a small region treated with the Kohn-Sham density functional theory within a larger system represented by classical potentials. We believe that a localized representation of the electronic structure is key to achieving an efficient embedding when covalent bonds cross the boundary between the regions. We describe and compare Green's-function-based and energy-minimization-based approaches to solving for this localized representation, and we discuss preliminary results for the behavior of water, ammonia, and the ammonium ion in Zeolite-4A. We will also summarize future work proposed in a pending submission ("Investigating the Chemistry of Nanopores Using a Localized Hierarchical Basis") to the joint BES/ASCR call Theory, Modeling, and Simulation in Nanoscience.

July 10, 2003
James Landry, Surface and Interface Science (1114)
Title: The Physics of Silos and Hoppers

I explore the formation and structure of granular packings using large-scale molecular dynamics simulations. The three-dimensional packings are created through pouring or sedimentation and then settle under the influence of gravity. The final packing state depends strongly on the history of construction. I compare the stress profiles in these packings to the classical theory of Janssen and show how the deviation of the stress from the Janssen form is related to the Coulomb failure criterion. I also investigate how to perturb the system to force it to the classical Janssen form.

Hopper flow has recently been suggested by many groups as an ideal system for studying the onset of jamming, both experimentally and through simulations. I present fully three-dimensional simulations of hopper flow and explore how the internal structure and force

distributions change with decreasing flow velocity. While changing flow velocities have only a small effect on the force distribution, they have a large effect on the impulse distribution. Finally, I will outline a new multi-scale modeling collaboration between Sandia and MIT based on a new model of hopper flow.

July 24, 2003
Chester Weiss, Geophysical Technology (6116)
Title: Anomalous Diffusion of Electromagnetic Fields in Hierarchical Geologic Media

Accurate subsurface imaging is important for a large number of applications including underground facility characterization, monitoring, defeat and damage assessment; resource exploration and recovery (oil and gas, geothermal, geologic sequestration of CO2); and environmental characterization, remediation and monitoring. Among the various geophysical imaging methods currently in practice, those based on the propagation of low-frequency (<1 MHz) electromagnetic (EM) fields are unique in their ability to identify deeply buried (>2 m) electrically conductive targets. However, a fundamental problem in the use of low-frequency EM methods is a basic understanding of anomalous diffusion of electromagnetic energy within highly complex, multi-scale geologic materials. A growing body of evidence suggests that the electrical structure of geologic materials is inherently fractal, arising from the dynamical systems that have generated and altered rocks through geologic time. These observations challenge the applicability of the usual macroscopic Maxwell equations which form the basis of all multi-dimensional numerical models used for subsurface EM imaging. As an alternative, the concepts of fractal signals and random walks through spatially-correlated heterogeneous media are currently under investigation as a means to describe the observed variations in EM earth response. This framework suggests that EM induction may be described by a modified, fractional-order diffusion equation which accounts for the inherently complex, multi-scale, hierarchical structure of geologic materials.

August 28, 2003
Gary Grest, Surface and Interface Science (1114)
Title: Spreading Dynamics of Polymer Nanodroplets

Simulation results for the spreading of polymer droplets will be presented. To study the dynamics of both the precursor foot and the bulk droplet, large drops of ~200,000 monomers are simulated using a bead-spring model for the polymer. Results for spreading on flat and atomistic surfaces will be compared for three different chain lengths 10, 20, and 40 monomers per chain. Comparison for different applications of Langevin and dissipative particle dynamics thermostats will also be presented. The dynamics of the bulk drop are fit to several continuum models. We find diffusive behavior for the precursor foot and good agreement with the molecular kinetic model of droplet spreading using both flat and atomistic surfaces. Despite the large system size and long simulation time relative to previous simulations, no evidence of hydrodynamic behavior in the spreading droplet is found.

September 25, 2003
Veena Tikare, Materials and Process Modeling (1834)

with Michael Braginsky (1834), Guadalupe Arguello, Solid Mechanics Engineering (9126), and Terry Garino, Ceramic Materials (1843).
Title: Numerical Simulation of Sintering at Multiple Length Scales

Sintering is one of the oldest processes used by man to manufacture materials dating as far back as 12,000 BC. While it is an ancient process, it is also necessary for many modern technologies such a multilayered ceramic packages, wireless communication devices, and many others. The process consists of thermally treating a powder or compact at a temperature below the melting point of the main constituent, for the purpose of increasing its strength by bonding together of the particles. During sintering, the individual particles bond, the pore space between particles is eliminated, the resulting component can shrinks by as much as 30 to 50% by volume, and it can distort its shape tremendously. Being able to control and predict the shrinkage and shape distortions during sintering has been the goal of much research in material science. And it has been achieved to varying degrees by many. The object of this project was to develop models that could simulate sintering at the mesoscale and at the macroscale to more accurately predict the overall shrinkage and shape distortions in engineering components.

The mesoscale model simulates microstructural evolution during sintering by modeling grain growth, pore migration and coarsening, and vacancy formation, diffusion and annihilation. In addition to studying microstructure, these simulation can be used to generate the constitutive equations describing shrinkage and deformation during sintering. These constitutive equations are used by continuum finite element simulations to predict the overall shrinkage and shape distortions of a sintering crystalline powder compact. Both models will be presented. Application of these models to study sintering will be demonstrated and discussed. Finally, the limitations of these models will be reviewed.

APPENDIX D - Draft Visitors Program plan

A Strategy for Growing Multiscale Materials Simulation Capabilities at Sandia

John Aidun, Computational Materials and Molecular Biology (9235), MS 0316
Charles Barbour, Nanostructure and Semiconductor Physics (1112), MS 1415
Eliot Fang, Materials and Process Modeling (1834), MS 1411
Hank Westrich, Geochemistry (6118), MS 0750

Sandia National Laboratories, 11 February 2002

Background:

Staff members in several departments have projects underway that either develop or apply multiscale methods for computational materials simulations ranging from quantum electronic to molecular scales. Multiscale simulation capabilities are important to Sandia's modeling and simulation capabilities, but they present a formidable challenge that is not likely to be universally solved by a single method. Moreover, successful solutions are likely to be multi-disciplinary approaches that cross-organizational boundaries.

It is in Sandia's interests for the current efforts in multiscale material simulation (MMS) to thrive, interact, and grow. Our immediate goal is to nurture these current efforts and foster communication and interaction among the separate MMS project teams. Additional goals for material modeling and simulation (M&S) at Sandia follow from this and some are detailed below. A long-term measure of success in these endeavors is for Sandia to become an acknowledged leader in numerical modeling and simulation of materials.

Here we propose developing a SNL program of summer visits by senior scientists in the field of material simulation. We see this as a versatile means for assisting the current MMS projects to progress rapidly and for facilitating communication and interaction among these project teams, as well as with the wider material M&S community within Sandia. Through this program we expect to realize many of the benefits of more coordinated research and development efforts in MMS: the R&D work having a greater impact and progressing faster than the aggregate of the parts would otherwise do; these pursuits gaining greater visibility both within and external to Sandia; aligning with opportunities for the sustained and increased funding that is required for long-term success; enabling the pursuit of exciting science that could not be done without multiscale capabilities. Through the summer visitors program we wish to encourage sufficient overlap among the sets of projects, either in technical approach or target applications, to achieve a desirable level of coordination of these efforts.

While a widely shared, long-term goal is to bridge from atomistic to continuum time and length scales, this is a daunting challenge that we do not propose to pursue in its entirety at this time. Instead, we choose initially to focus on computational and theoretic methods to bridge the time and length scales from discrete quantum electronic up to discrete or continuum mesoscale. This helps ensure a sufficient commonality of interest and issues among the different projects to make it feasible to develop the sought for interactions and coordination.

Proposed Activity – Visiting Senior Scientist Program: Summer visits by selected senior staff to collaborate with a specific SNL MMS project, participate in informal technical group discussions, and interact widely with SNL staff on the MMS project teams.

Initial Scope – Quantum electronic to mesoscale simulation methods and applications.

Purpose & Goals

Immediate (summer '02)– Encourage and facilitate communication and interaction among MMS project teams; obtain input from external experts in the field;

Near Term (FY'02 - FY'04) - Maintain summer program on a recurring basis; foster interdisciplinary interactions within SNL; establish formal collaborations with external experts; gain access to promising students in the area; increase SNL staff interest in MMS; provide MMS efforts visibility within SNL; develop external customers and funders.

Long Term – Expand multiscale R&D activities to extend to continuum modeling of materials; establish Sandia as a leader in (multiscale) material simulation; develop additional external customers and funders; establish internal organization, *e.g.,* LDRD Investment Area in MMS; (Multiscale) Material Simulation Initiative; Materials M&S Institute.

Potential Invitees for Summer '02

(solicit input from MMS project PIs)

Current MMS Projects

1. N. Modine (1112), "Modeling local chemistry in the presence of collective phenomena"
2. P. Schultz (9235), "Calibrated semi-empirical MD methods"
3. L. Frink / S. Rempe (9209), "Coupled quantum-classical solvation simulation"
4. L. Criscenti (6118), "Metal absorption onto oxide surfaces from aqueous solutions"
5. S. Foiles (1834), "Corrosion"
6. J. Zimmerman (8726) "A robust, coupled approach for atomistic-continuum simulation"

Leveraged Tie-Ins – Partners & Funders

CSRI; MESA Institute; CINT;
(SNL/CA summer intern program); other SNL/CA(?)
Campus Executive Prog.; Joint RF Support (MS&T, CIS, μE&P)

Format of Summer Interactions

1. Early on in visit, each visiting scientist gives a joint colloquium to MMS project teams on her/his area of interest and expertise.
2. Visiting scientists are jointly briefed on the set of MMS projects.
3. Each visiting scientist works on a MMS project (pre-identified).
4. Visiting scientists are encouraged to also look for opportunities to make an impact on additional MMS projects.
5. Hold weekly or bi-weekly informal technical colloquia / group discussions alternately lead by each of the MMS project teams. Opened to all; MMS project team staff particularly encouraged to participate.
6. Before departing, each visiting scientist presents summary of work and progress, and appropriate documentation (technical memo, SAND, journal article).

DISTRIBUTION:

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