SAND2007-4519P

Computing & Information Sciences External Review 2007
Computational Science R&D Group

The R&D programs in Computing and Information Sciences (CIS) at Sandia National Laboratories can be conveniently grouped into three areas: Applications Development, Algorithms and Enabling Technologies, and Systems. This grouping has traditionally provided the structure for our External Review presentations and write-ups and also largely reflects the Center 1400 structure. This year, this write-up will discuss the activities within the Computational Science R&D Group.

The focus of CIS work in the Computational Science R&D group is on computational methods for modeling phenomenology in specific areas of scientific or engineering interest to the Labs. In general, we develop methods and/or codes that others can use to solve problems or support scientific studies. We also, at a lower level of effort, use our codes to provide computational support on science or engineering projects for customers, both internal and external to the lab. These computational support projects typically involve some new, novel or otherwise unusual application of the code, which the customers are not currently employing, and which often illuminate the need for new or enhanced computational capabilities.

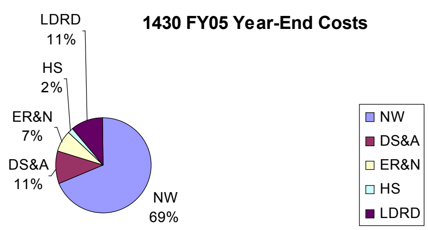
There is a wide range of application areas in science and engineering that a High Performance Computing (HPC) group such as CIS could pursue. In the end, we choose to invest time and resources in those application areas that meet a clear SNL mission need and that we believe will best exploit the HPC talent of the group. Since our work is applied research, a key metric of success is the impact on Lab missions. Another measure of success is the impact on the professional community, through publications and conference presentations, and through collaborations with other leading researchers in the professional community.

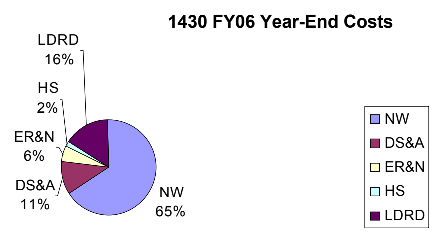
Our applications work also plays an important role in motivating and stimulating research in the other CIS focus areas. For example, our applications work provides important data on the characteristics of new HPC platforms that will be needed to get good performance on the studies of interest to the Lab. The applications also reveal areas where better solvers or algorithms are needed, and where such capabilities will enable us to more efficiently utilize our supercomputing resources.

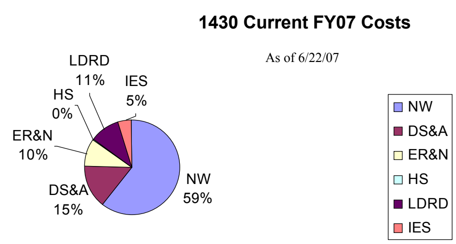
The R&D in our group is mission motivated, and there are five primary areas of mission responsibility, or Strategic Management Units (SMUs), at Sandia. These are Nuclear Weapons (NW), Energy Resources & Non-Proliferation (ER&N), Defense Systems & Assessments (DS&A), Homeland Security and Defense (HS&D), and Science Technology & Engineering (ST&E). In the past, roughly three quarters of the budget for CIS came from the Nuclear Weapons (NW) SMU, so work in our Applications area is particularly focused on the R&D needs of that part of the Lab mission. We do not, however, have sole responsibility for the development of computational capabilities to support the SNL NW program but, rather, share that responsibility with other organizations at the Laboratory; e.g., the Engineering Sciences and Materials Science Centers, among others.

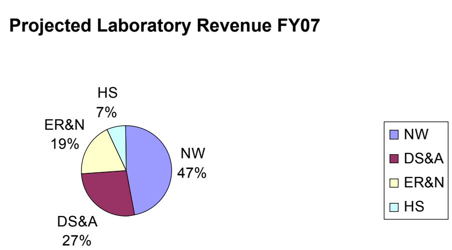
Accordingly, we have chosen applications development for our organization that (1) will have mission impact and improve our national security; (2) have a strong computational science/HPC component; and (3) will allow us to enhance our capability. Thus, for example, while the Engineering Sciences organizations at the Lab have major responsibility for mechanical and structural dynamics modeling R&D, the CIS groups have primary responsibility for R&D on the next generation software for large-scale electrical and electronic systems modeling. Likewise, while the Material Sciences Center has responsibility for understanding the science of materials behavior, staff members in CIS develop many of the codes that the SNL materials scientists use in their studies.

In the recent past, we have supported the NW SMU extensively. We are currently trying to expand our impact to include other SMUs. We want to support the other SMUs by bringing more advanced computational capability to solutions for their customers' needs. We are striving to more closely reflect the overall Laboratories' customer set.

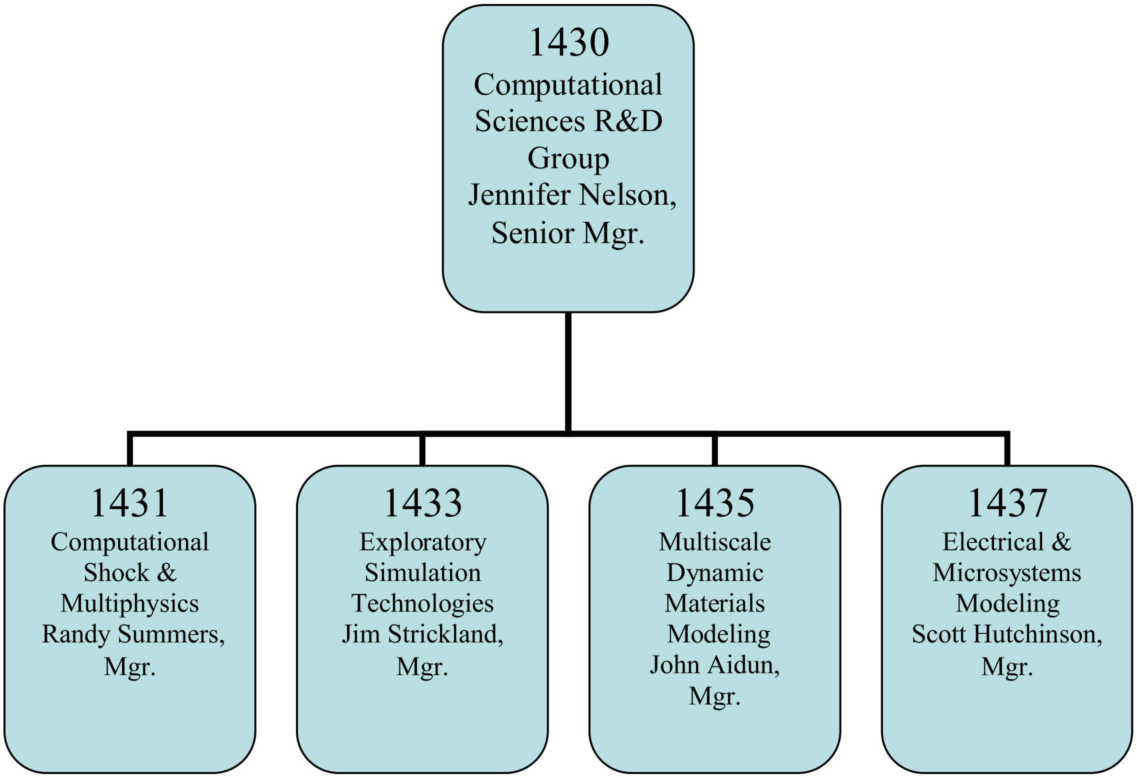








We have maintained the structure we transitioned to in the spring of 2005. This is giving the Lab a more direct focal point for our technologies and has helped facilitate our working with the other SMUs.



The following are more descriptive representations of the Departments within the Computational Science R&D Group:

Department 1431, Computational Shock & Multiphysics

The goal of this department is to develop simulation software for high strain rate and high energy density physics applications at Sandia that require large-scale computations with high resolution grids. Our primary focus is on specialized multiphysics applications for which general purpose hydrocodes or solid dynamics codes are not capable of fully addressing critical phenomena. Examples include many MHD applications that require careful attention to robust solution of coupled magnetic and hydrodynamic phenomena, such as experiments conducted on Sandia's Z machine, electromagnetic armor, and electromagnetic launch technologies, as well as applications focusing on complex failure mechanisms for critical systems and materials, such as ceramic, geologic, heterogeneous, composite, anisotropic, or biological materials. In particular, this area focuses applications with a very clear impact on national security and where the limitations of existing legacy or commercial tools have hindered progress in increasing basic scientific understanding and/or in developing technologies for national security missions. ALEGRA is the principal production code for implementing and demonstrating these capabilities, and Nevada is a common code base that contains the generic building blocks for ALEGRA and other applications and research efforts elsewhere at Sandia, including CHARON, a nonlinearly coupled drift diffusion model for semiconductor applications being developed by Dept 1437.

We have a long standing role and responsibility at the Lab for Applications support in the area of high-energy-density physics (HEDP). One of the most visible Sandia mission areas for this work is the Pulsed Power Program and the associated Z-machine for Above Ground Testing (AGT) of HEDP and radiation effects. This machine generates intense radiation fields through a magnetically driven implosion (Z-pinch) of a tungsten wire array. The complexity of the physics that must be understood to design and execute experiments on the Z-machine has led to our development of capabilities for modeling 3D coupled radiation-magnetohydrodynamics (MHD) phenomena. This HEDP modeling capability is a unique asset for Sandia, and extraordinary insights to details of 3D MHD processes are being obtained through use of our codes in Z-pinch simulations. Upcoming experiments on ZR, the recently completed upgrade to the Z machine, are critical to many science campaigns within the nuclear weapons program, and the ALEGRA-HEDP simulation capability for flyers and Z-pinches is essential to ZR success as the only tool currently available to model key phenomena. Successful completion of an ASC V&V Level 2 Milestone and subsequent application of ALEGRA to simulation of magnetically driven flyer plates have demonstrated a predictive capability for design of dynamic materials experiments. Recent application of this capability saved months of time and hundreds of thousands of dollars from the reduced number of Z shots necessary to characterize the shock melt regime for Beryllium. We have also made extraordinary progress in developing advanced multilevel solver technology for solving very difficult ill-conditioned and singular H-curl systems. Furthermore, we also have a long standing responsibility and sustained level of effort in the area of shock and high-strain-rate physics applications in support of various weapon projects, including shock-actuated component design and weapon effects analysis.

We have developed a significant collaboration with the Army Research Laboratory, in which we work closely with analysts and experimentalists there to apply the MHD technology we have developed for Z-pinch simulations to their unique problems in developing advanced armor concepts. Related work is focused on the implementation and application of statistical variability of material properties as the primary factor in achieving mesh-independent results for material failure. Failure of complex materials is extraordinarily difficult to simulate by traditional methods yet frequently is a showstopper for deployment of new technologies encompassing these materials. The statistical variability approach has demonstrated initial successes in applications for ceramic armor, and a JIEDDO proposal with ARL is expected to be funded to apply this methodology to debris fragmentation for traditional metal armor.

We are in the initial stages of developing collaborations with DoD to apply our MHD capabilities to better understand and resolve the wear mechanisms associated with electromagnetic launch technologies. These wear mechanisms and the influence of various parameters are very poorly understood but are believed to be dominated by MHD behavior at the interface between the rails and the projectile armature. An LDRD project has been funded with the objective of discovering the relative importance of these phenomena.

Department 1433, Exploratory Simulation Technologies

The mission of the Exploratory Simulation Technologies Department is to develop advanced or novel simulation capabilities that utilize high-performance computational methods to solve currently intractable problems of national importance. We currently have three strategic thrust areas; Consequence Simulation and Validation, Earth Systems, and Computational Mechanics. While each of these three areas is somewhat distinct, they are also complimentary. For example, some of the physics-based models that are associated with Earth Systems and Computational Mechanics are utilized in the development of decision support tools associated with our Consequence Simulation and Validation thrust area. Conversely, decision support tools may be useful in speeding up the convergence of numerical physics models. Also, there are a number of similarities in the numerical methods used for solving physics problems associated with the Earth Systems and Computational Mechanics thrust areas.

Consequence Simulation and Validation:

Consequence Simulation and Validation focuses on developing simulation and validation methodologies for high-consequence decision making that typically involves interacting physical, social, and economic systems. Furthermore, we work with established decision making organizations to ensure that such modeling and simulation technologies are effectively introduced into their environments. Although we are pursuing several computational approaches, our present work emphasizes agent-based modeling (ABM) and optimization (ABO). These simulation technologies use autonomous, computational entities (software agents) that perceive and act upon the simulation environment that, in some cases, represent real-world decision makers. As for ABO, agents are used to obtain Pareto optimization solutions that enable one to leverage large-scale parallel resources to analyze seemingly intractable multi-objective decision and control problems. Applications for our work include a wide range of so-called “wicked” problems (i.e., problems characterized by emergent behavior and unintended consequences), including healthcare policy modeling and analysis, climate change impact, the dynamics of conflict, as well as large-scale enterprise modeling for military logistics, nuclear power fuel cycles, and energy policy analysis. Presently, our major external customers are the Joint Warfare Analysis Center (JWAC) and Lockheed Martin Shared Vision (LMC SV).

Earth Systems:

An understanding of various Earth Systems related to climate, seismic and atmospheric wave propagation, as well as asteroid mitigation is becoming increasingly important from a National Security standpoint. For example, an improved understanding of climate change is of paramount importance for mission planning and facilities placement and design. Human societies will respond to climate change adaptation strategies that may lead to a shift in alliances and to civil unrest and conflict. Earth systems modeling includes biogeochemical cycles (such as the carbon cycle) and ocean circulation modeling, including loop currents and methane hydrate thermo-chemical feedbacks. The affects and mitigation strategies associated with asteroid impacts are being modeled by use of Sandia’s shock physics codes. Other codes are being utilized to simulate wave propagation through the Earth’s atmosphere and interior to study the ability to detect and characterize underground, surface, and atmospheric explosions as well as other noise generating activities. A major external customer is the DOE Office of Science that is providing us with funds to develop technology for the community climate model. We presently have CSRF funding to study mitigation of an asteroid-Earth strike and LDRD funding to model wave propagation through the Earth and the Earth’s atmosphere due to a subterranean, surface, or atmospheric explosion.

Computational Mechanics:

The mechanics associated with the development of modeling and simulation software requires a thorough understanding of the underlying physics along with a careful design of the numerical implementation. Here, computational mechanics is used as an umbrella term for the development of a set of physics applications and or associated numerical methodology. A common goal is to provide capability that is accurate, robust and amenable to high-performance computing. For some of our applications, exploratory methods are required which may have limited use outside of the particular application but which may, in fact, lead to use on a broader set of applications. In general, it is desirable to develop capability that has broad applicability (e.g., non-linear solvers, mesh enhancement, code coupling methodologies, etc.). Our present customers in this area are internal and include the ASC program, HEDP, and LDRD. The ASC code Premo has been developed to the point so as to allow initial calculations on the B61 to be made. The re-mesh capability that has been incorporated into Alegra has enabled our HEDP customer to make calculations that were previously impossible. We are in the process of expanding our compressible flow customer base to include AFRL. Code coupling activities for the burner reactor safety code and the Yucca Mountain project are underway.

Department 1435, Multiscale Dynamic Materials Modeling

"Enabling materials research with high performance computing"

We enable and promote high performance computing applications for investigating materials behavior; especially the properties and reactive processes of materials under dynamic and extreme loading conditions. Our core activity is thus extending, enhancing, and developing new computational simulation methods for materials investigations.

The core technical direction of Department 1435 has shifted since FY06, evolving with staffing changes. Two staff members whose work focused on biology departed and the three-member Peridynamics/EMU team was brought in from Department 1431. This addition gives us a secure foot-hold of expertise at the continuum scale and Peridynamics fits with our on-going focus on simulation methods development for materials investigations. The interests and expertise of the staff, collectively, now give the department a significant capability in modeling the dynamic response of materials, including the chemistry and reactivity that accompanies or drives dynamic response. As this area is of basic interest to Sandia, all the NNSA labs, and to DoD, we will emphasize this capability of the department and strengthen it. To this end, the department name was changed to "Multiscale Dynamic Material Modeling"; previously our name was "Multiscale Computational Materials Methods".

Robust, efficient, and relevant materials simulation methods cannot be developed without detailed knowledge and experience with applying the methods. Accordingly, department members also apply our simulation methods in investigations of the physics and chemistry of materials that are first-of-kind demonstrations of using a code or method, as well as for basic scientific investigations, to address issues of particular interest to Sandia that require their special expertise, and to support deployment of our simulation methods to interested groups.

Our efforts focused on material response to dynamic and adverse environments aim to support a range of customers within Sandia and in the DoD. Current and potential internal customers include: the High Energy Density Physics (HEDP) R, D, & A and dynamic material response experiments in Center 1600 (departments 1641, 1646, and 1647); the Explosives Applications department, 5434; the Penetrator Technology department, 5431; the High Power Microwave and RF Applications department, 5443; radiation effects interests of Center 1300; the explosives research in the Explosives Technology Group, 2550; meso-scale manufacturing technique development in Department 2455; and materials issues associated with advanced nuclear reactors in collaboration with Group 6770 and the developing GNEP program.

We have partners throughout the Labs. Most prominent are Departments 1814, 1516, 1111, 1112, 1114, 1132, 1726, 6334, 6338, 8756, 8776, and 8961 as well as our three sister departments in Group 1430. Our funding comes from several programs: ASC, CSRF, LDRD, the DOE-DoD MOU, ESRF, MICS, Campaign 2 (Dynamic Materials Response), QASPR, and WFO (ARL, Boeing, LMC).

Department 1437, Electrical & Microsystems Modeling

For decades Sandia has relied upon Electrical Modeling and Simulation (EM&S) tools to support its varied systems engineering missions. However, the historical reliance upon commercial tools has resulted in a fragmented user group and no leadership for developing a coordinated and focused approach to modern EM&S needs. With current and future high priority missions that rely on EM&S (e.g., the QASPR project), it has become clear that Sandia needs to enhance its EM&S capabilities, programmatic focus, and raise the visibility of 1430/1400's related work.

As noted, Sandia has and continues to rely on commercial tools for much of the design work in this area. However, the commercial software industry has not found a compelling business case for extending their products into the HPC and the prompt radiation effects regime. Sandia has many applications in these areas that are simply too demanding to be met by existing serial commercial tools. These include specific and unique requirements for electrical and electronic systems design that are not shared by the commercial electronics industry. In particular, system robustness in the presence of intense x-ray, gamma-ray and neutron radiation environments is a distinguishing requirement of Sandia weapon electronic systems. Accordingly, we are building on our parallel programming expertise to continue to develop and enhance the Xyce circuit-modeling code that not only scales to very large systems, but that also provides a user interface that is consistent with the commercial products traditionally used by Sandia's electrical designers. Additionally, we are developing a device-level application (Charon) that addresses these effects at the higher-fidelity device-scale behavior in a self-consistent manner. This new capability will be linked with the circuit-level analysis code to provide a crucial suite of tools for Sandia. One such important role for these applications is in support of certification of weapon reliability for hostile radiation environments after shutdown of the Sandia Pulse Reactor.

In FY07, program-development efforts have been undertaken to expand the EM&S support into other national security mission areas at the Lab. These include, primarily, Sandia's WFO work in supporting satellite programs and the design of key electrical components. If successful, such efforts will require circuit-level simulations at an unprecedented scale (~100M devices), potentially driving computational resources in many areas within Center

1400 from Algorithms to Computing to Applications. There is also a potential need from these customers for device-scale simulations that Charon may be well positioned to support.

So, to recap our program element relationships, the work in our Applications areas is motivated by mission needs and there are particular areas of science and engineering applications for which CIS has major responsibility. The Applications codes provide benchmarks concerning the characteristics of new HPC platforms that will be needed to get good performance on the simulations and calculations of interest to the Labs. Our Applications studies, in turn, motivate R&D in HPC Systems and Algorithms and Enabling Technologies, which provides new HPC capabilities to code development and analysis staff within CIS and across the Lab.

Last year's FY 06 external review:

In the course of last year's Application's Area external review session, questions, concerns and advice were generated by the panel and were featured in the outbriefing. The panel requested responses to their questions and concerns from some of the presenters which we have included below.

The FY 06 Applications Session topics were:

1. ALEGRA HEDP, Simulation of Z-Pinch, Allen Robinson
2. Xyce Parallel Electronic Simulator: Making an Impact, Eric Keiter
3. Peridynamics Capabilities and Applications, Stewart Silling
4. Substructured Multibody Molecular Dynamics, Paul Crozier

The panel had specific comments and questions relating to the Xyce (Keiter), Peridynamics (Silling), and Molecular Dynamics (Crozier) presentations.

- ***Panel comments regarding Xyce Parallel Electronic Simulator (Eric Keiter):***

  Panel Comment: The panel is surprised by the apparent difficulty in moving this technology out of the lab.

Response from Eric Keiter:

The Xyce circuit simulation project has continued to show great progress in FY2007, including the release of Xyce version 4.0 in May of 2007. Included in this release was a greatly improved DAE-based variable-order time integrator, which will enhance both the speed and accuracy of the simulator. Additionally, the multitime PDE algorithm is being supported for the first time, which will have a large impact on Xyce's ability to efficiently simulate oscillator circuits.

Under the auspices of the QASPR project, the Xyce team has developed a new compact model for the handling of transient neutron effects in bipolar junction transistors. Unlike previous circuit-level neutron effects models, this model is physics-based and should provide a predictive neutron effects capability. This represents a significant advance, as the conventional wisdom, within the neutron effects community had been that such a predictive model was not possible. By developing this model the Xyce team has significantly improved upon the state of the art for radiation effects modeling of circuits.

The Xyce team is expanding its impact and customer base both inside and outside Sandia lab. Within the lab's NW community, QASPR and RRW continue to be the main focus. However, non-NW customers, such as the satellite groups, are being developed. In addition, negotiations are nearing completion with an established Electronics Design Automation (EDA) vendor to commercialize the Xyce simulator outside the laboratory.

- ***Panel comments regarding Peridynamics Capabilities and Applications (Stewart Silling)***

  Panel Comment: Other efforts in the laboratory (ALE presented in 2005) related to modelling cracks are also being pursued. What is the relationship of this work to the ALE work?

Responses from Stewart Silling:

Alegra uses a continuum damage concept of fracture modeling, like most hydrocodes and finite element codes. In this approach, the stiffness and flow stress of elements are degraded according to some function of the local deformation history. This approach does not attempt to reproduce individual, discrete cracks, as Emu is designed to do. Emu models cracks explicitly, including their initiation, growth, and possible branching and arrest. This results in increased fidelity relative to continuum damage models in problems in which the discrete nature of cracks is important.

One area of commonality between Alegra and Emu is the ability to embed a random distribution of defects within a 3D continuum, then to run a deterministic calculation to evaluate the effect of this distribution on measurable response. In Emu, such random defects are easily created using a Weibull or other distribution of critical stretches for bond failure.

Panel Comment: This work appears similar to a body of work falling into the category of SPH and mesh-free Galerkin methods. Would be useful to better explain differences and unique opportunities.

Response: The mathematical system approximated numerically by Emu is fundamentally different from that solved by other meshless Lagrangian methods such as SPH and EFG. The latter methods solve the standard PDEs of the conventional theory of solid mechanics. Since these PDEs break down on discontinuities, they require special treatment of cracks, such as singular elements and element decohesion (or its meshless analog). They also require some means of tracking the location and configuration of cracks, adding greatly to the complexity of these approaches. They additionally require some means of prescribing the kinetics of crack growth, creating the need for a "crack growth law" and similar relations for crack branching, turning, and arrest. All of these supplemental relations are extraneous to the basic theory of solid mechanics. In contrast, the peridynamic approach is mathematically consistent with the fundamental physical nature of cracks as discontinuities, thereby avoiding the need for all of these "add-ons" to the PDEs. All of the features of crack growth emerge automatically from the basic peridynamic formulation.

Panel Comment: The panel would like to have seen more detail on the mathematical and physical foundations of his formulation.

Response: Although time limitations did not permit an in-depth discussion at the External Review presentation, the mathematical and physical foundations of the peridynamic method are discussed in a growing body of literature. The panel is referred for additional information to the following paper, which contains a thorough discussion, primarily from a continuum mechanics perspective, of the basic method:

S. A. Silling, "Reformulation of elasticity theory for discontinuities and long-range forces," Journal of the Mechanics and Physics of Solids 48 (2000) 175-209.

The following papers contain the basics of our approach to damage and fracture modeling:

S. A. Silling and E. Askari, "A meshfree method based on the peridynamic model of solid mechanics," Computers and Structures 83 (2005) 1526-1535.

S. A. Silling and F. Bobaru, "Peridynamic modeling of membranes and fibers," International Journal of Non-Linear Mechanics 40 (2005) 395-409.

Additional mathematical and physical discussion, including recent advances in the fundamentals of the theory and solution methods, may be found in the following references:

S. A. Silling, M. Zimmermann, and R. Abeyaratne, "Deformation of a peridynamic bar," Journal of Elasticity 73 (2003) 173-190.

O. Weckner and R. Abeyaratne, "The effect of long-range forces on the dynamics of a bar," Journal of the Mechanics and Physics of Solids 53 (2005) 705-728.

E. Emmrich and O. Weckner, "Analysis and numerical approximation of an integro-differential equation modeling non-local effects in linear elasticity," Mathematics and Mechanics of Solids 12 (2005) 1081286505059748v2.

K. Dayal and K. Bhattacharya, "Kinetics of phase transformations in the peridynamic formulation of continuum mechanics," Journal of the Mechanics and Physics of Solids 54 (2006) 1811-1842.

W. Gerstle, N. Sau, and S. Silling, "Peridynamic modeling of concrete structures," Nuclear Engineering and Design 237 (2007) 1250-1258.

P. N. Demmie and S. A. Silling, "An approach to modeling extreme loading of structures using peridynamics," Journal of Mechanics of Materials and Structures (accepted, 2007).

Summary of progress since the FY 06 External Review:
We have made fundamental advances in exploiting the intuitive similarities between the peridynamic continuum model and molecular dynamics. We intend to develop this area of re-

search in the coming years, with the goal of using the peridynamic model as a means to achieve atomistic to continuum coupling within a consistent mathematical framework (and without the need for code coupling). Our initial efforts are documented in the following paper:

R. Lehoucq and S. A. Silling, "Force flux and the peridynamic stress tensor," submitted to Journal of the Mechanics and Physics of Solids (2007).

We completed a manuscript reporting on peridynamic states, which offer a significant generalization of the earlier theory. Peridynamic states avoid the restrictions (such as Poisson ratio = 1/4) inherent in the assumption of pairwise interactions. By removing this assumption, peridynamic states allow a much wider spectrum of material behavior to be modeled while retaining the advantages of the basic approach in reproducing cracks. The state-based approach has now been implemented in the Emu code and is being tested. The manuscript documenting the theoretical work was accepted exactly as it was submitted, without any revision, by a major peer-reviewed journal:

S. A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, "Peridynamic states and constitutive modeling," Journal of Elasticity (accepted, 2007).

Sandia continues to work with The Boeing Company on application of the peridynamic model to impact, damage, and fracture in composites. Recent advances are reported in the following paper:

E. Askari, J. Xu, and S. Silling, "Peridynamic analysis of damage and failure in composites," 44^{th} AIAA Aerospace Sciences Meeting and Exhibit, AIAA2006-88 (2006).

- ***Panel comments regarding Substructured Multibody Molecular Dynamics (Paul Crozier):***

  Panel Comment: Sandia should be encouraged to find a customer to continue funding this promising work.

Response from Paul Crozier:

The SMMD project was funded through LDRD from FY04 through FY06. The primary motivation was to more efficiently simulate biological macro-molecules. When proposed in 2003, Center 1400 shared the mandate at SNL to pursue biology. Sandia's biology efforts are now consolidated into Group 8330 and Department 1435 has not invested effort into program development in biology; nor have there been significant opportunities for collaboration coming out of 8330's program development efforts. Consequently, the SMMD capability has lain dormant for the past year.

Though disappointing, this situation is not unusual. The project resulted in a significant new MD simulation capability that attacked some aspects of the multiscale challenge. We hold it in readiness to collaborate on applying it to suitable problems in biology and nanoscience, as they arise, and we promote its use on suitable problems as they come to our attention. When the opportunity arises to apply the method we will continue adding to it and refining it, as the project funding and goals permit, including developing an automatic substructuring algorithm.

Staffing/Funding Information:

The following is information regarding levels of funding and investment by major areas. The FTE or Full Time Equivalents include only permanent Sandia staff. Not included are limited-term employees, Post Docs, students, faculty etc.

The NW category includes our traditional customers like ASC and QASPR; the Other DOE category includes customers like MICS, and OBER; and the WFO category includes customers such as DoD, and NRC.

Computational Science R&D: FY07 Staffing (FTEs)

	FTEs	NW	CSRF	LDRD	Other DOE	WFO	Total
Computational Shock & Multiphysics							
"Z/Plasma Applications"	7.4	2,384		213			2,597
Advanced Armor Concepts	3.5					1,258	1,258
National Security Analysis	2.8		100			907	1,007
Advanced Methods	2.2	265	335	147		30	777
Exploratory Simulation Technologies							
Consequence Simulation and Validation	4.1		150	274		1044	1,468
Earth Systems	1.5			99	427		526
Computational Mechanics	5	973	590	258		300	2,121
Multiscale Dynamic Materials Modeling							
Atomistic Simulation Methods	4.7	1,275	300	97			1,672
Innovative Continuum Material Modeling	3.9	185	220	50	184	747	1,386
Meso-Scale and Bridging Methods	3	686	75	220		98	1,079
Electrical & Microsystem Modeling							
Electrical Modeling &Simulation	7.9	2,441		350			2,791
Microsystems	1.1	20			35	357	412
Enabling Solution Methods	5.4	415	475	623	391		1,904
Total	52.5	8,644	2,245	2,331	1,037	4,741	18,998