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Computing & Information Sciences External Review 2008
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Computational Science R&D Group

The focus of CIS work in the Computational Science R&D Group (1430) is on developing computational methods and application codes for modeling phenomena 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 ours 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 of Computer System and Algorithms & Enabling Technologies. 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.

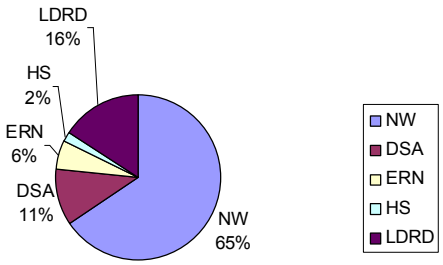
There are five primary areas of mission responsibility, or Strategic Management Units (SMUs), at Sandia. These are Nuclear Weapons (NW), Energy Resources & Non-Proliferation (ER&N), Defense Systems & Assessments (DS&A), Homeland Security and Defense (HS&D), and Science Technology & Engineering (ST&E). In the past, roughly three quarters of the budget for CIS came from the Nuclear Weapons (NW) SMU, so our Applications area has been 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 to improve US 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 organization at the Lab has major responsibility for mechanical and structural dynamics modeling R&D, we have primary responsibility for R&D on shock and multiphysics coupling R&D, and we have begun collaborating with Engineering Sciences to

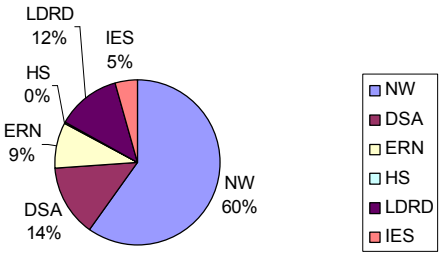
incorporate those technologies into the Sierra Mechanics software system to provide a broader range of integrated capabilities to internal and external customers. We work closely with the Microsystems Science, Technology, and Components Center to provide the next generation software for large-scale electrical and electronic systems modeling. Likewise, while the Material Sciences Center has responsibility for understanding the science of materials behavior, staff members in 1430 develop some 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 increasing our focus on other SMUs to diversify the set of programs we rely on for funding. We aim to support the other SMUs by bringing more advanced computational capability to meet their customers' needs. We want to more closely reflect the overall Laboratories' customer set in the present environment of shifting budgets and national priorities.

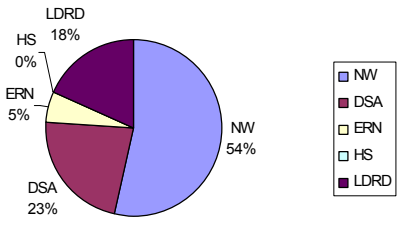
1430 FY06 Year-End Costs



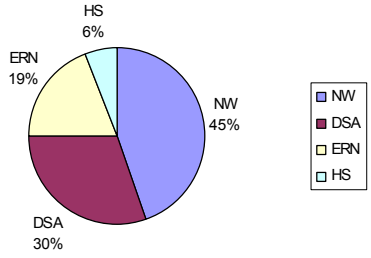
1430 FY07 Year-End Costs



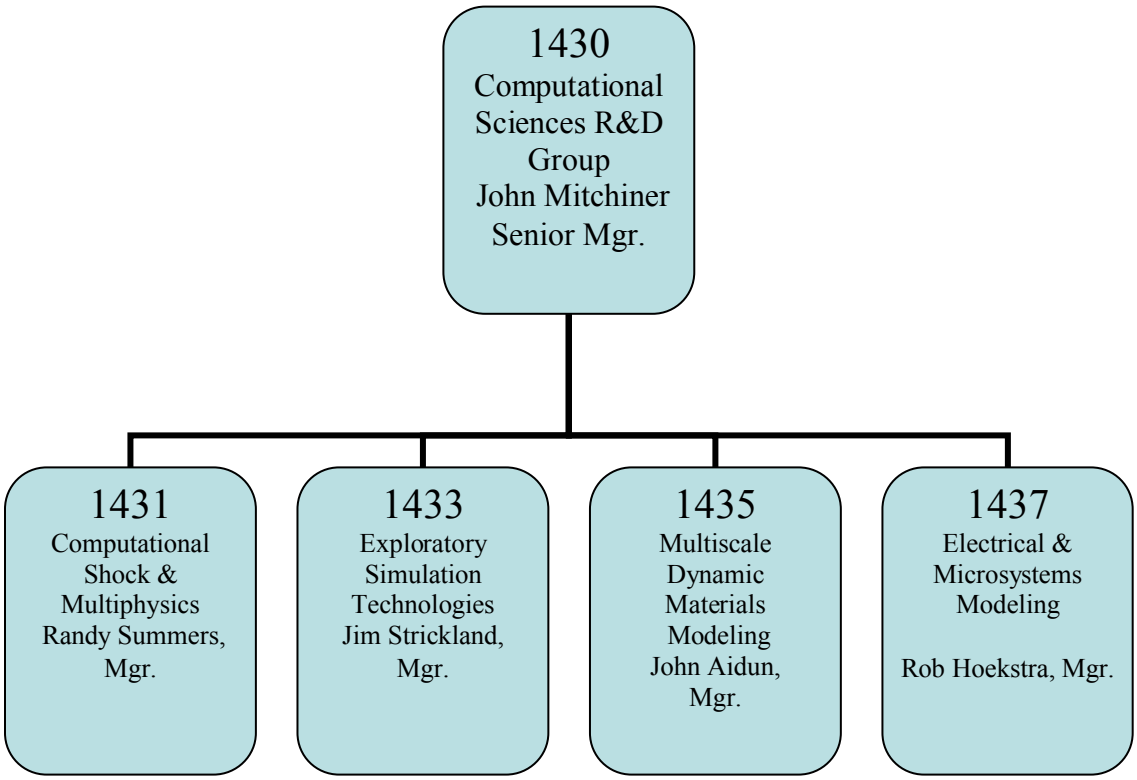
Projected FY08 1430 Revenue



Projected FY08 Laboratory Revenue



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.



A most notable change, however, was the reassignment in January 2008 of Jennifer Nelson from 1430 Senior Manager to the deputy to the VP for Energy, Security, and Defense Technologies (6000). The new Senior Manager, John Mitchiner, moved into 1430 from the Systems Engineering and Analysis Group (6320). John's education is in Mechanical Engineering Systems and Control Theory. John's career has focused on socio-economic-technical modeling and simulation for decision support and artificial intelligence programming. In his previous assignment he led the National Infrastructure Simulation and Analysis Center in support of the Department of Homeland Security.

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. Other applications focus on complex failure mechanisms for critical systems and

materials, such as ceramic, geologic, heterogeneous, composite, anisotropic, or biological materials. We intend that our simulation software have a very clear impact on national security in areas where existing legacy or commercial tools are unable to meet increasing requirements for predictive accuracy and uncertainty quantification.

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. Nevada supports other applications and research efforts 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. 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 new work has been funded by ARL to apply this methodology to debris fragmentation for traditional metal armor.

We have developed 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, and we are implementing new capabilities in

ALEGRA-MHD to simulate EM railgun performance with funding from the Bore Life Consortium within the Office of Naval Research.

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 socio-economic 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) British Petroleum (BP), and Special Operations Command Pacific (SOCPAC).

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 by using 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 LDRD funding to study asteroid-Earth strike phenomenon as well as LDRD funding to better understand the CO_2 cycle as it relates to climate.

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. 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 used to make validated calculations for the flow field over the B61 which includes modeling the spin-rocket fin interactions. The re-mesh capability that was 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 Boeing. Code coupling activities for the burner reactor safety code BRISC and the Yucca Mountain project were largely completed this year.

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 is modeling the dynamic response of materials, including the chemistry and reactivity that accompanies or drives dynamic response. 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 internal customers include: the ALEGRA and CHARON codes in sister department 1431and 1437, respectively; high energy density and dynamic materials response experiments in Center 1600; the Explosives Applications department, 5434; the Penetrator Technology department, 5431; the Information Operations Program , 5640; 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 nascent GNEP program.

We have partners throughout the Labs. Most prominent are Departments 1814, 1516, 1111, 1112, 1114, 1132, 1725, 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 Joint Munitions Project MOU, ESRF, DOE/OASCR, Campaign 2 (Dynamic Materials Response), QASPR, and WFO (ARL, Boeing, LMC, Orica U.S.A.).

Our work spans three technical thrusts, with staff members typically contributing in more than one area:
i) material mechanics – Methods to treat the mechanics of highly heterogeneous bodies or other complex geometries (*e.g.*, polycrystals and damaged structures). Current work in this are includes a set of projects developing and applying the peridynamics method to materials problems spanning a range of length scales, development and application of the extended finite element method (X-FEM), and equation of state modeling with associated improvements in methods and computational tools. This past year also saw an interesting study of early-time stress wave effects on traumatic brain injury.
ii) materials chemistry – Chemistry or reactivity of condensed matter coupled to the material's properties and mechanical response. This area sees development and application of a wide range of methods from quantum and classical atomistics through PDE-based continuum descriptions of charge carriers in semiconductors. Methods developments underway include automating creation of accurate interatomic potentials for classical molecular dynamics, creating a highly parallel, general purpose, kinetic Monte Carlo simulator, contributing to particle simulation (DSMC method) of non-ideal, reacting plasma in strong electric fields, and continual additions to Sandia's flagship MD code, LAMMPS. These capabilities are or will be applied to investigations of high explosives, plasmas behavior in neutron tubes, powering a plasma fuel engine, shock-induced phase transformation, and high dose radiation effects in materials.
iii) quantum methods – Highly functional codes empowered with basic physics and math theoretical advances. Most of the work in this area focuses on improving the accuracy and efficiency of quantum density functional theory (DFT) calculations. Mattsson has recently demonstrated exceptional performance in speed and accuracy from her new functional (roughly analogous to the material model in FEM). Others are extending and improving the efficiency of our local orbital, pseudopotential code, SeqQuest, and LANL's all-electron code RSPt. Basic research is underway into better solvers (density matrix minimizer), and new methods (orbital-free DFT and FEM-based implementation of Kohn-Sham DFT). These capabilities find application in studies of radiation-induced defects, electrochemistry, catalysis, high explosives, material aging, and nano-electronics. Also under this technical area, we are applying various other quantum and semi-empirical methods in studies to assist experimentalists to develop physical systems that can act as Qubits in a quantum computer.

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 program), 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 unique requirements for electrical 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, a device-level application, Charon, has been developed that addresses these effects at the higher-fidelity through finite element modeling of the drift-diffusion equations. As with Xyce, primary focus for this tool is on scalability and radiation effects, both areas of significant impact for the internal user community and built on the expertise developed in our center. This new capability will be linked with the Xyce 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 in hostile radiation environments. Until recently, Sandia relied on experiments using the Sandia Pulse Reactor (SPR) for system certification. SPR was shutdown permanently in FY06, thus creating a requirement for a new program to develop a Qualification Alternative to SPR (QASPR). Xyce and Charon play central roles in the methodology being developed in this program which seeks to utilize tightly coupled experimental efforts with physics-based modeling to form a framework for prediction of stockpile electrical systems response to prompt radiation environments. Charon has been successfully utilized in blind predictions with uncertainty for a single device prototype. We are in the process of an even more ambitious effort to predict circuit performance using Xyce where multiple devices are sensitive to radiation. If successful, QASPR will pave the way for a new certification methodology for weapons reliability.

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 national security mission needs. The Applications codes also provide benchmarks for new HPC platforms and, in turn, motivates R&D in HPC Systems and Algorithms and Enabling Technologies.

Last year's FY 07 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 out briefing. The panel requested responses to their questions and concerns from some of the presenters. The questions and responses are included below.

The FY 07 Applications Session topics were:

1. Graph-based Informatics for Decision Makers, Bruce Hendrickson
2. Charon, Rob Hoekstra
3. Applications of Agent-Oriented Software Engineering to Simulation and Optimization, John Siirola
4. A Mathematical Theory for Peridynamics, Rich Lehoucq

Panel comments regarding Graph-based Informatics for Decision Makers, (Bruce Hendrickson):

- The program was developed in a very professional and committed manner
- Congratulations on
  - Selection by NSF for hosting an XMT system as part of a consortium
  - 3 year LDRD
  - Substantial, new NSA support
  - Upcoming Kolda LDRD
  - Interesting work, good mathematics, well regarded by the outside community (NSA)
    - Graph-based informatics is key to a number of extremely important intelligence issues
- Encourage Sandia to build on this success, and branch out into other related opportunity areas that leverage Sandia's capability as the only discrete math research dept. in DOE
  - Biology may provide an important application domain
- There is a real need to develop deep application knowledge and apply it to benchmarking across all key architectures
- For Sandia to lead in graph-based informatics, including the access of structured and unstructured data is key

Response from Bruce Hendrickson:

We appreciate the constructive feedback the committee provided last year about our evolving strategy and activities in informatics. Considerable progress has been made in the past year in program development and technical advances in this area. Here we provide an update on some of these activities and respond to some of the questions raised last year.

We agree with the committee's comments that the analysis of large datasets is an enormously important issue that 1400 should address. We are pursuing this through several paths. First, we are conducting architectural research motivated by this class of problems. Unstructured data

analysis applications typically have much more challenging memory access patterns than traditional scientific simulations. Our early work on the Cray MTA and XMT systems highlighted the potential impact of non-standard architectures. This understanding is encapsulated in our vision for the X-Caliber architecture, a project led by Rich Murphy. Closely related, Bruce Hendrickson organized a workshop on behalf of the DOE Office of Science and NSA to explore the potential impact of XMT, Cell-based machines, and other emerging architectures on important DOE and DOD applications that perform poorly on current machines.

We continue to make progress on software and algorithms for analyzing large data sets. Our rapidly expanding Titan information visualization and analysis framework is the core unifying technology of our Grand Challenge LDRD on "Network Discovery, Characterization and Prediction". We have also made significant progress on algebraic analysis methods using higher-dimensional generalizations of matrices. In addition, we are continuing to develop new graph algorithms and multithreaded software for informatics applications. This latter activity is at the heart of a significant new work-for-others project that began this fiscal year.

The committee correctly recognized a shortage of expertise in high performance data access techniques. We are actively trying to hire in this area, and we are partnering with experts in Sandia's data warehousing organization. We have also purchased a Neteeza machine are working to explore its capabilities and to formulate a system architecture in which a high performance data server works with our current in-memory analysis tools.

Panel comments regarding Charon (Rob Hoekstra):

- Combination of unique need (radiation effect) with optimization for highly parallel computing is a great example of meeting a key NW need.
- Good progress in few years
- Good choice of practical algorithms to bridge across the multiple distance-time scales
- Good publications and exposure
- Good V&V methodologies
- Cutting edge research presented in a very clear and compelling way
- This is an outstanding example of a highly responsive, professional code development project. Careful incorporation of Verification and Validations from the outset is commendable

Response from Rob Hoekstra:

Since the last review, Charon has played a pivotal role in the success of the Qualification Alternatives to the Sandia Pulsed Reactor (QASPR) program. A blind prediction including quantified uncertainty taking advantage of DAKOTA was performed with outstanding results some of which you will see in the review talks. Significant algorithmic advances have been made including a new Constraint Volume FEM formulation which promises to reduce mesh sizes for QASPR relevant problems by at least a factor of 4. A vertical integration of Trilinos capabilities in Charon, an ASC Level II Milestone, with a strong reliance on automatic differentiation has produced key sensitivities for better physics understanding and opportunities for efficient optimization capability and intrusive UQ supporting future QASPR methodologies and goals.

Panel comments regarding Applications of Agent-Oriented Software Engineering to Simulation and Optimization, (John Siirola):

- CIS has a decade long history in investigating agent-based methods. Agent-based modeling is an important technology for Sandia to develop and invest in for a variety of problems including for Homeland Security/Defense
- Omega-AB could be a useful framework to integrate a number of these methods
  - Useful work-for-others for DoD although final application areas and research content are unclear
  - Will be good to hear about the project and its applications once it matures
- ABO: Interesting result on synthetic problem
  - The hybrid parallel optimization of ABO did meet the need for a new research approach to a very difficult problem.
  - A tangible example of a successful result of these tools would have been helpful, as would a comparison to an alternative approach

Response from John Siirola:

CIS has a decade long history in investigating agent based methods. Agent-based modeling is an important technology for Sandia to develop and invest in for a variety of problems including for Homeland Security/Defense

Omega-AB could be a useful framework to integrate of a number of these methods

- *Useful work-for-others for DoD although final application areas and research content are unclear*

  Omega-AB represents a unique capability for mixed-paradigm (agent-based, discrete event, sequential-modular, and systems dynamics) simulation. There is only one other package that advertises a multi-paradigm modeling capability (AnyLogic by XJ Technologies [St. Petersburg, Russia]), and it is significantly more restrictive in the manner in which it allows modelers to mix the paradigms.

  Specific research topics include:
  - Efficient representation of time in mixed-paradigm environments.
  - Coordination strategies between event- and integration-based components.
  - Visualization of mixed-paradigm models and complex network environments.
  - Parallelization strategies for event-based systems on both traditional MPP and non-traditional (massively multi-threaded) platforms.
  - V&V for continuous, discrete, and agent-based approaches to complex systems modeling. In particular, Omega-AB provides a unique tool for implementing multiple modeling approaches to a single problem within a single common environment. This allows for more direct "apples-to-apples" comparisons among the models and approaches, and may help define appropriate V&V approaches for each paradigm.

- *Will be good to hear about the project and its applications once it matures*

We are continuing development of the core capabilities within Omega-AB. Since the review, development on two new applications has begun. The first leverages the flexibility and extensibility of the Omega-AB framework to build a process development, planning, and scheduling tool. This tool is a specialized extension of the core Omega-AB application tailored to the customer's development and planning processes. It will provide an interactive planning environment that utilizes Omega-AB's underlying simulation capabilities to analyze uncertainty and risk in the final schedule. The second application is using Omega-AB as a test platform for investigating the development of mixed-paradigm modeling (agent-based and systems dynamics) for regional and national energy policy analysis.

ABO: Interesting result on synthetic problem

- *The hybrid parallel optimization of ABO did meet the need for a new research approach to a very difficult problem*

  Research and development on ABO has continued in FY08, targeting a releasable prototype version and integration into the DAKOTA toolkit.

- *A tangible example of a successful result of these tools would have been helpful, as would a comparison to an alternative approach*

  We are still in the research phase for this approach, and as such have not yet applied it to a production application. Work developing ABO has highlighted several new research topics, including management of heterogeneous data among multiple solvers and function evaluators, approaches to describing formulation properties, automatic reformulation based on solver-specific needs, and collection and distributed management of evaluation results. We have integrated much of our work addressing these issues into the forthcoming ACRO 2.0 / COLIN 3.0 releases, which will provide a powerful platform for rapidly developing, testing, and comparing hybrid optimization approaches. In addition, we have begun work integrating both ABO and an alternative hybrid algorithm based on pattern search (HOPSPACK) into the DAKOTA toolkit to support more rigorous testing, evaluation, and comparison.

Panel comments regarding A Mathematical Theory for Peridynamics, (Rich Lehoucq):

- Stated goal is modeling development of cracks in mechanics problems without special consideration.
- Theoretical basis for PD as a continuum version of molecular dynamics was thoroughly presented with reference to current published papers, meeting and/or exceeding the request from last year's review
- Interesting and promising approach to an important but difficult, indeed, unsolved, problem-fracture analysis, especially under strong shocks (e.g. armor penetration)
- Need additional capability for handling conventional materials issues before it can displace the standard codes in this area (e.g. CTH)

- Potentially a good technique for bridging the multi-scale issues from the atomistic to continuum
- Congratulations on Boeing CRADA, LDRD and DOE Office of Science funding

Response from Rich Lehoucq:

The paper discussed at last years external review "Force flux and the peridynamic stress tensor" has been published in the Journal of the Mechanics and Physics of Solids, 56, (2008) pp. 1566-1577. Silling and Lehoucq are revising "Convergence of Peridynamics to Classical Elasticity Theory" conditionally accepted by the Journal of Elasticity. The generalization of the originally proposed peridynamics framework published in "Peridynamics States and Constitutive modeling", 88, (2007) pp.151-184 has been implemented in EMU. An initial implementation of peridynamics within LAMMPS, a massively parallel molecular dynamics code, is under Sandia review for release under a public domain software license.

FY 06 external review (June 7-9, 2006):

In the course of the FY06 external review sessions, questions, concerns and advice were generated by the panel and were featured in the out briefing. The panel requested responses to their questions and concerns from some of the presenters which were included in previous read-ahead materials and listed 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 conven-

tional 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," 44th 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.

FY 05 external review (August 10-12, 2005):

In the course of the FY05 external review sessions, questions, concerns and advice were generated by the panel and were featured in the out briefing. The panel requested responses to their questions and concerns from some of the presenters which were included in previous read-ahead materials and listed below.

The FY 05 Applications Session topics were:

1. Parallel Circuit Simulator for Cell Biology, E. (Chi-Chi) May
2. Evolving Smart Agents, Alex Slepoy
3. Defects in Semiconductor: DFT and Supercell Approximation, Peter Schultz
4. Penetrator Simulations: Advancing ALE Technology, Tom Voth

Panel comments regarding Parallel Circuit Simulator for Cell Biology (Chi-Chi May):

Are there major hurdles for this work? The extraction of the various parameters needed for the simulations might pose a major challenge. The Panel would like to hear about the limits of this approach compared to other existing approaches.

Response from Elebeoba (Chi-Chi) May:

The committee has accurately identified a major hurdle for this work and for the area of systems biology simulation in general. One of the main challenges we are tackling is determining reaction rate parameters that result in simulation results that are well correlated to experimental data. We briefly describe how we are addressing this particular challenge.

A challenge in the development of accurate biological network simulations for systems biology is the availability of accurate rate data for metabolic reactions. Databases like BRENDA (*http://www.brenda.uni-koeln.de/*) contain empirically determined reaction rates for various organisms including *E. coli*. Incorporation of this data will reduce the number of unknown simulation parameters and provide boundaries for model refinement. We revisited our initial Xyce model of tryptophan biosynthesis and reformulated the *BSOURCE* metabolic reaction component in a format that lends itself to available data. Reaction kinetics is described using a form that explicitly incorporates the Michaelis-Menten constant, K_M, and the turnover rate, K_{cat}. Both rates are reported in the BRENDA database. We couple the Xyce model to the DAKOTA optimization framework to refine remaining model parameters based on experimental data that tracks the level of tryptophan in the system.

This approach (reformulation of metabolic reaction component, incorporation of empirical rate information, optimization) improves the BioXyce simulation framework, moving us towards the production of not only qualitative but also quantitatively relevant simulation results. Challenges remain including the applicability of the rate information reported in BRENDA. Rate information appears to be dependant on experimental conditions, including whether experiments are

conducted on wildtype or mutant forms of the organism. Hence, in some instances BRENDA values may not provide exact rate information but we can us it to extract a range of values for the optimization system to explore. Recent advances to Xyce, such as the direct incorporation of DAKOTA optimization capabilities into Xyce, will make this more feasible. Additional challenges include initial condition selection and avoiding over-fitting our model. We will be addressing these issues as part of the recently awarded NIH K25 grant (collaborating with UNM-HSC and Los Alamos); this project will use BioXyce as a framework for modeling host-pathogen interactions in an attempt to better understand latency and reactivation in *Mycobacterium tuberculosis*.

There are several approaches to modeling and simulating biological networks. For example the Berkley BioSpice (Adam Arkin, UC Berkley) project is a large-scale endeavor that incorporates empirical model construction and software development for integrating models into three-dimensional representations of cellular behavior. Such models would provide spatio-temporal information of intra-cellular activity. ChemCell (Sandia developed simulation platform) also provides this type of information. BioXyce does not provide this type of information at the intra-cellular level and given the electrical circuit simulation framework it is based on will most likely not provide such information. But there is the possibility of providing intercellular spatio-temporal information that can simulate a bacterial colony growing towards an energy source. This can be accomplished using the multi-cellular simulation framework demonstrated in the simulation of Drosophila development.

Flux Balance Analysis (Bernhard Palsson, UC San Diego), based on conservation of mass, performs steady state analysis of biological systems and uses a linear algebra approach to identify extreme biological pathways and correlating phenotypic planes. The BioXyce platform focuses on developing dynamic simulations as opposed to performing steady state analysis of the biological system. A current limitation is in using our platform to identify phenotypic regions that correlate to architectural changes (i.e., removal of a genetic or metabolic pathway) in our system. Towards this end our goal is to incorporate methods from control theory (specifically we are exploring collaborations in the area of hybrid-controls) into our simulation framework. The objective is to use a controls based approach to identify: i) Optimal initial conditions that correlate with empirical results or predefined desired results; ii) architectural changes (i.e., *in silico* gene knockouts) that push our system towards previously identified or un-identified phenotypic regions. These augmentations will also be pursued as part of the NIH K25 project.

Panel comments regarding Evolving Smart Agents (Alex Slepoy)

Parallelized Genetic Algorithm: Interesting initial results, evolving existing technology. Would like to see performance on real problems. Would like to see comparison to other Parallel GA work.

Not clear from presentation how genetic algorithms help agent-based modeling. Why genetic algorithms for evolving agents rather than other learning techniques that provide better insight in agent behavior? How does one optimize agents for altruistic behavior?

Response from Alex Slepoy:

The project is currently in the middle of the second year. The project hinges on the technology of "intelligent" agents for agent-based simulation. Such agents are not static programs, but are rather able to redefine themselves during the course of the simulation to fulfill some objective, defined by the user. Such agents are deemed critical to a number of agent-based simulations of robotic behavior or facility security problems at Sandia, where problems posed require evolution of strategy.

The over-all project deals with agent-based applications of "intelligent" agents. I did not attempt to describe this in great detail, since the implementation of the "intelligence" in the agents was targeted towards the later phase of the project.

The first year of the project focused on development of a generalized "thinking" model and its optimization. Early in the project, we selected a Genetic Programming [GP] formalism for this purpose. A GP is a computer program, created by a hierarchical nesting of elementary operators, termed a "tree", that can be optimized via a variant of a Genetic Algorithm [GA] or other methods. This formalism, as far as we know, is the most general formulation of a "thinking" model; it includes all other formulations as its sub-classes.

It is important to note that we are not using a Genetic Algorithm as a learning model. The model here is a functional tree of operators. The elementary operators represent a universal language. Genetic Algorithms are only one optional method for tree optimization.

In the first year, we focused on writing a software application GPPT that carries out a GP optimization on distributed memory clusters. This application was developed and demonstrated near-ideal scaling. Another first- and second-year target was the development of an improved optimization algorithm that would be able to take advantage of massively parallel architecture. We are currently comparing the performance of our optimization scheme to existing parallel GA methods. However, this is becoming less relevant as we have gradually diverged from a classical GA and have advanced into hybrid Monte Carlo methods using Parallel Tempering Metropolis strategies to speed up the search in a very large conformational space of the trees. We have been successful in obtaining significant speed-ups, as tested on an exciting surrogate problem we developed, as described in the following paragraph.

In the surrogate problem, we require the "agent" to recover the functional form of the interatomic potential that is hidden in "black box" fashion as an energy of a system of atoms. The "agent" is presented with a set of atom-filled boxes and their pre-computed total energies. From this information, the "agent" needs to recover the function that generated those energies. This "surrogate" problem in itself is a difficult unsolved problem of great importance to the computational materials community.

To our pleasant surprise, after thinking for over 20 hrs on 100 processors, the agents found the exact Lennard-Jones function that was used to generate the training data. This is an incredible feat, given that that they only sampled 10^8 of the 10^24 possible functions in the search space, and that the function values were strongly obscured when used to generate training data. We are currently writing up this result for publication in a peer reviewed journal.

Evolution of altruistic behavior has been demonstrated for computational models in game theory most notably as Nash equilibrium and its variants, as well as in many other guises. Hence, we also expect to observe an emergence of such behavior for our implementations of the prototypical game scenarios. Cooperative behavior emerges whenever it is a better strategy to achieve a defined objective, however self-serving that objective may be.

Panel comments regarding Density functional theory: Defects in Semiconductor (Peter Schultz):

Appreciate seeing the performance numbers-excellent performance results.

Response from Peter Schultz:

The preliminary results for the silicon defect properties were expanded, polished, finalized and submitted in a Report to Sandia's QASPR project and as a journal article accepted for publication in Physical Review Letters. The final validation study gave results with mean average absolute error of <0.1 eV, comparable to the experimental uncertainty for the same data (for those data that are available from experiment). The computed data are being used in device simulations, the next rung up on the multiscale simulation ladder in QASPR, which was the topic of last year's "Customer Perspective". The application is being extended to predict defect physics in more complex materials of interest to QASPR, such as gallium arsenide. The new method development that enabled this new application has since been released in an official production version of the SeqQuest DFT code, including the new task-parallel capability. Work is now ongoing to develop a data-distributed parallel code to enable the larger materials models that may be required for Sandia simulations.

Applying the method for determining defect properties this past year, I discovered previously unknown charge states for the phosphorous-vacancy pair defect and the boron-vacancy pair defect, which are both common secondary defects in irradiated silicon. New Pv(0/+) and Bv(/0) transitions are predicted, with deep levels near mid-gap that will be important recombination centers to consider in simulations of the electrical response of irradiated silicon devices.

Last year's Density Functional Theory (DFT) work relates to Eric Keiter's Xyce presentation this year. Xyce is two rungs higher on the "multiscale" ladder that comprises the modeling and simulation that CIS enables for Sandia's QASPR project. The defect transition energies determied from DFT contribute to the defect reaction constitutive relations that are solved in combination with the drift-diffusion equation in the electrical device modeler code CHARON. CHARON calculations are used in turn in developing radiation-aware compact device models that are used in XYCE to evaluate circuit performance in radiation environments.

Panel comments regarding Validation of ALE algorithms for penetration modeling (Tom Voth):

This mature project appears to be winding down-does SNL's strategic vision agree with this? SHISM shows potential, are there plans for technology transfer? If this work has new technology in the area of equipotential smoothers, please publish.

Response from Tom Voth:

The project in the form as presented at the CIS external review was at its end though the work has feed several ongoing and more recently completed projects. Specifically, the Verification and Validation work provided the foundation for a successful Level II ASC Milestone (PI: Mike Wong). Additionally, on-going penetration related work includes support for penetrator mechanics research in Org. 15000. Finally, requirements for better mesh smoothing algorithms provided by this work spurred the inclusion and improvement of mesh enhancement algorithms in ALEGRA by Voth and Brewer. These algorithms, as encapsulated in the MESQUITE code (PI: Pat Knupp), are beginning to allow truly Arbitary Lagrangian Eulerian (ALE) simulations of ALEGRA-HEDP/Z-Pinch physics. Until these developments, ALEGRA was primarily used in Eulerian mode as the remesh algorithms were often insufficient for the complicated physics associated with Z-Pinch simulations. Finally, one conference paper was presented and one journal article submitted describing the penetration related validation work.

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, BP, and Boeing.

Computational Science R&D: FY08 Staffing (FTEs):

	FTEs	NW	CSRF	LDRD	Other DOE	WFO	Total
Computational Shock & Multiphysics							
"Z/Plasma Applications"	4.3	1,673					**1,673**
Advanced Armor Concepts	5			380		1,700	**2,080**
National Security Analysis	1.5	337			75	243	**655**
Advanced Methods	3.5	719	250	209		370	**1,548**
Exploratory Simulation Technologies							
Consequence Simulation & Validation	8	13	865	638		1,103	**2,619**
Earth Systems	2.9			350	315	472	**1,137**
Computational Mechanics	3.2	995			157		**1,152**
Multiscale Dynamic Materials Modeling							
Atomistic Simulation Methods	6.8	1,037	200	560		655	**2,452**
Innovative Continuum Material Modeling	2.3	202	295			346	**843**
Meso-Scale and Bridging Methods	3.7	669		660		21	**1,350**
Electrical & Microsystem Modeling							
Electrical Modeling & Simulation	8.1	2,832	105				**2,937**
Microsystems	0.5					163	**163**
Enabling Solution Methods	6.9	404	675	1,036	372		**2,487**
Total	**56.7**	**$8,881**	**$2,390**	**$3,833**	**$919**	**$5,073**	**$21,096**