UCRL-ID-135209

Third Biennial Tri-Laboratory Engineering Conference on Modeling and Simulation

Abstract Book

November 2-3, 1999

Lawrence Livermore National Laboratory, Livermore, CA

Third Biennial Tri-Laboratory Engineering Conference on Modeling and Simulation

Organizing Committee Members

Lawrence Livermore National Laboratory

Arthur B. Shapiro
Principal Contact
Mail Stop: L-140
Phone: (925) 422-5066
Facsimile: (925) 422-5397
E-mail: shapiro1@llnl.gov

Ronna J. Oelrich
Mail Stop: L-113
Phone: (925) 423-3147
Facsimile: (925) 422-1509
E-mail: oelrich2@llnl.gov

Peter J. Raboin
Mail Stop: L-125
Phone: (925) 422-1583
Facsimile: (925) 423-4096
E-mail: raboin1@llnl.gov

Richard P. Ratowsky
Mail Stop: L-153
Phone: (925) 423-3907
Facsimile: (925) 423-5080
E-mail: ratowsky1@llnl.gov

Clifford C. Shang
Mail Stop: L-645
Phone: (925) 422-6174
Facsimile: (925) 422-1767
E-mail: shang1@llnl.gov

Joan R. Whitehead
Mail Stop: L-140
Phone: (925) 423-8812
Facsimile: (925) 422-5397
E-mail: whitehead1@llnl.gov

Tri-Laboratory Engineering Conference on Modeling & Simulation
Lawrence Livermore National Laboratory • Livermore, CA • November 2-3, 1999

Steven N. Kempka
Principal Contact
Mail Stop: 0835
Phone: (505) 844-8918
Facsimile: (505) 844-8251
E-mail: snkempk@sandia.gov

Martha M. Campiotti
Mail Stop: 9405
Phone: (925) 294-2998
Phone: (925) 294-3410
E-mail: mmcampi@sandia.gov

Paul E. Nielan
Mail Stop: 9405
Phone: (925) 294-2510
Facsimile: (925) 294-3403
E-mail: pen@sandia.gov

Los Alamos
NATIONAL LABORATORY

Jeff Hill
Principal Contact
Mail Stop: H821
Phone: (505) 667-9590
Facsimile: (505) 667-3559
E-mail: jhill@lanl.gov

Kay Matsumoto
Mail Stop: P946
Phone: (505) 665-5906
Facsimile: (505) 665-2137
E-mail: kay@lanl.gov

Table of Contents

Tri-Laboratory Engineering Conference on Modeling and Simulation

Schedule of Presentations

Tuesday, November 2, 1999

7:45 a.m. Sign-in . . . . . **Building 123 Auditorium Lobby**

8:15 a.m. Welcome and Introduction . . . . . **Building 123 Auditorium**

8:40 a.m. **Session 1**

Solid and Structural Mechanics 1 . . . . . **Building 123 Auditorium**

- Confinement Vessel Structural Analysis (U) . . . . . R. Robert Stevens
- The Conversion of a Confinement Vessel Structural Analysis from ABAQUS to DYNA3D (U) . . . . . Jason Pepin
- Computing the Pressure-Time History of Explosively Driven Vessels (U) . . . . . Stephen P. Rojas
- The Effects of Aging on the Structural Behavior of O-Ring Seals in Weapons Systems (U) . . . . . David Lo

Material Behavior and Characterization 1 . . . . . **Building 123 Conference Room A**

- Modeling Large Strain, High Rate Deformation in Metals (U) . . . . . Donald R. Lesuer
- Characteristics of Creep Damage for Pb-Sn Solder Material (U) . . . . . H. Eliot Fang
- Multi-Scale Material Modeling with Large Scale Atomistic Simulations of Plastic Deformation (U) . . . . . Mark F. Horstemeyer
- Grain-Scale Transient Dynamics Simulations of Polar Ceramics (U) . . . . . John B. Aidun

Hydrodynamics . . . . . **Building 132 Auditorium Room 1000**

- Debris Formation from Explosively-Loaded Spherical Metal Shells (U) . . . . . Marlin E. Kipp
- Progress in Lagrangian Hydrodynamics (U) . . . . . Tim L. Wilson
- Droplet Formation Caused by the Rapid Expansion of a Liquid (U) . . . . . William T. Ashurst
- High Resolution Experimental Results on Interfacial Physics (U) . . . . . P. M. Rightley

Manufacturing Process Modeling 1 . . . . . **Building 132 Room 1102**

- Determining Bottlenecks in JTA Operations at LANL using Extend Modeling (U) . . . . . William J. Parkinson
- Advanced Automatic Train Control Optimization (U) . . . . . Susanna P. Gordon
- KASSIM: Knowledge-Based Application for Stockpile Sustainment and Integration Management—Abstract (U) . . . . . Johnell M. Gonzalez-Lujan
- A Polymer Model Implementation For Simulation of Silylation Swelling (U) . . . . . Vincent C. Prantil

10:00 a.m. Break

10:20 a.m. **Session 2**

Solid and Structural Mechanics 2 . . . . . **Building 123 Auditorium**

- Simulating Distortion and Residual Stresses in Carburized Thin Strips (U) . . . . . Vincent C. Prantil
- Air-Bearing Guided Intercept and Line-of-Sight Experiments (AGILE) (U) . . . . . Lawrence C. Ng
- Updating of Finite Element Models for Highly Transient Structural Dynamic Events (U) . . . . . François M. Hemez
- Validation of a Finite Element Model Updating Procedure using High Velocity Impact Test Data (U) . . . . . Scott W. Doebling
- Design, Analysis, and Fabrication of the APT Superconducting Cavities (U) . . . . . Robert C. Gentzlinger

Material Behavior and Characterization 2 . . . . . **Building 123 Conference Room A**

- Modeling Polymers (U) . . . . . Matthew W. Lewis
- Modeling Microstructural Evolution in Polymers (U) . . . . . Richard V. Browning
- Modeling Decomposition of Confined, Rigid, Close-Celled Polyurethane Foam (U) . . . . . M. L. Hobbs
- Strong Incremental Objectivity and Integration of Hypoelastic Constitutive Laws (U) . . . . . William M. Scherzinger
- Non-Linear Magnetic Effects in Magneto-Rheological Fluids (U) . . . . . Janine L. Fales

Computational Heat Transfer 1 . . . . . **Building 132 Auditorium Room 1000**

- The Effect of Heat Transfer Coefficient Temperature Dependence on Tensile Thermal Stress During the Active Cooling of a Heat Capacity Laser Slab (U) . . . . . Lisle B. Hagler
- Thermal Sensitivity Analysis for the W-76 Accelerometer (U) . . . . . Kevin J. Dowding
- Thermal-Mechanical Analysis of the NIF Target Positioner (U) . . . . . Wayne O. Miller
- Thermal Analysis of the Passively Cooled Vault Within the Los Alamos Nuclear Material Storage Facility (U) . . . . . C. N. Ammerman
- Thermal / Structural Analysis and Frequency Shift of the CCL Cavities for the Spallation Neutron Source (U) . . . . . Snezana Konecni

Manufacturing Process Modeling 2 . . . . **Building 132 Room 1102**

A Fully Coupled Finite Element Model of the Silylation Process (U) . . . . William S. Winters

Modeling the Silylation Process-Mass Transfer and Chemical Reaction in a Swelling Resist (U) . . . . Greg Evans

LANL Detonator Production Simulation Model (U) . . . . Robert J. Burnside

Comparison of Traditional Algorithms with Modern Computer-Aided Design Tools (U) . . . . Wilbur D. Birchler

The Application of Massively Parallel Computing to Characterize Furnace Brazing Processes (U) . . . . Steven E. Gainoulakis

12:00 p.m. Lunch

1:00 p.m. **Session 3**

Solid and Structural Mechanics 3 . . . . **Building 123 Auditorium**

Particle Accelerator Facility Background Vibration, Causes, Effects, and Mitigation (U) . . . . Stephen Ellis

Limit Cycle Measurements from a Cantilever Beam Attached to a Rotating Body (U) . . . . Christopher L. Lee

Computational Aspects in *hp* Cloud Solutions of Schrödinger's Equation (U) . . . . J. D. Becker

Structural Finite Element Analyses for Support of the Design and Manufacturing of a Weapons Component (U) . . . . Vicki L. Porter

Residual Stresses in an Inconel 718 Clad Tungsten Tube Processed by Hot Iso-static Pressing (U) . . . . . . D. W. Brown

Material Behavior and Characterization 3 . . . . **Building 123 Conference Room A**

Application of ALE3D to Modeling Non-Eroding Penetrators into Concrete (U) . . . . Douglas R. Faux

Multi-Scale Material Modeling Multi-Scale Damage Progression Analysis: Monotonic Loadings (U) . . . . Mark F. Horstemeyer

Modeling Discontinuities and Long-Range Forces with an Alternative Theory of Continuum Mechanics (U) . . . . Stewart A. Silling

Failure in Dynamically Expanding Thin Shells (U) . . . . Michael B. Prime

Coupling a Dislocation Dynamics Model with the ALE3D Continuum Model (U) . . . . Andrew T. Anderson

Computational Heat Transfer 2 . . . . **Building 132 Auditorium Room 1000**

Subsurface Gap Depth Detection by Infared (IR) Imaging Using a Surface Heat Pulse (U) . . . . . . Charles S. Landram

An Investigation of Cutting Tool Temperatures Distributions during Orthogonal Machining (U) . . . . . . Mark R. Miller

Frequency Shift Studies for the Spallation Neutron Source Drift Tube Linac (U) . . . . Lucie M. Parietti

Modeling of Some Thermal and Fluid Flow Issues Related to the Design of the National Ignition Facility (U) . . . . William G. Houf

Comparison of Simple Algorithms for Heat and Mass Transfer during Ablative Reentry (U) . . . . Mark A. Havstad

Manufacturing Process Modeling 3 . . . . **Building 132 Room 1102**

100% Quality Assured Processing for Precision Small Lot Manufacturing: Applications to Brazing (U) . . . . Vivek R. Dave

As-built/As-is Assessment of Geometric and Material Properties for One-Hundred Manufactured Products (U) . . . . Ronald M. Dolin

Confederation of Models to Perform Assessments in Stockpile Stewardship (U) . . . . Michael M. Johnson

Sheffield Inspection Rotary Gage Post-Processing Algorithms (U) . . . . Wilbur D. Birchler

Lean Manufacture of Assemblies for the National Ignition Facility (U) . . . . Lychin Chang

2:45 p.m Break

3:15 p.m. **Session 4**

Solid and Structural Mechanics 4 . . . . **Building 123 Auditorium**

Symmetry Considerations in Finite Volume Solutions in Axis-Symmetric Geometries (U) . . . . Raymond L. Bell

A Highly Efficient Enhanced Assumed Strain Physically Stabilized Hexahedral Element (U) . . . . Michael A. Puso

Segment to Segment Sliding Interface Algorithms for Contact Between Edges (U) . . . . Jerry I. Lin

An Investigation of the Use of Shell Elements for Modeling Inflation of Fabric Structures (U) . . . . Vicki L. Porter

Unconditionally Stable, Implicit Dynamic Analysis of Coupled Flexible Finite Element—Rigid Systems (U) . . . . Michael A. Puso

Comparison of Modeling Techniques for a Three-Layered Shell in ABAQUS (U) . . . . Carole A. Le Gall

9:45 a.m. Break

10:15 a.m. **Session 6**

Mesh Generation and Visualization . . . . **Building 123 Auditorium**

Graphical Programming Tools for Control System Development (U) . . . . .Gary W. Johnson
New Flexibility in Analysis Results from the MDG Code Family (U) . . . . .Douglas E. Speck
Three-Dimensional Geometry Reconstruction from Photogrammetry and Radiograph Data (U) . . . . .Jill Hefele
Pandemonium: A New Tool for Glovebox Process Dose Modeling (U) . . . . .Drew E. Kornreich

Structural Dynamics 1 . . . . **Building 123 Conference Room A**

Seismic Analyses of NIF Structures (U) . . . . .Stanley C. Sommer
To Detail or Too Detailed, That Is the Modeling Question (U) . . . . .Michael A. Gerhard
NIF Target Area Transport Mirror Wavefront Evaluations (U) . . . . .David J. Trummer
Calculation of von Mises Stress in a Random Vibration Environment,
Part I: An Efficient Method for Calculating RMS von Mises Stress (U) . . . . .Daniel J. Segalman
Calculation of von Mises Stress in a Random Vibration Environment,
Part II: Predicting the Probability Distribution for Cases of Gaussian Loads (U) . . . . .Richard V. Field, Jr.

Classified 1 . . . . **Building 132 Auditorium Room 1000**

Amy N. Robertson
Thomas A. Butler
Ramsey C. Chun
Steven L. Creighton
Brian H. Aubert

Computational Fluid Dynamics 2 . . . . **Building 132 Room 1102**

Lattice Boltzmann Simulation of Particulate Media in Microfluidic Systems (U) . . . . .David S. Clague
Computation and Measurement of Turbulent Dispersion of
Toxic Aerosols or Gases In Enclosures (U) . . . . .Richard A. Martin
Homogeneous Charge Compresson Ignition Engine Combustion Modeling (U) . . . . .Daniel Flowers
Modeling Thermal Batteries using a Multi-Dimensional Stefan-Maxwell Framework (U) . . . . .Ken S. Chen
Simulation of High Speed Gas Flow in a Reservoir-Receiver-Valve System (U) . . . . .Robert W. Meier

12:00 p.m Lunch

1:15 p.m. **Session 7**

Parallel Methods and Algorithms . . . . **Building 123 Auditorium**

Moving NIKE3D Towards Parallelism: Exploratory Efforts with Sparse Direct Linear Solvers (U) . .Robert M. Ferencz
Zoltan: A Dynamic Load-Balancing Library for Parallel Applications (U) . . . . .Karen D. Devine
Salinas—A Massively Parallel Sparse Eigensolver for
Structural Dynamics Finite Element Analysis (U) . . . . .Brian J. Driessen
Parallel Implicit Electromagnetics using the Vector Finite Element Method (U) . . . . .Daniel A. White
A Parallel Contact Algorithm with Dynamic Load Balancing for Explicit/Implicit Finite Element
Methods and Applications in Solid and Structural Mechanics (U) . . . . .Anthony J. De Groot

Structural Dynamics 2 . . . . **Building 123 Conference Room A**

Structural Dynamics Analysis of an Extreme Ultraviolet Lithography Optical System (U) . . . . .Clay Fulcher
Modal Survey of a Medium Energy Superconducting Radio Frequency Cavity
for Accelerator Production of Tritium Project (U) . . . . .Gretchen W. Ellis
Design Parameter Sensitivity of the B61 Nose Structural Dynamics Model (U) . . . . .Howard P. Walther
Seismic Fragility Models for Reinforced Concrete Moment Frames with Masonry Infill (U) . . . . . .Michael W. Salmon
On the Use of Inverse Dynamic Analysis to Determine Hostile Shock Component Specifications
for the MC4380 Neutron Generator (U) . . . . .Jeffrey L. Dohner

Classified 2 . . . . **Building 132 Auditorium Room 1000**

Lara D. Daily
Allen G. Baca
Francisco M. Guerra
Francisco M. Guerra
Kin L. Lam
Susurla S. Murty

Welcome

The Organizing Committee welcomes you to the Third Biennial Tri-Laboratory Engineering Conference on Modeling and Simulation at Lawrence Livermore National Laboratory, Livermore, CA.

Abstract Book

This Abstract Book has been printed for your convenience and for future reference. The individual abstracts have been approved by the security organization at each laboratory. They are printed as received from the authors.

The Book is organized by sessions and then by topic areas. The abstracts are listed in the order of presentation.

Session 1: Tuesday, November 2, 1999, 8:40 a.m. – 10:00 a.m.

Solid and Structural Mechanics 1
Building 123 Auditorium

Confinement Vessel Structural Analysis (U)

R. Robert Stevens
Los Alamos National Laboratory

Hydrodynamic experiments involving high explosive (HE) detonations have traditionally been done in "open air," but there is now increasing emphasis on conducting these experiments inside of large steel vessels so that no materials or gases generated during the explosive tests are released to the environment. These confinement vessels are subjected to severe blast loading and must reliably prevent any environmental release of material over their expected lifetime.

The structural analysis of these confinement vessels is currently being performed on the ASCI Blue Mountain computer using a combination of two numerical techniques: the transient pressures acting on the inner surfaces of the vessel are computed using an Eulerian hydrodynamics code, and the vessel's structural response to these pressures is analyzed using an explicit finite element structural dynamics code.

The presentation will focus on the modeling techniques that were used to represent the bolted joints attaching the vessel's massive doors to their nozzles. Also, the strategy used to create the million-plus element mesh will be described, and some modeling details that are important for good performance with the structural analysis code "ParaDyn" (the massively parallel version of Dyna3D) will be discussed.

The Conversion of a Confinement Vessel Structural Analysis from ABAQUS to DYNA3D (U)

Jason Pepin
R. Robert Stevens
Los Alamos National Laboratory

Confinement vessels are currently being designed to contain hydrodynamic experiments involving high explosive (HE) detonations. These confinement vessels are subjected to severe blast loading and must reliably prevent any environmental release of material over their expected lifetime.

The structural analysis of the ports (doors and nozzles) of these confinement vessels was previously performed using ABAQUS Standard and Explicit. In order to analyze the entire vessels structural response, it was necessary to convert the ABAQUS model to DYNA3D as a blueprint for running "ParaDyn" (the massively parallel version of DYNA3D) on the ASCI Blue Mountain computer.

This presentation will focus on the modeling techniques that were used to convert an ABAQUS model containing separate implicit and explicit steps into a DYNA3D model. Specifically, the method used to preload the bolted joints attaching the vessel's doors to their nozzles will be discussed. Also, the strategy used to eliminate hourglassing will be described, as well as some modeling details that are important when preparing the DYNA3D model for use with "ParaDyn."

Computing the Pressure-Time History of Explosively Driven Vessels (U)

Stephen P. Rojas
Ralph R. Stevens
Gary A. Dilts
Los Alamos National Laboratory

The Eulerian hydrocodes CTH and MESA were used to estimate the pressure-time response of spherical vessels used to contain detonation products. Data from MESA and CTH are compared to experimentally determined pressure-time and impulse histories. Parametric studies were conducted to investigate the effects of detonation location and explosive mass on the characteristics of the resulting pressure-time profile. Tracer particle data was averaged and handed off to the Lagrangian structural dynamics code ParaDyn in order to study the detailed structural response of the vessel. Global stress and strain results for the subsequent ParaDyn model will be compared to the hydrocode modeling results which used similar material modeling assumptions.

As a supplement to this work, the smooth particle hydrodynamics code SPHINX was investigated as a candidate to incorporate the effects of fragmentation into the pressure induced vessel response. SPHINX calculations were performed which yielded pressure-time data as well as fragment mass distributions and penetration depths.

Comparisons between available test data and SPH calculations will be presented.

The Effects of Aging on the Structural Behavior of O-Ring Seals in Weapons Systems (U)

Linda A. Domeier
Wei-Yang Lu
Vera D. Revelli
Sandia National Laboratories, Livermore, CA

C.S. (David) Lo
Kenneth T. Gillen
Daniel J. Segalman
Sandia National Laboratories, Albuquerque, NM

Mark H. Wilson
Allied Signal, Inc., Kansas City, MO

All weapon systems depend on the ability of elastomeric O-ring seals to guarantee environments over long periods of time. This project is developing a predictive model for the reliability of butyl rubber O-rings after long-term aging in the field, including the physical and chemical effects on aging. The model utilizes rheological experiments to quantify material model parameters. Stress relaxation, compression set, leakage rate, sealing force experiments, and mechanical properties (i.e. tensile strength) are used to identify important features needed in the model. A constitutive model for butyl rubber is being implemented in the JAS finite element code. The JAS results are in turn used in the Advance Mean Value method to develop statistical measures of the lifetime of butyl rubber O-rings in stockpile weapons.

This work includes O-rings from the W76, W80, and W87, but all weapon systems depend on the ability of elastomeric O-ring seals to guarantee environments over long periods of time. For the original design lives of approximately 20 years it was appropriate to assume that the behavior of the joints did not change over time. However, recently life requirements of greater than 50 years have been proposed for nuclear weapons in the enduring stockpile. This project is focused on characterizing butyl elastomers and developing deterministic models for use in statistical prediction of o-ring reliability. The question addressed is at what point does degradation in O-ring material behavior compromise the integrity of a sealed joint?

This is a continuing project. In FY00, the focus will be on developing a practical method to measure the sealing force of stockpile return O-rings; characterizing the time dependent material behavior utilizing parameters obtained with new state-of-the-art equipment; understanding inherent variability shown in current data; completing the new additions to the JAS code for modeling effects of physical relaxation on O-rings in fluctuating temperature environments; and updating probabilistic analyses.

Material Behavior and Characterization 1
Building 123 Conference Room A

Modeling Large Strain, High Rate Deformation in Metals (U)

Donald R. Lesuer
Gregory J. Kay
Mary M. LeBlanc
Michael J. O'Brien
Lawrence Livermore National Laboratory

Many modeling problems require accurate representation of the high-rate, large-strain deformation response of metals. Examples include processing operations (such as metal cutting, rolling and forging) as well as the in-service performance of metals (such as ballistic penetration and perforation, munition performance and explosive fragmentation). In this paper, we examine the large strain deformation response of 6061-T6 and Ti-6Al-4V over a range in strain rates from 10-4 s-1 to over 104 s-1. The results have been used to critically evaluate material models used for simulations involving large strains and high deformation rates, including the Johnson-Cook material model. Two new models that address the shortcomings of the Johnson-Cook model were then developed and evaluated. One of the models is derived from the rate equations that represent deformation mechanisms active during moderate and high rate loading while the other model accounts for the influence of void formation on yield and flow behavior of a ductile metal (the Gurson model). The characteristics and predictive capabilities of these models are then reviewed.

Characteristics of Creep Damage for Pb-Sn Solder Material (U)

H. Eliot Fang
Michael K. Neilsen
Sandia National Laboratories, Albuquerque, NM

C. L. Chow
University of Michigan, Dearborn, Michigan

A critical consideration in characterizing aging of solder joint material for electronic packaging is its viscoplastic behavior. This is because the Pb-Sn eutectic solder material is highly rate sensitive and time dependent. Recently, a viscoplastic model incorporating the grain size and damage as internal state variables has been developed to examine the characteristics of creep damage in 60Sn-40Pb solder material. Based on the theory of damage mechanics, a two-scalar damage model is developed by introducing the damage variables and the free energy equivalence principle. An inelastic potential function is proposed to derive an inelastic damage evolution equation by applying the concept of inelastic damage energy release rate. It is postulated that a material element is said to have been ruptured when the total accumulated damage in the element reaches a critical value.

The damage coupled viscoplasticity model is discretized and incorporated into a finite element program. To illustrate the application of the model, several case examples are devised to analyze, both numerically and experimentally, creep behaviors of the material at several stress levels at room temperature (22 °C). The results demonstrate that the proposed model can successfully predict the behavior of the solder material.

Multi-Scale Material Modeling with Large Scale Atomistic Simulations of Plastic Deformation (U)

Mark F. Horstemeyer
Mike I. Baskes
Steven J. Plimpton
Sandia National Laboratories, Livermore, CA

Large scale, large strain atomistic simulations were performed with the Embedded Atom Method (EAM) to determine various parametric effects on yield and plasticity of single crystal nickel: (1) size scale (from nanometers, 40 atoms, to 1.6 microns, 100 million atoms), (2) crystal orientation (single slip, double slip, quadruple slip, and octal slip), (3) strain rate (1e6/sec to 1e12/sec), (4) temperature (100K to 900K), (5) various stress states (simple shear, torsion, and compression), and (6) different initial dislocation densities. In particular, we focused on the effects of dislocations on the stress state to motivate continuum theory plasticity models. Implications of these atomistic results on continuum theories of plasticity will be discussed. A discussion on the spatio-temporal constraints of atomistic simulations will be discussed in the context of serial and parallel computing.

Results show that the nucleation of dislocations plays a critical role on the determination of yield (and the stress state througout the deformation). Further, a length scale parameter relating the volume to surface area of a critically stressed volume is introduced to model the length scale trend of yield. Plasticity is categorized into three length

scale domains with appropriately related continuum equations. We first examined other orientations and their averaged stresses, axial stresses, and distributions throughout the block of atoms. Results related to crystals oriented for single slip, double slip, quadruple slip, octal slip and a pseudopolycrystal, in which the single crystal results were averaged, are described. Non-Schmid effects are shown to arise during the deformation process. Finite element calculations of simple shear were performed and show the same locations of stress and strain gradients under "simple shear" boundary conditions as the atomistic simulations. Strain rate effects related to yield (and stress state at different strain levels) are illustrated by the phonon drag effect that has been experimentally observed. Kinematic variables related to an atomic strain tensor have also been defined and results related to dislocation populations will be examined.

Grain-Scale Transient Dynamics Simulations of Polar Ceramics (U)

John B. Aidun
Rebecca M. Brannon
David M. Hensinger
Mark D. Rintoul
Allen C. Robinson
Veena Tikare
Sandia National Laboratories, Albuquerque, NM

The ferroelectric ceramic, lead zirconate titanate (PZT) is the heart of shock-actuated power supplies that have been in used reliably in the stockpile for decades. The power supplies are well engineered with a highly nonconservative design for high performance. However, because details of their performance are not well understood, it is difficult to make successful design modifications. Consequently, in the current environment of reduced testing, numerical simulations are being used to add understanding and predictive capability to available experimental observations. This capability will facilitate successful design modifications to suit the power supply for new size and performance requirements. In support of both component-level numerical simulations of the power supply and development of a new ceramic production process, an effort is underway to simulate, at the grain scale, shock wave propagation in PZT. The approach will be described for performing grain-scale simulations of stress wave propagation in the porous, phase-transforming, polarized ceramic in the presence of quasi-static electric fields. The status of efforts in microstructure generation, meshing, extensions to the ALEGRA-EMMA code, and modeling of the ferroelectric material will be presented.

Hydrodynamics
Building 132 Auditorium Room 1000

Debris Formation from Explosively-Loaded Spherical Metal Shells (U)

Marlin E. Kipp
Sandia National Laboratories, Albuquerque, NM

The formation of debris resulting from explosive loading of metal shells continues to be an area where substantial experimental and computational effort is directed. When the metal shell is on the interior of an explosive charge, and the explosive is one-point initiated, the post collapse behavior of the metal is of interest. As the metal expands, the debris created during the fracture process becomes a source term for dispersal of any respirable particles that form either promptly or during subsequent motion.

Many small-scale explosive experiments using hollow spherical metal shells have been performed, and the effort to model the response with numerical simulations is ongoing. Both two and three dimensional calculations with the CTH Eulerian shock physics code have addressed this geometry, focused on the fragmentation aspect of the metal. The goal has been to obtain a fragment source term that could be used as input to a more global model that accommodates the local environment and models other processes that lead to the aerosols which are eventually dispersed into the atmosphere.

Full three-phase equations of state are required to capture the material response to the intense shock loading and subsequent release that is experienced by the metal. Methods to determine the fractions of solid, liquid, and vapor have been pursued, and techniques to obtain explicit fragment characteristics (size, velocity, state) have been implemented.

Numerical simulations of metals loaded in this manner include silver, steel, and tantalum. The calculated steel motion displays excellent agreement with available radiographic data, including the observed jet formation.

Progress in Lagrangian Hydrodynamics (U)

Tim L. Wilson
Edward J. Caramana
Charles H. Neil
Los Alamos National Laboratory

Historically, Lagrangian methods formulated on two-dimensional quadrilateral meshes and used to compute multi-material compressible flow have been plagued with several difficulties such as lack of symmetry for unequal angular zoning, anomalous grid distortion (hourglass and spurious vorticity), mesh tangling, lack of energy conservation and arbitrary artificial viscosity effects.

Herein we present a new method, developed by Caramana et al.[1-4], that eliminates the above mentioned difficulties and show results for applications of interest. The new method is formulated on a standard staggered grid: density, internal energy and pressure are zone-centered while velocity is located at the nodes. In addition to this principle mesh, the computational domain is also discretized with a median mesh that connects mid-points of opposite zone edges. Thus, the median mesh subdivides a principle zone into subzones.

The heart of the method is a discrete compatible formulation for three evolution equations—total energy, specific internal energy and momentum—that guarantees total energy conservation to machine roundoff. When applied to subzones where differences in subzonal densities produce differences in subzonal pressures, the compatible formulation gives rise to differential forces that resist spurious distortion. A modification of the pressure gradient operator preserves symmetry when symmetry is present in the physical solution and gives results close to the unmodified gradient operator when the solution is asymmetric. A new edge-centered artificial viscosity possesses the desirable properties of dissipativity, Galilean invariance, self similar motion invariance, wave front invariance and viscous force continuity.

Results from complex problems are presented and compared with results from an older Lagrangian method.

References:

1. J. Comput. Phys. 141, 174 (1998).
2. J. Comput. Phys. 142, 521 (1998).
3. J. Comput. Phys. 144, 70 (1998).
4. J. Comput. Phys. 146, 227 (1998).

Droplet Formation Caused by the Rapid Expansion of a Liquid (U)

William T. Ashurst
Sandia National Laboratories, Livermore, CA

Brad Lee Holian
Los Alamos National Laboratory

Atomization of a diesel fuel jet occurs over microsecond time scales and over sub-millimeter distances. The liquid

jet breakup may depend upon cavitation and involves creation of new liquid surface area. Neither of these effects are well described by continuum models of fluid dynamics.

To obtain a direct numerical simulation of the atomization process, we have used the molecular dynamics (MD) method which directly computes the atomic motion. However, simulations at the atomic scale have the disadvantage of being small in size and short in time: an MD simulation at nano-scales (nanometers and nanoseconds) represents a huge task. Therefore, instead of the complete fuel jet breakup, we have simulated a much smaller homogeneous volume of liquid which undergoes atomization during an applied rapid expansion. In the calculations, the liquid volume is composed of only 32,000 atoms, and it is expanding into a vacuum. The resulting fragments are the droplets and they are examined for their size and temperature.

The mean droplet size has a power-law dependence upon the initial expansion rate, in agreement with two continuum models of fragmentation. The continuum model which converts elastic energy into surface energy at a critical time has the better agreement with the MD results. But neither continuum model describes the droplet size distribution. The MD simulation results also appear to be in agreement with experimental results obtained with the free-jet expansion of liquid helium in which the largest drop contains 40 million atoms—over a thousand times larger than those in the simulations. A brief summary of the work is available at: http://www.ca.sandia.gov/CRF/Research/Basic/ashurst_physrevE99/index_4.html

High Resolution Experimental Results on Interfacial Physics (U)

P. M. Rightley
R. F. Benjamin
R. A. Pelak
K. P. Prestridge
P. V. Vorobieff
W. J. Rider
J. R. Kamm
J. E. Hammerberg
Los Alamos National Laboratory

The cornerstone of code credibility is the resolution and accuracy of the comparisons with experimental reality. Fundamental to such comparisons, accurate, high-resolution experimental data must be produced in quantity. In support of this goal of validation, we have designed and performed two innovative, inexpensive experiments on interfacial dynamics. We describe the results of laboratory-scale experiments on metal-on-metal friction and fluid instability.

One study endeavors to better understand the physical interactions at the contact interface between two metals sliding relative to one another at high speeds and loads. Current knowledge (both experimental data and models) is quite limited when the relative velocity becomes a significant fraction of the sound speed in either material. The data obtained in the course of this experimental study as well as the computations required to infer interfacial conditions are enhancing our understanding of the interfacial dynamics and providing an important benchmark for ASCI validation studies.

In the second project, results with high spatiotemporal resolution from shock-driven gas curtains provide valuable benchmarks for quantitative hydrocode validation. We visualize a vortex-dominated flow of a thin curtain of heavy gas accelerated by a shock with laser-sheet illumination and multi-frame imaging and use the Particle Image Velocimetry (PIV) technique to produce 2D velocity fields. The 2D perturbation initially applied to the curtain interfaces causes an unstable flow that is deterministic at early times and turbulent at late times. Thus the experimental data contain both deterministic and stochastic features that can be compared in detail with simulations and theory. Analysis techniques that explore all of the scales present in the flowfield have been applied to both the experimental data as well as simulations of the experiment. These techniques have shown that the simulations both agree and disagree with the experiments—depending on the quantities of interest.

Manufacturing Process Modeling 1
Building 132 Room 1102

Determining Bottlenecks in JTA Operations at LANL using Extend Modeling (U)

William J. Parkinson
Wilbur D. Birchler
Lee F. Brown
Scott A. Schilling
Los Alamos National Laboratory

Several simulation models of the JTA (Joint Test Assembly) production process at Los Alamos National Laboratory are developed using the simulation language Extend. The aim of the models is to describe the process in detail from design to assembly. An important goal of the modeling process is the determination of inefficiencies and bottlenecks in the operation. An unusual aspect of our models is that they track design and engineering as well as the manufacturing process. In other words, we are tracking both materials and information. The first simulation model is very general. It is used to encourage subject-matter experts to provide more specific information for the development of more detailed models. The process is iterative—continued feed back and improvement. This technique can be successful, though there often is a reluctance of some subject-matter experts to provide information. Communications from subject-matter experts are frequently in a semantic form such as rules of thumb. We are also using historical data and data from the Enterprise Resource Planning tool (ERP). This tool has potential to provide much information in statistical form. All forms of information are helpful in building the models.

The current model differentiates between weapons systems, system assemblies, parts, and materials. Utilization of the various machines and personnel is determined for various scenarios. This study provides insight into possible bottlenecks in the operation for several different situations. In this paper details of the most current model are described. Difficulties in programming and obtaining data are also discussed. Results of the more interesting simulation scenarios will be provided.

Advanced Automatic Train Control Optimization (U)

Susanna P. Gordon
Pamela J. Williams
Sandia National Laboratories, Livermore, CA

A new era of automatic train control has begun, in which mass transit trains will be commanded with precision beyond the capabilities of past systems. Although transit districts such as San Francisco's Bay Area Rapid Transit (BART) have controlled their trains automatically for decades, the control systems have provided limited capability in terms of train position location and speed control. Increases in capacity now require trains to run closer together than these systems can accommodate. Therefore new systems, such as the Advanced Automatic Train Control (AATC) system, are under development.

On a daily basis, BART's current system experiences approximately 20 delays of five or more minutes. The resulting backups lead to uncomfortable rides for passengers and wasted energy, and can cause power shortages. With more trains on the system, such problems will become more the rule than the exception. Our goal is to use optimization within the AATC system to smooth out train operations and to reduce energy consumption and power infrastructure requirements. We are initially focusing on a schedule-constrained problem with the primary objective of improving passenger comfort. Passenger comfort may be measured in terms of the smoothness of the ride, which is related to train acceleration.

Using JAVA, a simplified simulator of train control has been developed. The simulation will permit the evaluation and testing of optimization algorithms under development. First, we model the schedule-constrained problem as a discrete-time nonlinear optimal control problem. Then, we use o3d, a sequential quadratic programming algorithm, to solve the optimal control problem. We will present results that demonstrate the effectiveness of optimization techniqes to manage train interference during acceleration.

KASSIM: Knowledge-Based Application for Stockpile Sustainment and Integration Management-Abstract (U)

Johnell M. Gonzalez-Lujan
Robert Y. Parker
Los Alamos National Laboratory

The Knowledge-Based Application for Stockpile Sustainment (KASSIM) is a high-level discrete-event computer simulation model of the nuclear warhead production complex. This model serves as a prototype used to define and understand the issues associated with maintaining the U.S. Nuclear Stockpile. KASSIM version 0 was developed at Los Alamos National Laboratory under the Stockpile Life Extension Program Thrust Area (SLEP) within TSA Division. This model provides a graphical means for understanding the relationships of the structure of the complex and the behavior resulting from these relationships.

KASSIM is designed to analyze the capability of the nuclear production complex to respond to warhead refurbishment plans and START treaty scenarios. The model can simulate refurbishment that takes place either in the field or within a specified refurbishment facility. Currently, KASSIM simulates the material and information flow of seven weapon types and seven subsystem types for a total of 49 different part types. However, the model can easily accommodate the quantities required to simulate the movement of all weapons in the stockpile. Model inputs include refurbishment schedules, subsystem production schedules and present stockpile data. Model metrics include plant utilization, inventory levels, lead-time impacts, transportation requirements, stockpile levels and queue levels. Pre-production of subsystems is assumed to be two years, regardless of subsystem or weapon type.

Model output has helped analysts evaluate various refurbishment plans and START scenarios as a function of the capabilities of the complex. By modifying system parameters via a spreadsheet, the analyst is able to generate graphs of output results to compare to previous simulation runs.

A Polymer Model Implementation For Simulation of Silylation Swelling (U)

Vincent C. Prantil
Sandia National Laboratories, Livermore, CA

Extreme UltraViolet Lithography (EUVL) has been demonstrated as a viable candidate for fabrication of integrated circuits having features on the scale of 100 nm. The EUVL process utilizes thin layer imaging (TLI) to photochemically transfer imaged patterns in the top thin layer of a polymer resist. The purpose of the polymer layer is to act as a mask for subsequent etching of the circuit board to realize a particular stenciled pattern dictated in the chip design.

The thin polymer layer, if it is to perform well, must accomplish two things. It must be possible to lay down the polymer stencil array while maintaining channels with sharp contrast through which accurate etching can occur. Also, the polymer must be able to be placed on the substrate and form channels not in excess of 100 nanometer width. Current technologies are characterized by channel widths of 0.25 microns.

A pilot study was undertaken to determine if such channel widths could be obtained with prescribed polymer masks. For the polymer mask to work properly, it must be illuminated with ultraviolet light, a process called silylation, causing it to uptake gaseous aminosilanes which chemically react with the resist. A detrimental side effect of this reaction is a mechanical swelling of the polymer thin film. If the swelling is excessive, the polymer mask will not produce the proper stencil for the underlying circuit on the substrate.

From the analysis perspective, we couple the chemical reaction driving force for swelling expansion with a nonlinear material model for the inelastic behavior of a long-chained molecular polymer which predicts the silylation swelling to first order. Herein, we discuss the large strain, inelastic polymer model of Boyce *et al.* and its numerical implementation in the simulation software. We present particular validation examples of one-dimensional swelling as well as use of the model in more realistic two-dimensional boundary value problems.

Session 2: Tuesday, November 2, 1999, 10:20 a.m.–12:00 p.m.

Solid and Structural Mechanics 2
Building 123 Auditorium

Simulating Distortion and Residual Stresses in Carburized Thin Strips (U)

Vincent C. Prantil
Melvin L. Callabresi
James F. Lathrop
Sandia National Laboratories, Livermore, CA

Ganesh S. Ramaswamy
General Electric Company, Schenectady, NY

Mark Lusk
Colorado School of Mines, Golden, CO

This paper illustrates the application of a new multiphase material model for simulating distortion and residual stresses in carburized and quenched gear steels. Heat treatment is simulated in thin, metallic strips that are carburized on one side to introduce a non-symmetric carbon profile and subsequently quenched. Because the material properties are strongly dependent on the carbon content, quenching results in significant transverse deflections. The material model accounts for temperature and rate dependent elastic-plastic flow in a multiphase alloy structure. The model is fit to an extensive matrix of experimental data for low carbon steels (0.2 – 0.8%) whose transformation kinetics and mechanical response are similar to the 4023 and 4620 alloys used in experiments reported in the literature. These experiments provide detailed data for both transverse deflections and near-surface residual stresses that were measured using x-ray diffraction for a variety of strip thicknesses. Deflections and in-plane stresses compared favorably with finite element predictions using a User MATerial (UMAT) interface in the finite element code ABAQUS. The heat treatment cycle is simulated in an uncoupled serial analysis of carburization by diffusion, quenching by conduction and convection including phase transformation kinetics and finally a structural analysis incorporating TRansformation-Induced Plasticity (TRIP). Accurate residual stress profiles require detailed knowledge of the heat transfer coefficients of the quench media as well as alloy-dependent descriptions for phase transformation kinetics and TRIP strains.

Air-Bearing Guided Intercept and Line-of-Sight Experiments (AGILE) (U)

Lawrence C. Ng
Eric F. Breitfeller
Lawrence Livermore National Laboratory

This paper describes a ground based test and evaluation concept for testing an agile, lightweight, interceptor's performance. The interceptor is mounted on a four/five degrees-of-freedom (DOF) test apparatus consisting of either a linear air-rail (one translational DOF) or flat air-table (two translational DOFs), upon which is mounted an air bearing which provides an additional three rotational DOFs. "Dynamic air-bearing" (DAB) is the term used to define this test apparatus. The key attribute of the DAB, when coupled with a target projection system, is that it allows for a rapid turnaround test and evaluation of a fully integrated vehicle's ability to detect, acquire, and track a closing target with real-time closed loop attitude control and divert guidance. In addition, it also provides a testbed for the rapid development and evaluation of new hardware components and software functionality. The testbed can be configured to support both indoor and outdoor tests. Indoor air-table implementations of the DAB, however, limits the test vehicle's divert acceleration to less than 1g. For vehicles equipped with greater than 1g acceleration and employing hypergolic propellants, other approaches such as the out-door air-rail DAB or the captive tether flight [1] may be more applicable. Unlike other hardware-in-the-loop (HWIL) tests, the final measure of performance of an intercept experiment is a vehicle's actual miss distance—a direct measure of an interceptor's "hit" capability. By conducting multiple intercept experiments, statistical estimates of a vehicle's intercept capability can be obtained, and these statistics can then be used to independently calibrate a 6-DOF computer simulation. The DAB can also be used to evaluate the performance of a new class of agile micro-satellites for proximity inspection of low-earth-orbit (LEO) space assets. Despite more than a decade of intensive flight testing, reliable hit-to-kill (HTK) technology has not been demonstrated. Therefore, we believe that the DAB provides a low-cost ground test capability that may be used to improve flight test performance.

Updating of Finite Element Models for Highly Transient Structural Dynamic Events (U)

François M. Hemez
Scott W. Doebling
Winston Rhee
Paula Beardsley
Los Alamos National Laboratory

This paper presents the development of a novel technique for updating the parameters of a finite element model using data from short duration, highly transient structural dynamic events. For the type of events involved, the time scale of interest is on the order of the wave speed of the materials. Thus, the explicit solution method must be used to perform the finite element time integration. Because a frequency domain (modal) solution is inappropriate, conventional finite element model updating techniques are not applicable to this type of problem. A novel approach is proposed that combines a previously developed optimization metric based on principal component decomposition with a previously developed inverse problem formulation based on a two-point boundary value problem and solved with an optimal control approach. The approach is designed to allow for general types of nonlinearity in the problem. The types of parameters of interest for updating include material constitutive relations, contact surface properties, test initial conditions, and test boundary conditions. The overall motivation for the method is to improve individual material and contact models as well as improve general modeling rules for simulating highly transient events. The development and formulation of the method are presented along with a verification problem to demonstrate the application of the method.

Validation of a Finite Element Model Updating Procedure using High Velocity Impact Test Data (U)

Scott W. Doebling
François M. Hemez
Winston Rhee
Paula Beardsley
Los Alamos National Laboratory

This paper describes the validation of a novel finite element model updating technique to improve the accuracy of simulation for a highly transient impact event. A series of impact-loading experiments was performed on a test article containing both metal and hyperelastic material. The velocity change during impact is on the order of 500 in/sec. Because the dynamics of this short-duration event are on the order of the wave speed in the materials, an explicit finite element code was used to perform the simulation. However, conventional finite element model updating techniques are dependent upon the identification of normal vibration modes to formulate their objective functions. A novel technique was developed to update the constitutive parameters of the viscoelastic material, the contact parameters in the model, and the initial conditions of the impact test. The updated parameters significantly improve the correlation of the explicit finite element model with the experimental results. The results confirm the validity of the technique as a means to improve the accuracy of explicit finite element simulations.

Design, Analysis, and Fabrication of the APT Superconducting Cavities (U)

Robert C. Gentzlinger
Russell R. Mitchell
Los Alamos National Laboratory

The Accelerator Production of Tritium (APT) high-energy linac utilizes superconducting radio frequency (SCRF) niobium cavities that are enclosed inside titanium helium vessels. The helium vessels are filled with liquid helium, flooding the cavities and maintaining the 2K operating temperature. Structural analyses were performed on the cavities and its surrounding helium vessel for various loading conditions and temperature environments. An overview of the design, supporting analysis, material testing, and prototype cavity fabrication will be discussed.

Material Behavior and Characterization 2
Building 123 Conference Room A

Modeling Polymers (U)

Matthew W. Lewis
Charles A. Anderson
Los Alamos National Laboratory

We have modeled the behavior of elastomeric foams, rigid foams, and hyperelastic polymers with the *HYPERFOAM, *FOAM, and *HYPERELASTIC material models in ABAQUS. We have included viscoelastic effects. A large set of data for short and long term behavior of these materials is being developed. Test data and long term relaxation data are predicted adequately by these models.

The higher rate forms of these models are also being put into PRONTO and DYNA. The algorithms for the hyperelastic foam model require eigenvalue solutions of the stretch tensor, but these can be performed without a large computational penalty. Additionally, we are trying to include routines like those used in ABAQUS to provide fitted model parameters from test data.

Modeling Microstructural Evolution in Polymers (U)

Richard V. Browning
Scott G. Bardenhagen
Los Alamos National Laboratory

Many polymers exhibit time dependent changes in their properties over very long periods. One example is physical aging as described by Struik, another is growth of hard segment domain structures in thermo-plastic polyurethanes. We will show some experimental results to illustrate the behavior and then discuss models that are under development and evaluation. These models are macroscopic constitutive equations, intended for implementation in finite element codes, with parameters that can be obtained from experiments or from microstructural numerical models.

Modeling Decomposition of Confined, Rigid, Close-Celled Polyurethane Foam (U)

M. L. Hobbs
K. L. Erickson
T. Y. Chu
T. H. Fletcher
Sandia National Laboratories, Albuquerque, NM

The decomposition of rigid polyurethane foam has been modeled by a kinetic bond-breaking mechanism to form polymer fragments such as toluene diisocyanate, toluene aminoisocyanate, toluene diamine, trimethylol propane, etc. Dominant decomposition pathways were found to be dependent on confinement as well as pressure. As pressure increases, the dominant reaction pathways form more CO_2 than at ambient pressure. The bond-breaking scheme is resolved using percolation theory to describe evolving polymer fragments. The polymer fragments vaporize according to individual vapor pressures.

Kinetic parameters for the Confined PolyUrethane Foam decomposition (C-PUF) model were obtained from Thermal Gravimetric Analysis (TGA) performed at atmospheric pressure. The effect of pressure between 1 and 20 atm were investigated by using a high pressure TGA (HPTGA). A sensitivity and uncertainty analysis was also performed using the C-PUF model. The agreement between the C-PUF model and the TGA data is not exact but within experimental uncertainty.

Scale-up effects were examined by simulating the response of a partially confined 8.8-cm diameter by 15-cm long right circular cylinder of foam containing an encapsulated component. Predictions of center temperature, mid-radial temperatures, and component temperatures as well as regression of the foam surface were in agreement with measurement's using thermocouples and X-ray imaging.

Strong Incremental Objectivity and Integration of Hypoelastic Constitutive Laws (U)

William M. Scherzinger
Sandia National Laboratory, Albuquerque, NM

Two concerns regarding the integration of hypoelastic constitutive models are of importance in obtaining accurate solutions in finite element applications. One is the choice of an appropriate objective stress rate. In particular, two different stress rates are commonly used: the Jaumann rate and the polar rate. They are best known for the extremely different behavior that they exhibit in large deformation, simple shear problems. A second consideration concerns the actual numerical integration of the stress rate over a time step. In most finite element codes the configuration of the body is known at the beginning and end of a time step. The deformation history over the time step, however, is not known. The assumptions made about this deformation history can greatly affect the resulting stress field, sometimes leading to very non-physical behavior. This can be seen for small deformation, cyclic shearing problems.

In addressing these issues, a stress integration routine is developed using the polar stress rate along with a specific deformation history for the time step. This deformation history is based on the strongly objective, incremental routine of Rashid (1993), and it gives accurate solutions for the finite deformation simple shear problem and the small deformation cyclic shear problem. Implementation of this stress integration routine into JAS3D requires the accurate evaluation of the logarithmic strain, and a simple method for this evaluation is presented.

Non-Linear Magnetic Effects in Magneto-Rheological Fluids (U)

Janine L. Fales
Los Alamos National Laboratory

When introduced to the concept of magneto-rheological fluids, one can envision numerous applications to serve both civilian and military sectors. When exposed to the physical strength of model MR fluids, enthusiasm grows—only to be tempered by the lack of commercial devices. The sheer complexity of the fundamental science of these materials has dictated deliberate increases in understanding over the last fifty years.

Important advances have been made in modeling but adequate predictive modeling is not yet available. Common simplifications to the composite physics include dipolar approximation and linear magnetization of monodisperse, spherical particles. Outstanding areas of research to better understand the disparity between computational predictions and experimental results include effects of non-linearity of particle magnetization, particle shape and size distribution, and influences of neighboring particles.

This presentation will report on progress toward the inclusion of non-linear particle magnetization effects on the rheology of typical magneto-rheological fluids. The explicit introduction of non-linear particle magnetization on interparticle forces is expected to yield insight into the subquadratic dependence of yield stress found at modest applied fields.

Computational Heat Transfer 1
Building 132 Auditorium Room 1000

The Effect of Heat Transfer Coefficient Temperature Dependence on Tensile Thermal Stress During the Active Cooling of a Heat Capacity Laser Slab (U)

Lisle B. Hagler
Mark D. Rotter
Lawrence Livermore National Laboratory

In heat capacity laser operations it is highly desirable to bring the glass laser slabs to an isothermal condition as quickly as possible to reduce the time interval between 'shots.' The isothermal condition is necessary to eliminate the wavefront distortions due to slab deflections and stresses induced by thermal gradients. Active cooling is used to reduce the slab temperature between shots. However, care must be taken during the cooling process. Cooling the glass slabs too rapidly will result in the fracture of the slab from thermal stresses.

Current techniques for the 'optimal' forced convective gas cooling of a laser slab to an isothermal condition between shots rely on the assumption of a constant heat transfer coefficient. These methods are based on the ability to determine analytical expressions for the temperature distribution and thermal stress field. This can only be done when the heat transfer coefficient is constant. In reality, for forced convection with gases, the heat transfer coefficient is a decreasing function of temperature. The rate of decrease with temperature depends on the type of gas employed.

A perturbation technique, based on the assumption of a slowly varying heat transfer coefficient, is used to obtain approximate analytical expressions for the temperature distribution and thermal stress field. Additionally it is shown that peak thermal stress is not only highly dependent on Biot number, but that a temperature dependent heat transfer coefficient can significantly increase this stress.

An ANSYS finite element analysis (FEA) model of a laser glass slab is used to verify and extend the perturbation method results.

Thermal Sensitivity Analysis for the W-76 Accelerometer (U)

Kevin J. Dowding
Bennie F. Blackwell
Sandia National Laboratories, Albuquerque, NM

Programmatic requirements are forcing the analyst to perform simulations for situations other than the nominal set of model input parameters. In addition to computing the response for the nominal model parameters, we need to know the sensitivity of the response to uncertainties in the input parameters. A measure of the sensitivity of the response (temperature, velocity, displacement, etc.) to changes in model parameters (thermal conductivity, viscosity, Young's modulus, etc.) is the sensitivity coefficient. Mathematically, the sensitivity coefficient is defined as the partial derivative of the field variable (output) with respect to the parameter of interest. One method of computing sensitivity coefficients is the Sensitivity Equation Method (SEM). This approach involves differentiating the conservation equations with respect to model parameters. New "conservation like" equations for the sensitivity coefficients result from this process. These "conservation like" equations are solved using the same algorithm as was used to solve the original conservation equations. We have implemented this methodology in a general-purpose thermal analysis code. Implementation experiences as well computational results for a sensitivity analysis for the W-76 accelerometer will be presented.

Thermal-Mechanical Analysis of the NIF Target Positioner (U)

Wayne O. Miller
Lawrence Livermore National Laboratory

The target positioner for the National Ignition Facility is required to repeatedly position and hold laser targets within a radius of 7 µm from the 10-m dia. target chamber center. From this overall stability budget, only 1.5 µm is allocated to thermal effects. The challenges in meeting this thermal budget are significant. The positioner is a 6-m cantilevered boom constructed of composites and aluminum. The boom is withdrawn after each shot and subject to thermal cycling from venting and subsequent evacuation for target replacement. The positioner is then reinserted into the evacuated target chamber, which is at an elevated temperature from past laser shots. The support frame for the positioner is outside the chamber and is subject to transient thermal motions from variations in the target bay air temperature. The floor supporting the frame is also subject to thermal transients and must be considered.

The analysis of the thermal stability of the target positioner was likewise multifaceted, and the approach was to divide and conquer. The support frame and floor were analyzed as a kinematic mechanism subject to transient thermal expansion of the links. The room air temperature transients are unknown and so were bracketed by several assumed behaviors. The transient thermal upsets from venting and evacuation were analyzed using a coupled fluid/solid heat transfer model. The warm evacuated target chamber was treated as a fully nonlinear 3-D radiation problem to allow the study of several nonsymmetric thermal source locations. The composite material forming the main structure of the positioner was not defined, so several orthotropic material studies were included to help specify the material requirements. Operational timing and scheduling of the target positioner were also considered since the stability budget is based on the combined transient response. An envelope of acceptable design and operational parameters was found which meets the stability budget.

Thermal Analysis of the Passively Cooled Vault Within the Los Alamos Nuclear Material Storage Facility (U)

C. N. Ammerman
J.D. Bernardin
W.S. Gregory
S.M. Hopkins
Los Alamos National Laboratory

The Los Alamos Nuclear Materials Storage Facility (NMSF) is being renovated for long-term storage of heat-generating nuclear materials. The heat removal will be achieved using a passive cooling scheme that relies on free convection and radiation heat transfer to maintain storage material temperatures below a limit of 140 °C. The NMSF storage concept involves placing radioactive materials inside a set of nested steel canisters. The canisters are, in turn, placed in holding fixtures and positioned vertically within steel storage pipes (6.10 m length, 45.7 cm outer diameter, and 1.27 cm wall thickness), referred to as a drywells. Several hundred drywells, arranged in linear arrays within a large storage bay, will dissipate waste heat to the surrounding air. The heated drywells will create a passive, buoyancy-driven airflow pattern that will draw cool air into the storage bay and exhaust heated air through an outlet stack. To test the feasibility of this cooling concept, a full-scale experiment was conducted in which 36, in-line drywells were heated in a passive flow environment. Experimental facility air flow rates and corresponding drywell surface temperatures were investigated. A 3-D CFD model was created to complement the full-scale, 36-drywell experiment. The CFD model has been generated and benchmarked against the full-scale experiment using the CFX4.2 commercial code. Comparisons of air temperature, drywell surface temperature, and facility mass flow rate are made between the numerical and experimental data. The model provides detailed flow and temperature information within the experiment that would have been too costly to acquire from the full-scale test. The results of this effort provide confidence that CFD can be used as a design tool for applications with buoyancy-driven airflow in large enclosures, such as the NMSF facility.

Thermal / Structural Analysis and Frequency Shift of the CCL Cavities for the Spallation Neutron Source (U)

Snezana Konecni
Nathan K. Bultman
Los Alamos National Laboratory

The Spallation Neutron Source (SNS) is an accelerator-based facility that produces pulsed beams of neutrons by bombarding a mercury target with intense beams of 1-GeV protons. Los Alamos National Laboratory is responsible for the design, fabrication, installation, and testing of the Linear Accelerator (linac) for the SNS project. The linac accepts beam from the front end system and accelerates it from 2.5 MeV to 1.0 GeV. The linac consists of a drift-tube linac (DTL), a coupled-cavity drift-tube linac (CCDTL), and a coupled-cavity linac (CCL). The DTL operates at an RF resonant frequency of 402.5 MHz, while the CCDTL and CCL operate at 805 MHz. CCL cavities are figures of revolution about the beam axis. An automated tuning program sets up the geometry for a symmetric accelerating cavity and runs a physics code SUPERFISH repetitively, varying geometry to tune each cavity to desired frequency. One of the SUPERFISH outputs is a file that contains geometry and heat flux per segment on the cavity due to the electric field. This information is used to create the geometry and heat loads for the thermal/structural analysis of the CCL cavities. The analysis includes temperature distributions and structural response for both steady state and transient conditions of the RF heating. Several cooling schemes were looked at. The original scheme includes four parallel annular paths around the cavity nose in the septum, fed and collected by internal plenums as shown in the 3-D model. The general purpose finite element code COSMOS was used for the 2-D temperature and structural calculations. A FORTRAN code was used to interface between SUPERFISH and COSMOS in determining the frequency shift analysis due to thermal distortion of the CCL cavity. The local heat transfer coefficient was determined based on the flow rate. The general purpose finite element code ANSYS was used for the 3-D temperature and structural calculations.

Manufacturing Process Modeling 2
Building 132 Room 1102

A Fully Coupled Finite Element Model of the Silylation Process (U)

William S. Winters
Sandia National Laboratories, Livermore, CA

Extreme Ultraviolet Lithography (EUVL) is expected to have an essential role in the development of next-generation smaller feature (100-130nm) semiconductor devices. The post-exposure silylation process is one of several thin layer imaging technologies being considered for EUVL. During silylation, gaseous aminosilanes are absorbed at the resist surface and diffuse into the imaging layer. A reaction takes place in the layer that results in an uptake of silicon, localized increases in volume and the evolution of a product gas. Volume increases on the order of one hundred percent are typical and result in complex stress states in the resist material. This and two other companion presentations will describe a new computational model of the positive tone silylation process. The model is two-dimensional and transient and accounts for the combined effects of mass transport (diffusion of silylation agent and reaction product), the chemical reaction resulting in the uptake of silicon and material swelling, the generation of stresses, and the resulting material motion. The influence of stress on diffusion and reaction rates is also included. Both Fickian and case II diffusion models have been incorporated. The model provides for the appropriate mass transport and momentum boundary conditions and couples the behavior (stress/strain) of uncrosslinked and crosslinked materials as well including the influence of underlying device topology. Finite element mesh generation, problem setup, and post processing of computed results is sufficiently mature to permit investigation of a broad parameter space which includes material properties and geometry issues, e.g., alternate crosslinking distributions, resist thickness, etc.). This presentation will focus on the solution of the material momentum equations, coupling of the mass transport, chemistry and material models and 2D model validation. Results from a nominal 2D transient simulation will be presented. The two companion presentations will focus on the mass transport, chemistry, and material constitutive models as well as model validation.

Modeling the Silylation Process-Mass Transfer and Chemical Reaction in a Swelling Resist (U)

Greg Evans
Rich Larson
Sandia National Laboratories, Livermore, CA

Silylation is a process for incorporating silicon into unexposed areas of resist and thereby rendering them resistant to subsequent etching. In the process, considered at Sandia in the EUVL project, a gas containing silicon (e.g., dimethylaminopentamethyldisilane) diffuses into the resist material (e.g., a cresol novolac) and reacts with it, producing a large (factor of two) volume change of the resist. Silylation is one of the factors that can affect line edge roughness (others are acid diffusion, aerial image quality, and etching). Issues include (1) the sensitivities of the silylation process (reaction, diffusion, and swelling) to feature size, (2) determining the optimum silylation process conditions (pressure, temperature, time, initial thickness, etc.), and (3) knowledge of the fundamental properties and relationships (reaction rate, diffusion coefficient, glass transition temperature, equation of state, stress-strain behavior, etc.). A silylation modeling effort was initiated to address these issues.

This talk focuses on the formulation and the solution of the governing equations for mass transport and chemical reaction in the resist. Two models are discussed; the first is a transient one-dimensional model in which a coordinate transformation that takes into account the movement of the swelling resist is applied to the differential equations. Model results using a simple elastic stress model show the effects of model parameters on the silylation process in the small deformation regime. The model is used primarily as a basis for verifying the solution of more complex two-dimensional models. The second model is a control volume mode, formulated for implementation into a two-dimensional finite element thermomechanical code; to be compatible with material models developed for the swelling resist, the formulation requires that resist material (unsilylated and silylated) remain within control volume boundaries. The model provides an unconstrained volume expansion rate used in the material model. Results from the two models are compared.

LANL Detonator Production Simulation Model (U)

Robert J. Burnside
Nelson S. DeMuth
Richard F. Farman
Steve M. Nielson
Los Alamos National Laboratory

Los Alamos has developed an object-oriented, discrete-event, detonator production simulation model. The model provides system information to management to help handle the increasing detonator requirements. A simulation model is necessary to handle the time dependence of material flows and decision points in the production process. The model determines equipment utilization and product pinch points to assist in managing the increasing workload. Also, conduct-of-operation options can be evaluated easily and quickly to improve production and safety. The model has been successfully used to analyze additional equipment needs and evaluate conduct-of-operation options. Some of the issues addressed in developing the model are described below.

Detonator production is a complex process with many products and product pathways using a fixed set of resources. Certain steps can be preformed simultaneously while others must be done in sequence. Development and qualification lots have much different manufacturing and rejection rates than the final fabrication lots. A fraction of a given lot must be test fired and the fraction varies up to 100% depending on the detonator lot type.

Detonators are produced in fixed-size batches that contain both certified product and rejected product. As later inspections occur, a larger portion of the batch will be rejected product. As the various components are assembled into the final product or detonator, the handling of excess components must be addressed. Both bonded and work in progress storage requirements need to be identified, both in size and location, to efficiently support production.

Comparison of Traditional Algorithms with Modern Computer-Aided Design Tools (U)

Wilbur D. Birchler
Scott A. Schilling
Bradley G. Baas
Los Alamos National Laboratory

The Nuclear Weapons Complex is under going major changes in the areas of design, analysis, and manufacturing. Many of the weapons components were represented with long standing traditional algorithms and now modern Computer Aided Design (CAD) tools are replacing these traditional design and manufacturing activities. These new solid-based models are intended to capture the total design and manufacturing features. The goals of this presentation are to demonstrate how well the traditional and modern data algorithms compare.

This work describes numerical comparisons between the traditional algorithms and the equivalent data extracted from modern CAD tools. An algorithm called Wilson-Fowler Splines was used in the design and manufacture of several components in the Nuclear Weapons Stockpile. Today, the Nuclear Weapons Complex is utilizing and evaluating the capabilities of the Parametric Technology, Inc. Pro/Engineer suite of tools to aid in the design and manufacture these components, if the need arises.

This presentation consists of three major segments. The first segment compares the accuracy of the Wilson-Fowler Spline algorithm with several analytical functions. The effects of the number of significant figures in the input data stream are discussed.

In the second segment, comparisons are made with results from the Pro/Engineer solids-based model representations to the traditional Wilson-Fowler algorithm. Several cases are presented. The impact of end angles on the results are presented and discussed.

The last segment compares the Pro/Manufacture Cutter Location output data with the traditional Wilson-Fowler algorithm. Several cases are presented. The effects of Pro/M tolerance settings on the final tool paths are demonstrated.

The conclusions of this work demonstrated that the differences between the traditional and modern CAD tools are insignificant to the design and manufacturing processes.

The Application of Massively Parallel Computing to Characterize Furnace Brazing Processes (U)

Steven E. Gianoulakis
F. Michael Hosking
Robert G. Schmitt
Louis. A. Malizia
Sandia National Laboratories

A braze process is typically defined by a time-temperature profile. This profile includes specified temperature ramps, and plateaus to ensure that the braze material experiences an appropriate thermal history. The braze material must be held above a certain temperature for a specified time, and must be cooled in a controlled manner to minimize residual stresses. Knowing the appropriate time-temperature profile for a specific braze alloy in not sufficient to ensure acceptable joint formation within a furnace. Braze furnaces are typically controlled based on sensors on the furnace itself, not the workpieces. Therefore, one must understand the coupled thermal response of the furnace and workpieces to be able to develop a control program which results in the desired temperature profile at the braze. In the past, this characterization was accomplished through time consuming and expensive trial-and-error experimentation. Sandia National Laboratories has developed a thermal model of a production braze furnace, including the internal support structure and detailed representations of the work pieces. The predominant mode of heat transfer within the furnace is radiation, and because of the geometric complexity of the model, the resulting enclosure radiation problem was intractable using conventional computing. The largest model includes over one million finite elements and nearly 25 billion viewfactors. This size of model was easily handled using Sandia's TFLOP massively parallel computer. Simulation results and validation data will be presented demonstrating the utility of such a modeling approach. Thus far this modeling effort has resulted in a 10 X reduction in experiments necessary to identify the furnace control parameters, a 30–100 percent increase in throughput for various components, and a 10 percent reduction in braze cycle time.

Session 3: Tuesday, November 2, 1999, 1:00 p.m.–2:45 p.m.

Solid and Structural Mechanics 3
Building 123 Auditorium

Particle Accelerator Facility Background Vibration, Causes, Effects, and Mitigation (U)

Stephen Ellis
Los Alamos National Laboratory

Background vibration input of even small magnitude acting on various particle accelerator components at unfavorable frequencies can cause significant degradation of accelerator performance. Certain accelerator components, such as focusing magnets, are very sensitive to small dynamic motions. Vibratory excitation from background sources at frequencies corresponding to the natural mechanical modes of a focusing magnet can cause excessive dynamic motion of the magnet which in turn can cause defocusing and misalignment of the beam, severely degrading beam quality.

Other high tech facilities, such as space telescope installations, silicon chip fabrication facilities or micro-machining facilities, also utilize equipment that is very sensitive to low level dynamic motion.

Sources of vibratory energy include systems common to all industrial buildings such as HVAC systems, shop air compressors, sump pumps, machine tools, cranes and elevators. Low frequency background seismic vibratory input is also always present. Input from nearby vehicular traffic as well as vibratory input from any nearby residential, commercial, or industrial activities may be present as well. Additional sources common to accelerator facilities include the pumps and blowers and related flow turbulence associated with thermal control systems, and the various vacuum and roughing pumps associated with the vacuum systems.

Design methodology for new equipment and facilities aims to isolate vibration sources within the facility as much as possible. For example, incorporating vibration isolation devices on pumps and installing this equipment with maximum reasonable distance to sensitive equipment. When designing new dynamically sensitive equipment, attempts should be made to design such that fundamental mechanical modes are above the anticipated frequency range where the majority of the background vibratory energy exists.

During assembly, installation, and subsequently operation of the APT/LEDA RFQ particle accelerator, background vibration levels were measured and vibration sources within the facility were identified. Response of the RFQ to this background vibratory input was measured and compared with numerical estimates obtained using ABAQUS.

Limit Cycle Measurements from a Cantilever Beam Attached to a Rotating Body (U)

Christopher L. Lee
Lawrence Livermore National Laboratory

The simple model of a cantilever beam attached to a rigid, rotating body captures the characteristic dynamics of flexible rotating mechanical systems such as helicopter blades, robot arms, and satellite appendages. Theoretical studies of nonlinear dynamic response under periodic, near-resonant excitation have identified distinct classes of periodic responses associated with saddle node, pitchfork, and Hopf bifurcation points. The Hopf bifurcation points indicate regions where stable limit cycle responses characterized as an amplitude modulated time series may exist.

Results from an experimental study of a cantilever beam attached to a rotating body demonstrate the existence of stable, amplitude modulated limit cycle responses following theoretical predictions. Starting from a periodic response, a single system parameter (the excitation frequency) is varied and the periodic response loses stability giving way to a stable limit cycle. As is possible with a nonlinear system, a periodic input can yield a non-periodic output.

Computational Aspects in *hp* Cloud Solutions of Schrödinger's Equation (U)

J. D. Becker
Los Alamos National Laboratory

The *hp* Cloud method is a meshless descendant of the finite element method. Use of a partition of unity allows an arbitrarily smooth representation of the solution. A set of clouds provides an open cover for the problem domain. Associated with each cloud is a basis which provides compact support (as in fem), and a great flexibility with respect to the choice of function classes (unlike traditional fem). As with other meshless methods, enforcement of boundary conditions and optimal integration schemes are some of the main unresolved issues. The treatment of Dirichlet boundary conditions (periodic and semi-infinite) that arise in the eigensolutions of Schrödinger's equation are discussed. The use of non-polynomial basis sets appropriate for singular potentials are explored, and the problems of quadrature in conjunction with these bases are treated via various integral transforms.

Structural Finite Element Analyses for Support of the Design and Manufacturing of a Weapons Component (U)

Vicki L. Porter
Sandia National Laboratories, Albuquerque, NM

This presentation will describe ongoing efforts in the modeling and simulation of structural deformation of a weapon component during manufacturing and hostile environment testing. Analyses are being conducted on the present design as a demonstration of capability.

Simulation efforts are focused on analyzing the present method of forming the component between two dies. Simulation of the forming operation and the subsequent springback is being accomplished with JAS3D, a finite element code for the nonlinear analysis of structures subjected to quasi-static loading, which, in this problem, is contact-driven. Due to symmetry, only a section of the component is modeled during the forming analyses. Computational results will be compared with measurements of actual parts after they are removed from the dies.

The response of the formed component to shock loading is modeled with PRONTO3D, a finite element code for nonlinear, transient dynamic analysis of structures. The dynamic analysis is started from the last JAS3D output and thus includes the effects of residual stresses incurred during forming. Because the dynamic loading and boundary conditions do not necessarily coincide with the symmetry of the component, a larger portion of the part is modeled, requiring the shock analysis to be run on the massively-parallel machine.

Residual Stresses in an Inconel 718 Clad Tungsten Tube Processed by Hot Iso-static Pressing (U)

D. W. Brown
R. B. Parker
P. Rangaswamy
Los Alamos National Laboratory

The Accelerator Production of Tritium (APT) has been developed as a possible supplier of Tritium to the nation's Nuclear Weapon Stockpile. To produce Tritium, tungsten rods are bombarded with high-energy protons releasing neutrons, via a spallation reaction, which are then captured by ^{3}He, yielding the necessary Tritium. Design requirements and safety consideration do not allow coolant to be in direct contact with the tungsten, necessitating cladding of the rods. Inconel 718 has been chosen as the cladding material for its superior mechanical, thermal, and neutronic properties. Because the cladding must be in intimate contact with the tungsten at operating temperatures, the materials are diffusion bonded by Hot Iso-static Pressing (HIP) at 1080 °C. However, the difference in thermal expansion coefficients of Inconel 718 and tungsten produce large residual stresses upon cooling. We have utilized X-ray diffraction (XRD) to study a tungsten tube clad with Inconel 718 on both the inner and outer surface. The classical XRD (*d vs. sin²_*) technique was used to determine the stresses in the outer layer of Inconel 718. These results are used to benchmark Finite Element Analysis (FEA) calculations, and a direct comparison will be made in this paper.

Material Behavior and Characterization 3
Building 123 Conference Room A

Application of ALE3D to Modeling Non-Eroding Penetrators into Concrete (U)

Douglas R. Faux
Lawrence Livermore National Laboratory

A new technique has been added to ALE3D to model non-eroding penetration. Nearly rigid penetrators transfer too much momentum to the target in standard Eulerian treatments because there are not multiple velocity fields available for both the target and the penetrator. ALE3D can utilize its slide surface capabilities to eliminate that problem. In a typical simulation the penetrator is treated Lagrangian with a slide surface surrounding it. ALE elements are then used to define the surrounding medium. The target is overlaid on this surrounding mesh and allowed to flow through it. With this technique, the mesh is allowed to move in concert with the penetrator in order that significant amounts of deflection and tumbling can take place without the mesh tangling. The target flows through the mesh as the mesh moves through space.

A new material model has been implemented in ALE3D to model materials such as concrete, geological material and ceramics. The model consists of a porous-crush equation of state, a constitutive model that recognizes the existence of both undamaged and damaged material, and a damage model that transforms material from its initial state to its damaged state. ALE3D simulations were performed on non-eroding deformable steel penetrators penetrating into concrete targets to evaluate the new concrete damage model.

A heavy tapered steel penetrator is molded with ALE3D utilizing both the non-eroding penetrator mesh logic and the concrete damage model. The penetrator's rigid body dynamics are recorded while its case and generic payloads are evaluated for survivability.

Multi-Scale Material Modeling Multi-Scale Damage Progression Analysis: Monotonic Loadings (U)

Mark F. Horstemeyer
Sandia National Laboratories, Livermore, CA

A damage framework will be discussed that spans many spatial size scales. A macroscale internal state variable damage model is included within the Bammann-Chiesa-Johnson (BCJ) plasticity framework to determine effects of void nucleation, growth, and coalescence separately. Because the BCJ equations have been implemented into finite element codes, the damage model can be used for large scale component or systems level analyses. An A356 cast aluminum alloy is used as the model material to discuss each component of the damage progression. Void nucleation occurs mainly at the scale of 1-20 microns as particles fracture or debond from the adjacent aluminum matrix. The void nucleation rate has been quantified by tension, compression, and torsion experiments and at different temperatures. Further micromechanical simulations revealed that the first order influence factor to initiate voids is temperature over the spatial distribution, size, or shape. Void growth occurs from pre-existing casting pores and from void nucleation from silicon particles at scale from 2-100 microns. Micromechanical simulations were performed on SEM micrographs to understand the relation between pores initiated from silicon particles and pre-existing pores from the casting process. Experiments were performed to quantify the pore growth at different temperatures. Coalescence can be quantified at this scale and also at the next higher scale where pore-pore interaction takes place. From 20-200 microns, pore-pore interactions can dominate, so micromechanical simulations were performed to show the importance of temperature, spatial distribution, size effects, and shape effects. Separate macroscale equations for void nucleation, growth, and coalescence were developed from these simulations and included in the BCJ framework for finite element analysis of notch tensile tests, the B83 weapons carrier, and the control arm of a Chrysler Viper. Atomistic simulations were also performed to show the mechanisms related to silicon fracture and interface debonding.

Modeling Discontinuities and Long-Range Forces with an Alternative Theory of Continuum Mechanics (U)

Stewart A. Silling
Sandia National Laboratories, Albuquerque, NM

In the conventional formulation of continuum mechanics, partial differential equations are used to model the forces between material particles and the motion of these particles. This approach is in some ways ill-suited to the study of problems in which discontinuities such as cracks and phase boundaries are present, since the necessary partial

derivatives with respect to the spatial coordinates are undefined on these discontinuities. An alternative way of modeling continua will be described in this talk. In this approach, the spatial derivatives are not needed or used. Therefore, the equation of motion and constitutive model apply without regard to the presence of discontinuities. This alternative approach may be thought of as a continuum version of molecular dynamics.

Force on a material particle due to deformation of a body is determined by integration of a force-displacement function that characterizes interaction between pairs of particles. Therefore, the model is formulated in terms of integral equations rather than partial differential equations. This avoids the need to evaluate partial derivatives in space along discontinuities. It also allows for the incorporation of long-range forces between material particles. It also provides for the modeling of dispersive linear waves, as in lattice dynamics.

It will be shown that this method may have potential for the modeling of problems in which singularities of various types arise spontaneously as a result of loading. The theory permits damage and fracture to be modeled without separately specified relations for crack velocity and trajectory, and even without criteria for crack growth. Instead, crack advance emerges naturally from the constitutive model and from the basic equation of motion. Numerical examples using this approach appear to give insight into phenomena that are observed experimentally in dynamic fracture mechanics. These include crack instabilities and branching.

Failure in Dynamically Expanding Thin Shells (U)

Michael B. Prime
Rick L. Martineau
Los Alamos National Laboratory

A model was developed to predict the initiation of instabilities in thin, metallic cylindrical shells subjected to internal explosive detonations. In several experiments, fast framing camera pictures were used to observe the formation of instabilities on the outer surface of the cylinders and eventual fracture. The explicit finite element code ABAQUS was used to model the cylinder expansion and formation of instabilities. A viscoplastic constitutive, equation-of-state, and damage model was implemented as a user material subroutine. Using uniform material properties and either Johnson-Cook or Mechanical Threshold Stress constitutive law, the model was unable to correctly material instability. The failure prediction was improved by incorporating either spatial variation in initial material strength or a Gurson-Tvergaard-Needleman microvoid growth model with a spatial variation in initial void volume fraction. A special routine was developed to initialize the material or void properties with variations on the length scale of the typical grain size.

Coupling a Dislocation Dynamics Model with the ALE3D Continuum Model (U)

Andrew T. Anderson
Moono Rhee
Lawrence Livermore National Laboratory

Plastic deformation at high strain rates, especially at low temperature, may lead to such phenomena as shear band formation and flow localization, resulting in a large number of dislocations generated in a local region. During this process, the mechanical energy is converted to heat which dissipates into the surrounding medium. Our goal is to quantify the temperature rise due to dislocation motion as a function of strain rate and surrounding initial temperature. Since the dislocation mobility changes with temperature, the temperature rise due to high speed dislocations may be an important factor in determining the characteristics of dislocations, with direct effects on the overall macroscopic deformation properties.

Determination of the temperature rise is done by coupling the Micro3D dislocation code with the ALE3D finite element code by using the former as a subroutine called from the continuum code. ALE3D is a large multi-physics code developed at LLNL to handle hydrodynamics, structural dynamics, heat transfer, and chemistry effects. In the present application, the code runs in a thermal-only mode, with follow-on work to explore coupling of stress fields.

Initial runs of coupled dislocation and continuum codes have been completed on a single Frank-Read source in one plane of a molybdenum cube 10 µm on a side. Small temperature increases, on the order of a milliKelvin, are seen by the time the source has generated three or four loops. Additional runs will be performed with a variety of interacting dislocation sources to explore changes in aggregate dislocation motion resulting from thermally-enhanced mobilities.

Computational Heat Transfer 2
Building 132 Auditorium Room 1000

Subsurface Gap Depth Detection by Infared (IR) Imaging Using a Surface Heat Pulse (U)

Charles S. Landram
Richard W. Martin
Nancy K. DelGrande
Philip F. Durbin
Lawrence Livermore National Laboratory

The depth of gaps located below a lamp-heated surface can be determined from IR surface temperature images following a single pulse of heat. The gaps are assumed to reside at a fixed depth in a plane parallel to the surface. Both the magnitude of the image spatial contrast (in temperature) as well as the time at which it is the sharpest (brightest) provide two unique quantities whose measurements can be used to determine gap depth. This determination requires (direct) numerical solution to the unsteady, multidimensional heat conduction equation based on a tentative buried gap shape similar to that observed at the surface. The procedure is illustrated for a cylindrical gap buried 3/8 inch from the surface of a 3 inch slab of stainless steel.

An Investigation of Cutting Tool Temperatures Distributions during Orthogonal Machining (U)

Mark R. Miller
Los Alamos National Laboratory

High temperatures in the cutting zone of a machining process increase cutting tool wear, which reduce cutting tool life, decrease part quality and adversely influence the economics of machining. Although theoretical models have been constructed to provide mechanical and thermal data to determine cutting tool life, experimental work has not yet provided accurate or sufficient temperature information for comparison with theoretical predictions. During this investigation digital infrared imaging was used to gather temperature data in the highly deformed region near a cutting tool edge. The data has proven more accurate and offers higher resolution than techniques that have been applied to orthogonal machining in the past. The testing involved machining with non-coated carbide cutting tools and an AISI 1025 steel work piece using typical industrial cutting speeds. Results from the tests are compared to a finite element simulation of the metal cutting process.

Frequency Shift Studies for the Spallation Neutron Source Drift Tube Linac (U)

Lucie M. Parietti
Nathan K. Bultman
Los Alamos National Laboratory

The Spallation Neutron Source (SNS) is an accelerator-based facility that will be built at Oak Ridge National Laboratory by 2005. The SNS will produce pulsed beams of neutrons by bombarding a mercury target with intense beams of 1-Gev protons. The drift tube linac (DTL) of the Spallation Neutron Source accelerates the beam from 2.5 MeV to 20 MeV at the operating frequency of 402.5 MHz. This pulsed operating linac is about 9 meters long and consists of 84 cells with 83 permanent magnet quadrupole drift tubes. Under normal operation (beam on), about 80% of the radio frequency (RF) power is dissipated in the cavity walls. This amounts to 76 kW at a 7% RF duty factor. The power dissipated causes thermal distortions (i. e., shape change) which result in a shift of the RF resonant frequency of the accelerating mode. To maintain the desired resonance frequency, each cavity is cooled by forced water circulation to compensate for the thermal distortions caused by RF heating.

Size and location of the cooling channels must provide adequate cooling and resonant frequency control. Frequency shift studies are performed to guide the design of the cooling channels. The DTL tank and 83 drift tubes are cooled on two separate circuits. The thermal deformations resulting from RF heating are evaluated separately for both the tank and eight individual drift tubes using finite element models. The frequency shift of these eight cells are then computed based on the calculated deformations using the Slater perturbation theory for RF cavity analysis. A uniform frequency shift for all 84 cells can be obtained by balancing the flow rate and tailoring the cooling channels for each individual drift tube. An average acceptable resonant frequency for the DTL system is maintained by dynamically adjusting the water temperature in the drift tube circuit.

Modeling of Some Thermal and Fluid Flow Issues Related to the Design of the National Ignition Facility (U)

William G. Houf
Sandia National Laboratories, Livermore, CA

Thermal and fluid flow calculations have been performed to examine the extent of thermal gradients that might occur inside the argon gas of the target area beamtubes of the National Ignition Facility (NIF). The beamtubes are used to carry the propagating laser beams to the target chamber in the facility. Temperature gradients in the argon gas perpendicular to the direction of the propagating laser beam, produce refractive index gradients that can cause the laser beam to bend. If the temperature gradients are strong enough and persist over a long enough length of the beam, they could cause the laser beam to deflect significantly and become misaligned with the target. The total misalignment of a beam on the target is the accumulation of the misalignment that it experiences as it propagates through the entire NIF optical system. Each component of the system has a specified amount of allowable misalignment budget that it is allocated. Detailed three-dimensional calculations of buoyant convection and heat transfer have been computed to estimate thermal gradients in the argon gas and to compute an estimate of the expected misalignment do to beamtube thermal gradients.

Comparison of Simple Algorithms for Heat and Mass Transfer during Ablative Reentry (U)

Mark A. Havstad
Lawrence Livermore National Laboratory

Techniques for estimation of heat and mass transfer effects within and from reentry bodies have varied in complexity greatly. Conduction effects have been treated with zero dimensional, volume integrated, one-dimensional, two-dimensional and three-dimensional models. Surface chemical effects have been treated assuming both equilibrium and non-equilibrium reaction rates. The variation of subsurface density in time and space has been ignored, treated with a fixed or variable "charring" temperature and solved consistently within the formulation using an Arrhenius-type reaction rate expression. The motion of pyrolysis products within the solid matrix has been treated with and without a momentum conservation equation.

A series of models of varying complexity have been formulated in order to compare estimates of the heat and mass transfer effects in and on the surface of the outermost material of a reentering body with a carbon based shell. Volume integrated, one-dimensional and three-dimensional conductive treatments are compared using the heat balance integral, finite difference and finite element methods respectively. Non-equilibrium reaction rates are compared to equilibrium calculations for each model. The charring temperature formulation within the heat balance integral is compared to two formulations for the evolution of the subsurface density within the finite difference and finite element models. Pyrolysis gas flow effects are compared using "instantaneous" flow within each time step of the heat balance integral and finite difference models and a one-dimensional momentum equation for the porous media flow within the finite element model. Results for surface temperature during flight, surface recession and net conductive flux to the surface will be compared for the various formulations with an emphasis on which modeling assumptions are most in need of revision.

Manufacturing Process Modeling 3
Building 132 Room 1102

100% Quality Assured Processing for Precision Small Lot Manufacturing: Applications to Brazing (U)

Vivek R. Dave
Frank M. Smith
Stephen W. Quintana
Los Alamos National Laboratory

Precision small lot manufacturing is characterized by highly critical or man-rated components, low production volumes, high product diversity, and high quality requirements. Furthermore, the manufacturing capability required to produce such components must be maintained over long time frames with little or no opportunity for destructive testing or validation. Considering the ubiquitous nature of such manufacturing challenges in both aerospace and weapons applications, it is somewhat surprising that a 100% quality-assured methodology has not been more widely implemented. The current work describes a CRADA project aimed at implementing such an approach.

100% quality-assurance implies a complete reliance on in-situ process monitoring and control, and the complete absence of post-process inspection. This approach has been successfully implemented in the joining of critical components for next-generation military aircraft, and is therefore feasible in a 'real world' precision small lot manufacturing environment. The approach will here be described for brazing, and it will be shown that it is possible to achieve similar results, subject to some fundamental physical limitations such as CTE mismatch and drastically dissimilar material combinations. Examples of implementation strategies will be given, and insights will be presented on how this methodology can be extended to other related processes, such as heat treatment and casting.

As-built/As-is Assessment of Geometric and Material Properties for One-Hundred Manufactured Products (U)

Ronald M. Dolin
Chris Treml
Edward Rodriguez
Nirav B. Shah
Los Alamos National Laboratory

As part of an overall effort to enhance the predictive capability of analysis codes, we focused on generating precise numerical models of test products. One-hundred marine floats were purchased from a commercial vendor. The vessels were to be spherically manufactured, but they varied. The classic modeling approach would have been to generate a single nominal model of a sphere and assert that however this nominal model behaved in analysis, so would all the individual floats. However, as is always the case, none of the physical spheres matched this classical model. So in order to enhance the fidelity of analysis predictions we treated each part as being deterministically unique. This differs from the classic approach which asserts, in an ad hoc manner, that a nominal model is the probabilistic mean for all products.

Our approach provided an individual and deterministic model for each product. This approach, called as-built/as-is modeling, has been under development for several years at Los Alamos. The goal of as-built/as-is modeling is to capture and characterize the unique state of a part in a numerical model. Because not every aspect of a part can be captured through inspection and measurement, model parameters must be inferred to fill the information voids. To accomplish this, Bayesian inference techniques in a decision analysis framework are used. The process of mapping from sparse product information to numerical model parameters is discussed. Results of the as-built/as-is modeling of the marine floats are presented.

This allows multiple users to simultaneously participate in a simulation.

Confederation of Models to Perform Assessments in Stockpile Stewardship (U)

Michael M. Johnson
Todd D. Plantenga
Ann S. Yoshimura
Sandia National Laboratories, Livermore, CA

CoMPASS, a Confederation of Models to Perform Assessments in Stockpile Stewardship, is a distributed enterprise simulation of the Department of Energy (DOE) Nuclear Weapons Complex. The DOE NWC can be viewed as an inter-related network, or confederation of systems—each with specialized functions—structured to meet our stewardship responsibilities today and into the future. Components of the NWC enterprise requiring detailed analysis include aging weapons, shrinking complex resources, reduced budgets, proposed new directions (e.g., SLEP SWPP, Enhanced Surveillance Program CTBT, ADAPT Start III), etc. CoMPASS is the basis of a unified tool for use by domain experts in answering system questions. System questions the tool may ultimately be able to answer vary with the perspective of the person posing the question. For example, someone from DOE/HQ might ask, "How might START III change my production needs?" For each question, there may be a different, valid set of system assumptions that affects the way the user sees the complex.

CoMPASS has two primary goals, one each for Enterprise Modeling and Simulation. Under Enterprise Modeling, the primary goal is to provide an information unification framework for the DOE/NWC. To do this, we are capturing a static description of NWC products and processes, understanding and codifying the information flow between entities, and unifying stockpile information sources into a dynamic, queriable repository.

For Enterprise Simulation, our primary goal is the linkage of (1) disparate system simulation models from domain experts with, (2) policy driven resource allocation to allow DOE/NWC tradeoff analyses. This framework supports multi-mode and multi-fidelity simulation confederates, complete with weapon Record of Assembly (RoA) component detail. Furthermore, resource allocation policies, including core surveillance and dismantlement, interact with weapon degradation models to affect the stockpile reliability.

Hence, CoMPASS is a confederation of component simulation and data models, each constructed and managed by domain experts. CoMPASS provides a software framework to coordinate interactions between confederates. The ultimate goal of CoMPASS is a linkage across the NWC of geographically disparate confederate models. Here, CoMPASS confederate models, databases, and user interfaces are spread and run across the entire nuclear weapons complex.

Sheffield Inspection Rotary Gage Post-Processing Algorithms (U)

Wilbur D. Birchler
Christopher J. Scully
Los Alamos National Laboratory

The Nuclear Weapons Complex is undergoing major changes in the areas of design, analysis, and manufacturing. Because of these changes, the possible manufacturing roll of Los Alamos may be increased. Coupled with these possible new manufacturing activities are the part inspection requirements. The Sheffield Inspection Rotary Gage has been satisfactorily utilized by Rocky Flats and Lawrence Livermore to inspect manufactured parts. Now, Los Alamos is expanding its capabilities to use the Sheffield Inspection Rotary Gage.

Many tasks were required to make the gage functional at Los Alamos. The two tasks presented are associated with the post-processing of the inspection data. The first task was to understand the existing pre- and post-processing algorithms used at Rocky Flats. The second was to determine if modern Computer Aided Design (CAD) tools could be utilized to display and evaluate the inspection data.

In the first task, both the pre- and post-processing data algorithms were evaluated. The input data for the Sheffield is described. This description includes with the theoretical (probe) touch points on the part surfaces relative to the radial measurement lines. An understanding of the positions of the probe tips to the surfaces is required for knowing how to post-process the data. A Pro/Engineer procedure was developed to automatically generate the input data for the Sheffield.

The second task was to understand the post processing tasks used at Rocky Flats. A description of their process presented along with the assumptions used. Because of some of the these assumptions and the use of a Parametric Technology, Inc. Pro/Engineer tool call Pro/Verify a new post processing algorithm was developed. Its is PRO/Engineer based with input obtained form a standalone data processor. Both of these programs are discussed.

Lean Manufacture of Assemblies for the National Ignition Facility (U)

Lychin Chang
Lawrence Livermore National Laboratory

The concept of Lean Manufacturing, which was pioneered at Toyota, emphasizes continuous improvement through the identification of the value stream and the reduction of waste, and making value flow at the pull of the customer. The Lean concepts have been applied to many manufacturing applications in industry, most notably the major automotive plants.

The National Ignition Facility's (NIF) Lean Enterprise Team at Lawrence Livermore National Laboratory is working to apply the concepts of Lean Manufacturing to the production of the mechanical and optical assemblies which will comprise the NIF system. Application of the Lean concepts requires the identification of the value stream, along with streamlining of the production process, such that unnecessary steps are eliminated, and production flows according to the demand schedule in a "just-in-time" manner.

A fully animated, discrete-event simulation model is being developed which captures the production flow of Line Replaceable Units (LRU) of the NIF. The model simulates the production steps, resource requirements, and material flow through the Optics Assembly Building (OAB) and the Optics Processing and Development Laboratory (OPDL). The overall goal is to ensure that the "leaned" procedures are adequate to meet the overall activation schedule. The model may be used to identify either where additional cost saving reductions may be taken or additional steps or resources are required.

Session 4: Tuesday, November 2, 1999, 3:15 p.m.–5:00 p.m.

Solid and Structural Mechanics 4
Building 123 Auditorium

Symmetry Considerations in Finite Volume Solutions in Axis-Symmetric Geometries (U)

Raymond L. Bell
Sandia National Laboratories, Albuquerque, NM

The current version of the CTH code uses the Benson (1992) Half Index Shifted (HIS) momentum scheme for the solution of the momentum conservation equation. This scheme eliminates the usual staggered mesh needed for momentum advection. Instead, each face centered velocity (momentum) is shifted one half index to the center of each cell sharing the face. This results in twice the number of momentum advection calculations as the earlier method, but improves the overall accuracy of the simulation.

CTH has six different geometry options: 1D rectangular, 1D cylindrical, 1D spherical, 2D rectangular, 2D cylindrical, and 3D rectangular. While running 2D cylindrical calculations we noted that spherical shocks tended to become very asymmetrical after many computational cycles. Corresponding 2D rectangular calculations did not show the same asymmetry. This led us to consider potential modifications to the HIS scheme that would cure the asymmetry in 2D cylindrical calculations without corrupting rectangular geometry calculations.

We show the modifications which improve the 2D cylindrical results without changing any of the rectangular geometry results. These modifications involve the weighting scheme used to recover the face centered velocities from the residual cell centered HIS momenta after the advection step is completed.

A Highly Efficient Enhanced Assumed Strain Physically Stabilized Hexahedral Element (U)

Michael A. Puso
Lawrence Livermore National Laboratory

A method which combines the incompatible modes method with the physical stabilization method is developed to provide a highly efficient formulation for the single point 8 node hexahedral element. The resulting element, implemented into DYNA3D and NIKE3D, is compared to well-known enhanced elements in standard benchmark type problems. It is seen that this single point element is nearly as coarse mesh accurate as the fully integrated EAS elements. A key feature is the novel enhanced strain fields which do not require any matrix inversions to get the internal element degrees of freedom. This combined with the reduction of hourglass stresses to four hourglass forces produces an element that is only 6.5% slower than the perturbation stabilized single point brick element commonly used in many explicit finite element codes.

Segment to Segment Sliding Interface Algorithms for Contact Between Edges (U)

Jerry I. Lin
Lawrence Livermore National Laboratory

Modern computational mechanics codes often include the Sliding Interface feature to simulate interactions between mechanical bodies. In most finite element codes, e.g., LLNL's DYNA3D and NIKE3D, interference detection algorithms that investigate the geometric relationship between a node and a segment are preferred in the Sliding Interface feature. Though algorithms of this nature have their advantages, they often fail to detect interference under certain conditions, such as contact between edges of plate or shell structures. This drawback can be attributed to the loss of sight of the nodal connectivity for one contact entity.

Sliding Interface algorithms that examine the interference between two segments are designed to overcome this shortcoming. This new method will be integrated into the explicit finite element code DYNA3D. The contact force, which is the force necessary to separate the interfering segments, is distributed among nodes defining the segments. The magnitude and direction of the contact force is determined based upon the severity of the interference and the segment orientations and motions. The new Sliding Interface algorithms can be used for general contact or penetration detection.

An Investigation of the Use of Shell Elements for Modeling Inflation of Fabric Structures (U)

Vicki L. Porter
Sandia National Laboratories, Albuquerque, NM

An on-going ASCI project is research and development of a fluids/structural analysis code for the coupled analysis of parachutes. The current project plan calls for development of a new 3D fluids code to be coupled with PRONTO3D, a three-dimensional finite element code for the nonlinear, transient dynamic analysis of structures. This presentation will describe structural analyses performed with the shell element in PRONTO3D on test problems involving fabric structures in anticipation of the future coupled analyses of parachutes.

In the initial stages of parachute inflation, the structural problem is mass-driven with very little stiffness. Because there is very little strain energy during this phase, the under-integrated shell elements common in explicit dynamics codes are susceptible to hour-glassing modes. In addition, actual fabrics cannot carry a compressive load and will simply deform out-of-plane, i.e., wrinkle. Modeling of wrinkling behavior with a standard shell element is highly dependent on mesh density unless compensation is made in the constitutive model to eliminate compressive stresses. This presentation describes efforts to reduce hourglassing behavior, as well as analyses performed to investigate the effects of mesh density on the modeling of wrinkling behavior without modifying the constitutive model. The shell element used in this study is one developed by Key and Hoff as an improvement to the Belytschko-Lin-Tsay element. The Key-Hoff element has improved representation of warping modes because it is based on structural geometry rather than treating the geometry as flat, and it possesses a true warping stiffness rather than a warping hourglass mode.

Thin fabric structures are often assumed to lack bending stiffness and modeled with membrane elements rather than shell elements. Comparisons of shell and membrane element behavior will also be presented.

Unconditionally Stable, Implicit Dynamic Analysis of Coupled Flexible Finite Element—Rigid Systems (U)

Michael A. Puso
Lawrence Livermore National Laboratory

Many dynamic events, such as vibrations of transportation containers, re-entry vehicles undergoing gravitational and spin up loadings, seismic loading of structures, etc., occur over long time spans and can be potentially simulated using implicit dynamic analysis. This is because the system response of these events are often dominated by the low frequency behavior of the structure and implicit analysis can exploit large time steps (compared to explicit) to handle these long duration's. On the other hand, the classical implicit integrators such as Newmark's method and the generalized midpoint rule are not unconditionally stable in the nonlinear regime. Recently, implicit dynamics algorithms which are unconditionally stable for nonlinear problems with contact have been developed. In our work, we improve these algorithms and also generalized them to handle both flexible finite elements and rigid bodies. That is, we can handle dynamic systems with bilateral constraints of rigid materials directly connected to flexible materials and unilateral constraints due to flexible-flexible, rigid-flexible and rigid-rigid contact. These are original contributions and have been implemented into NIKE3D and demonstrated on number of examples.

Comparison of Modeling Techniques for a Three-Layered Shell in ABAQUS (U)

Carole A. Le Gall
Sandia National Laboratories, Livermore, CA

Computational methods are often used to evaluate the structural response of weapon systems. In many cases, this requires that finite element (FE) models of the conical outer aeroshell be developed. The aeroshell is composed of three layers, in which a carbon phenolic outer shell is bonded to an aluminum substrate with a thin layer of bond material. The primary difficulty in modeling this structure lies in characterizing the behavior and properties of the thin, soft bond material.

To compare different modeling techniques, several FE models were developed and the frequency responses were calculated using ABAQUS. Two general studies were performed. In the first study, a thin-walled cylinder was modeled using each of three different modeling techniques to allow for comparison of the techniques. The cylinder was modeled using solid elements, shell elements, or a combination of solid and shell elements ("mixed" modeling). Comparison of solid and shell modeling techniques suggest that the laminate shell theory used in these evaluations does not accurately represent the structural response when the material properties of the laminate are extremely dissimilar. Comparison of solid and "mixed" modeling techniques suggest that the "mixed" method more accurately represents the structural response of this type of shell structure. The studies suggest that this type of configuration can efficiently be modeled in ABAQUS using a combination of linear solid and offset shell elements.

In the second study, the bond modulus was varied in both the shell and solid models to assess the influence of the elastic modulus of the bond layer on the error in frequency response of shell models. The results of these analyses showed that the laminate shell theory for the test geometry appears to be applicable only when the ratio between dissimilar material moduli is less than approximately two orders of magnitude.

Material Behavior and Characterization 4
Building 123 Conference Room A

The Mystery of Deep-Focus Earthquakes (U)

Charles A. Anderson
Los Alamos National Laboratory

Gerald Schubert
University of California, Los Angeles

J. Philippe Devaux
Ecole Normale Superieure, Paris, France

The cause of deep-focus earthquakes is a major puzzle in geodynamics because at great depth rocks should flow rather than break to relieve stress. In general, failure can occur by either brittle fracture or ductile flow. Fracture and frictional sliding are strongly inhibited by pressure, but not by temperature, because they involve the opening of tensile microcracks. The stress at which rocks flow, on the other hand, is strongly reduced by increasing temperature, but is essentially unaffected by pressure. Thus, because temperature and pressure increase with depth in subducting slabs, the response to tectonically-imposed stresses deep in slabs should be ductile flow rather than abrupt seismic failure. Nevertheless, deep-focus earthquakes are common in slabs that descend far into the mantle such as the largest deep earthquake on record (M = 8.3), which occurred 650 km beneath Bolivia on June 9, 1994.

In this talk a thermo-mechanical numerical model of a subducting slab in which the olivine→spinel phase transformation occurs will be described. The thermal structure of a meta-stable olivine wedge has been simulated by the model. The stress field caused by this thermal structure has been determined and adds corroboration to the hypothesis that transformational stresses in subducting slabs could cause deep-focus earthquakes.

Aluminum Honeycomb Constitutive Model Validation for the B61 Radar Nose Crush Model (U)

Terry D. Hinnerichs
Michael K. Neilsen
Vesta I. Bateman
Thomas G. Carne
Barry D. Boughton
Sandia National Laboratories, Albuquerque, NM

Wei-Yang Lu
Sandia National Laboratories, Livermore, CA

The Advanced Weapon Projects Department 2167 and its design team plan to qualify the new B61 Common Radar Nose crush performance by a combination of model-based simulations and by full-scale hardware testing on the Sandia-Albuquerque Rocket-Rail test facility. A PRONTO3D finite element nose crush model is being used for qualification process. Significant forward and aft volumes of the new Radar Nose are composed of aluminum honeycomb and are the major shock mitigation materials. This presentation will focus on the validation of the constitutive model used to model the aluminum honeycomb crush within the PRONTO3D finite element code.

The B61 Radar Nose qualification testing is currently being performed at conditions thought to be worst case based on past nose crush tests and relatively simple analyses. The purpose of this higher fidelity validated nose crush model will be to fully explore the design space and make predictions on what are the most demanding conditions, e.g., impact pitch and roll angles.

An overview of the constitutive model validation process will be given that includes constitutive testing and model validation testing under the MAVEN program and the construction of a Phemonena Identification and Ranking Table. Also, through sensitivity analyses, the model parameters with significant uncertainties will be identified and the process of propagating these through the analyses will be described. Finally, the criteria for excepting the model as being validated will be discussed.

A Damage Accumulation Model for Thermomechanical Fatigue of a Metal Matrix Composite Based upon a Finite Element Analysis Approach (U)

Michael J. O'Brien
Choi K. Syn
Donald R. Lesuer
Lawrence Livermore National Laboratory

Finite element modeling was used to simulate the volumetric average stress-strain response of discontinuous Kaowool-fiber reinforced aluminum-matrix composites under combined cycles of temperature and mechanical loading. The finite element model accounted for rate independent plasticity, rate dependent creep and residual stress due to mismatches in coefficient of thermal expansion and solved for the stress-strain history of the composite's components. The accumulated elastic, plastic and creep strains were calculated as functions of time for the cyclic loading and used in a damage accumulation model to predict the thermomechanical fatigue life of the composite. It was assumed that fatigue damage is governed by mechanical strain range and that creep damage is governed by the exhaustion of ductility. The calculated results were compared with experimental results for three different applied loading profiles. It was found that stress relaxation due to creep accounted for the observed difference in thermomechanical fatigue life for the three different profiles.

An Evaluation of Several Hardening Models using Taylor Cylinder Impact Data (U)

Marvin A. Zocher
Paul J. Maudlin
Elane C. Flower-Maudlin
Los Alamos National Laboratory

Efforts are currently underway at Los Alamos to enhance our ability to predict the behavior of metals undergoing finite deformation. A key ingredient in correctly modeling finite deformation plasticity is the hardening model. Several models have been proposed. Which model is "best" is as yet an open issue. It may be that "model A" does a better job in "low" strain-rate regimes while "model B" does a better job in "high" strain-rate regimes, and "model C" does better in-between. It may be possible to develop a single model that does well throughout the full range of strain-rates that may be of interest.

The objective of this work is to begin to answer the question of which hardening model is best. We shall investigate the ability of several different hardening models to predict the finite deformation resultant in Taylor cylinder impact tests. The models to be evaluated are Johnston-Cook, PTW, MTS, and Steinberg-Guinan. All four models have been written into a single continuum mechanics code and can consequently be evaluated in such a way that all other factors are equal. The Taylor cylinder test produces strain-rates on the order of 103 to 105. An evaluation in other (higher) strain-rate regimes awaits further work.

Discrete Dynamic Fracture With Finite Elements (U)

Jobie M. Gerken
Joel G. Bennett
Fred W. Smith
Los Alamos National Laboratory

A method to model discrete dynamic crack propagation in 2 dimensional structures has been developed and implemented in the implicit finite element code ABAQUS/Standard. First, a new 2 dimensional bilinear finite element is formulated from the Hu-Washizu energy principle, which includes standard plane stress/plane strain behavior with an additional load due to a small crack on the edge of the element. This new element is then used to define an Interface Crack Element (ICE), which consists of two adjacent finite elements with a small crack located at the interface. Each adjacent element is uniquely defined so that the elements are allowed to separate to model discrete crack growth along any element interface. The two adjacent elements are allowed to separate when defined failure criteria for the small interface crack have been met. These failure criteria are based solely on information available from the two adjacent elements. This precludes the need for any *a priori* assumptions about the fracture behavior of the structure and allows for arbitrary crack growth based on the solution to the boundary value problem. Investigation is ongoing into the appropriate interface failure criteria. Discussion of several possible interface failure criteria is presented. Preliminary results of crack propagation in both linear elastic and rate dependent, damage prone materials, such as PBX 9501, are presented and compared with some recent experimental results. The results indicate that although the crack initiation loads may be somewhat in error, the crack propagation paths can be reproduced.

Size Effects in Brittle Materials (U)

Robert A. Riddle
Lawrence Livermore National Laboratory

Brittle materials, such as ceramics, glasses, salts, and composites of metals and ceramics are distinguished not only by their inability to sustain plastic deformation on the macroscale, but also by the variability in their apparent strength and other mechanical and thermal properties.

Various statistical methods have been used to describe the variable strength of brittle materials. Among these methods is the statistical distribution and failure prediction method developed by Weibull.

The failure prediction method by Weibull is based on the concept of the 'weakest link.' For brittle solids this means that the failure is initiated by the largest flaw in a region of tensile stress. Because larger solids have a greater probability of larger flaws, it is expected that larger volumes of brittle materials will have lower strengths. Because brittle materials experience crack grow in regions of tensile stress, but not compressive stress, the failure predictions are influenced by the extent as well as the magnitude of the tensile stresses.

The two parameters of the Weibull failure model characterizing the failure of specimens are the dimensionless modulus m and the characteristic strength σ_θ with units of stress. The characteristic strength changes with specimen size and geometry. The characteristic strength is transformed into the Weibull scale parameter, which defines strength relative to a unit size, and has units of stress•volume$^{(1/m)}$.

Weibull parameters for failure analysis are presented for 5 different materials: a ceramic, a salt, and three types of glass. Predictions of the volume effect based on the Weibull modulus are compared. Potential correlations between the Weibull parameters and fracture toughness values are put forth with the object of predicting critical flaw size and flaw distributions within the brittle materials.

Computational Heat Transfer 3 and Radiation Transport
Building 132 Auditorium Room 1000

Finite Element Analysis of Liquid Flow, Energy Transport, and Deforming Interfaces in a Ti-6Al-4V Evaporation Melt (U)

Matthew A. McClelland
Kenneth W. Westerberg
Lawrence Livermore National Laboratory

Chrispian E. Shelton
Jonathan Storer
3M Company, St. Paul, MN

The electron-beam evaporation of Ti-6Al-4V is an important step in the fabrication of metal matrix composites for aircraft components. The energy from an electron beam is used to evaporate metal from the top of a rod which is fed vertically through a water-cooled crucible. The evaporation rate is strongly influenced by thermal convection in the liquid pool at the e-beam impact site. The flow is driven by thermally-induced buoyancy and capillary forces and is in the transition region between laminar and turbulent flow. The MELT finite element code is used to calculate steady-state, two-dimensional flow and temperature fields along with liquid-solid and liquid-vapor interface locations. These interfaces are tracked using a mesh structured with rotating spines.

Model results are compared with measurements from 3M's Advanced Development Coater. The electron-beam footprint dimensions were obtained from video images, and the evaporation rate was determined from feed rate measurements. Crucible heat flow rates were calculated from temperature rises in the cooling water, and the final melt pool shape was obtained by sectioning the top of the rod. A single thermal transport parameter was adjusted in the MELT model to provide a good representation of the measured evaporation rates, crucible heat flows, and lower pool boundary locations. The MELT model predicts a significant increase in evaporation rate from an improvement in e-beam trajectory.

High Explosive Violent Reaction (HEVR) From Slow Heating Conditions (U)

Armando S. Vigil
Los Alamos National Laboratory

The high explosives (HEs) developed and used at the Los Alamos National Laboratory are designed to be insensitive to impact and thermal insults under all but the most extreme conditions. Nevertheless, violent reactions do occasionally occur when HE is involved in an accident. The HE response is closely dependent on the type of external stimulus that initiates the reaction. For example, fast heating of conventional HE will probably result in fairly benign burning, while long-term, slow heating of conventional HE is more likely to produce an HEVR that will do much more damage to the immediate surroundings. An HEVR (High Explosive Violent Reaction) can be defined as the rapid release of energy from an explosive that ranges from slightly faster than a deflagration (very rapid burning) to a reaction that approaches a detonation. A number of thermal analyses have been done to determine slow heat/cook-off conditions that produce HE self-heating that can build up to a catastrophic runaway reaction. I will specify the conditions that control reaction violence, describe experiments that produced an HEVR, describe analyses done to determine a heating rate threshold for HEVR, and list possible HEVR situations.

Thermal-Hydraulic Design of a Blanket for the Accelerator Production of Tritium (U)

Richard J. Kapernick
Ray M. Guffee
Los Alamos National Laboratory

The Accelerator Production of Tritium (APT) Project, sponsored by the U. S. Department of Energy, has developed a conceptual design of an accelerator-based system to produce tritium. In the design, high-energy protons impact a tungsten target and, through a process of spallation, produce high-energy neutrons. These neutrons are moderated and captured in a blanket structure surrounding the target. This blanket structure contains lead, which serves as a neutron multiplier and moderator; ^3He, which captures thermalized neutrons and produces tritium; aluminum, which

serves as the structural material because of its low neutron capture cross-section; and light water, which cools the structure. The blanket structure is approximately 400 cm high, 120 cm thick, and is divided into 18 modules. Each module weighs up to 100 tons.

The blanket thermal power is 30 MW, with power densities in the lead varying from 40 W/cc down to values much less than 1 W/cc. The challenge presented in the thermal-hydraulics of the blanket is to produce a design that accommodates this large variation in power density, maintains turbulent single-phase flow throughout the system, produces a coolant temperature rise that is large enough to allow the heat exchangers to be reasonably sized, meets the low-temperature operating limit for aluminum, and maximizes the production of tritium.

This paper describes the blanket design that has been developed to meet the thermal-hydraulic requirements summarized above and that is structurally adequate. Also presented are the thermal-hydraulic methods that have been developed to produce the design and assess its performance.

Modeling of Packages Transporting Weapons Components Using the MCNP-4B Code (U)

Luisa F. Hansen
Lawrence Livermore National Laboratory

The MCNP-4B code is a useful tool for modeling radioactive material packages, such as shipping containers bearing nuclear weapon components, and for performing shielding and criticality calculations required by Title 10, Code of Federal Regulations, Part 71 (10 CFR 71).

MCNP-4B is a Monte Carlo transport code, which is used to analyze transport of neutrons, photons and electrons or to carry on coupled channel calculations for neutron/photon/electron transport. MCNP is able to describe any complex three-dimensional body containing any number of materials in different configurations, as a combination of geometric cells limited by first- and second-degree surfaces and fourth degree elliptical tori.

Starting from the mechanical drawings of the packaging and weapon components to be shipped calculational models have been done for the Model FL, AT400A and ALR8-SI packages. Together with the detailed geometry of the different sections of the packaging and its content, the density of each one of the materials found in the package is required by the code in order to accurately calculate the masses and volumes of each section. In addition to the density, an accurate isotopic composition for each material is required to account for the nuclear interactions of the neutrons and photons emitted by the radioactive content of the package containing these materials. These interactions (cross sections) govern calculations of the dose rates outside the package and its multiplication factor k_{eff}.

A detailed description of the input files and calculational models obtained for the above containers will be shown, together with a comparison of the total dose rates and k_{eff} values for these three packages for the same enclosed pit. The sensitivity of the dose rate calculations to the specific isotopic composition of the choice of materials in the overpack of the ALR8-SI will be illustrated.

Analysis of Heat Transfer During Quenching of a Gear Blank (U)

Vivek Sahai
Salvador M. Aceves
Lawrence Livermore National Laboratory

This paper presents experimental and numerical results for the quench of a gear blank in agitated and stagnant oil. Heat transfer within the gear blank is analyzed with a whole domain-optimizer technique inverse solution method, to calculate the time history at every point in the gear blank. The development of this procedure represents the first stage in an overall analysis of the quench process that will later include material phase transformations and deformation.

The paper presents ten variations in setting up the inverse problem, to analyze which combination of independent variables and decision variables results in the best match between experimental and numerical results. The results indicate that dividing the boundary of the gear blank into four zones and assigning a fixed heat transfer coefficient or heat flux to each zone yields an average RMS error (average difference between experimental and numerical results) of the order of 40 K. This error can be reduced by either increasing the number of zones, by reducing the number of thermocouples being matched, or by allowing the heat transfer or heat flux to vary within the zones. Of these possibilities, variation of heat transfer within the zones gives the best improvement in the quality of the match for the amount of extra effort required to run the problem.

Uncertainty and Sensitivity
Building 132 Room 1102

A Framework for Efficient Treatment of Variability, Uncertainty, and Discretization Error in Optimization Problems (U)

Vicente J. Romero
Sandia National Laboratories, Albuquerque, NM

Incomplete convergence in numerical simulation such as computational physics simulations and/or Monte Carlo simulations that might enter into the calculation of the objective function in an optimization problem produces noise, bias, and topographical inaccuracy in the objective function. These affect accuracy and convergence rate in the optimization problem. Accordingly, an optimization framework has been developed that acknowledges discretization/convergence error and manages model resolution to efficiently reduce uncertainty in the final optima. The framework employs a structured-sampling optimization scheme devised for noise-tolerance and efficiency in global searching leading to local optimization. Uncertainty due to variability and uncertainty of critical model parameters such as material properties, constitutive equation constants, boundary condition coefficients, etc. that can be treated as random variables is efficiently handled as an optimization "post-problem." An illustrative application of the framework to an "industrial" test problem will be presented.

Effect of Initial Seed on Monte Carlo Probabilities (Computational Confidence Intervals for Simple-Random and Latin-Hypercube Sampling) (U)

Vicente J. Romero
Sandia National Laboratories, Albuquerque, NM

In order to devise an algorithm for actively monitoring and terminating Monte Carlo sampling when sufficiently small and reliable confidence intervals (CI) are achieved on calculated probabilities, the behavior of computationally calculated CI must be explored and mapped out. This knowledge is also required in assessing the accuracy of other probability estimation techniques against Monte Carlo sampling (Monte Carlo results often [and many times inappropriately] being held as the standard for comparison). Based on 100 trials in a simple random sampling (SRS) statistical-inference test problem, computed CI are examined for level of significance in conformance to CI theory over valid spectrums of probabilities (population proportions) for population sizes of 500 and 10,000 samples. Significant differences between "ideal" and "computational" statistics are found to exist. With regard to Latin Hypercube sampling (LHS), empirical comparison reveals that at a 0.1 level of significance LHS is over an order of magnitude more efficient that SRS for similar CI on probabilities (population proportions) between 0.25 to 0.75. Contrary to a somewhat commonly held belief, however, the efficiency advantage vanishes as the probability extremes of 0 and 1 are approached. More generally, the statistical reliability of applying CI theory to SRS and LHS in a computational environment that calculates sampling variance directly by "sample grouping" or "replicated sampling" is presently being assessed.

Bayesian Inference Techniques in a Decision Analysis Framework to Determine Valve Reliability (U)

Ronald M. Dolin
Edward Rodriguez
Los Alamos National Laboratory

Bayesian analysis and inference techniques are used to determine the reliability of a valve design. Since only forty valves are available for testing it is not pragmatic to assess reliability using frequentist probability methods. Also, there exists a vast amount of historical and antidotal information on valves that should be incorporated into the reliability assessment. Bayesian analysis is a branch of probability theory that allows diverse information to be synthesized into a single comprehensive framework.

By combining Bayesian analysis with hypothesis testing in a decision analysis framework we hope to develop an intelligent outline for how the forty valves should be tested. Rather than just test all forty and analyze the statistical results, we want to take an incremental approach, integrating the results of the most recently completed test with the results of all the other previous tests to predict how the next test should be performed. For example, whether the next test should be in a hot, cold, or at ambient environment. Each test is conducted so as to strengthen the confidence in a given hypothesis. This approach allows us to learn as we go. It is hoped that enough knowledge can be

gained by the time we complete the forty tests that we have a high confidence in the computed reliability number.

Using Bayesian Belief Networks for Quantifying and Reducing Uncertainty in Prediction of Buckling Characteristics of Marine Floats (U)

Christine Treml
A. Sharif Heger
Los Alamos National Laboratory

The goal of this project is to develop a method using Bayesian belief networks (BBN) to quantify and reduce the uncertainty in scientific predictions. The uniqueness of this method lies in the BBNs ability to handle both qualitative and a variety of quantitative data in modeling a decision and/or prediction process. This area has become increasingly important to the analysis of complex systems in light of difficulties associated with their testing. Programs involving small numbers of units and limited production rates are often forced to rely on past data, current nondestructive observations, and numerical simulations to predict the effects of events such as material replacements, manufacturing changes, and aging on their performance.

To determine the effectiveness of this method, it will be applied to the investigation of buckling characteristics of spherical stainless steel marine floats. A constitutive model for these spheres has been developed. A sample group of 100 will be used, and will be examined qualitatively for surface, contour, and weld quality. Forty of these spheres will be subjected to an as-built dimension inspection to obtain distributions on the actual geometry, and the constitutive relations such as stress-strain curves. Another 40 of the spheres will be instrumented and subjected to a load supplied by a hydraulic press until buckling occurs. Probabilistic distributions for the constitutive and qualitative properties as related to the buckling characteristics will be determined from the qualitative, as-build, and experimental observations. These distributions will be used in conjunction with a Bayesian belief network to help update the constitutive model and to make predictions about the possible behavior of any given sphere subjected to a buckling force. The BBN will also provide a unified handling of all of the available information, such as, qualitative observations, past quantitative measurements and experimental data, and the results from the numeric model.

Propagation of Uncertainties in Bayesian Belief Networks: A Case Study in Evaluation of Valve Reliability (U)

A. Sharif Heger
Edward A. Rodriguez
Christine A. Treml
Roberta J. Shaw
Los Alamos National Laboratory

We have used Bayesian belief networks (BBN) to investigate the reliability of a subset of valves as they are currently used. A BBN is a graphical model that encodes causal and probabilistic relationships among variables of interest. It is a visually effective method for modeling complex systems, which may contain both qualitative and quantitative variables. It models the relationship among the components and processes that make up the system and has an intuitive representation of information flow.

When used in conjunction with statistical techniques, a BBN model of a complex engineering system has several advantages for data and decision analysis over existing methods such as fault trees and event trees. First, a BBN encodes dependencies among all variables and, therefore, can accommodate scenarios where data are missing. Second, a BBN can encode causal relationships to gain understanding about a problem domain, and to predict the consequences of intervention. Third, since a BBN combines both causal and probabilistic relationships, it is an ideal representation for combining prior knowledge and experimental data. Finally, using Bayesian statistical methods, the BBN approach to modeling a system provides an efficient and principled approach for avoiding overfitting of data.

We have used Bayesian belief networks to construct a model of a valve from prior knowledge and existing data. Further, we have extended the method to evaluate the reliability of the valves within the framework of their application. Within this context, we consider several plausible scenarios that can occur during the operation of the valve and evaluate their effect on its parts and its overall reliability.

In general, the BBN method is an effective decision-theoretic tool for assessing the performance of a system in the absence of data. This method may be used for decision making to modify or upgrade the actual valve based on a mathematically sound and tractable method. We must emphasize that we have limited the application of this method to a simple example to focus on demonstrating its potential benefits. A comprehensive decision analysis requires detailed knowledge of decision alternatives, which include costs of options, policy, and manufacturing infrastructure.

Session 5: Wednesday, November 3, 1999, 8:00 a.m.–9:45 a.m.

Solid and Structural Mechanics 5
Building 123 Auditorium

A Segment-Based Automatic Contact Algorithm for Explicit Finite Element Calculations (U)

Edward Zywicz
Lawrence Livermore National Laboratory

In complex multi-body finite element simulations, contact detection and its subsequent resolution are pivotal in generating physically correct and accurate results. This work describes recent enhancements made to DYNA3D's automatic contact algorithm that greatly improve its robustness and efficiency. The new approach is based upon the concepts that 1) a finite contact domain (i.e., volume) exists for each segment, 2) potential contact can be identified using the slave node's position and the current contact domain, and 3) a single slave node can be in simultaneous contact with multiple segments. The salient features of the global sorting, rough screening, and local contact detection algorithms based upon these concepts are discussed.

The periodically performed global sort constructs a list of nodes that are potentially in contact with each segment. In the global sort the segments are first grouped together based upon their size and an estimate of the overall sorting cost. Then each segment group and all the nodes are bucket sorted via traditional methods (Benson and Hallquist, 1986) using the group's largest characteristic dimension. Next, a velocity-modified pin-ball screening criteria is applied to the bucketed data to construct the list of candidate nodes per segment. The interval between sorts is modified on-the-fly to "minimize" the overall cost of the global sort and rough screening.

At each step (or iteration), the segment-based sub-lists of nodes are further reduced, i.e., rough screened, based upon a planar idealization of the segment, segment warpage and thickness, and the current geometry. The reduced segment-based lists are then inverted to form a list of candidate segments for each node before the local search is performed.

The local contact detection algorithm uses a fixed-iteration, closest point projection method to determine the slave node's isoparametric position on each candidate segment. The isoparametric coordinates, penetration rate and depth, and other segment-based geometrical factors are used to assign a hierarchical rank to the potential contact and identify a master node on the segment. Constraint equations are then generated for the "top" ranking segments of each master node identified.

3D Toolboxes for Semiconductor Modeling using LaGriT: From Deposition and Etch to Microstructure Evolution and Capacitance Extraction (U)

J. Tinka Gammel
Neil Carlson
Andrew Kuprat
Robert Walker
David Cartwright
Denise George
Los Alamos National Laboratory

Michael Coltrin
Pauline Ho
Sandia National Laboratory, Albuquerque, NM

We discuss several tools for semiconductor modeling which make use of the Los Alamos LaGriT adaptive unstructured grid generation and optimization software package. TopoSim3D is a three-dimensional profile simulation tool being developed at Los Alamos to model surface motion during deposition and etch, with the surface reaction mechanisms described using ChemKin and Surface ChemKin software libraries, developed at Sandia National Laboratory. Grain3D is a three-dimensional Gradient Weighted Moving Finite Element code being developed at Los Alamos to model microstructural evolution and annealing, and allows for both material anisotropy and coupling to a time-dependent, diffusive field such as a temperature gradient. These codes also interact to model grain growth during processing. Both TopoSim3D and Grain3D rely upon the unique optimization capabilities of LaGriT, which ensure that interfaces and grid quality are maintained in these moving-mesh applications even as interfaces change geometrically and topologically in response to both surface and volume fields, which can themselves be the solutions of time-dependent PDEs on the surface or volume meshes. LaGriT also has the ability to adapt a grid so as to minimize the error in the solution of PDE's, allowing for accurate solution using a small number of grid nodes. We will briefly discuss a new tool we are developing based on this feature of LaGriT, which calculates the capacitance matrix for complex, asymmetric, 3D interconnect structures where sharp corners and non-smooth features lead to singularities in the solution. These codes provide a capability, integrated via LaGriT, for studying three-dimensional effects in semiconductors at a feature-scale level.

OPL—A Ray-Trace Code for Determining Wavefront Distortion in Optical Elements (U)

Mark Rotter
Steve Sutton
Lawrence Livermore National Laboratory

When an optical element such as a lens or the active medium of a solid-state laser is subjected to stresses due to mounting or thermal loading, the properties of the element are perturbed relative to the non-stressed state. These perturbations manifest themselves as surface distortions which lead to refractive-index variations throughout the optic. Two of the more well-known effects arising from these perturbations are thermal lensing in rod-geometry solid-state lasers and stress-induced birefringence.

We have developed a ray-trace code, OPL, which calculates the distortion an initially-plane wave experiences as it propagates through the optic as a result of stresses and/or thermal loading. This code is designed to be used as a post-processor to either the NIKE3D/TOPAZ3D suite of finite-element codes, or with ANSYS, a commercially-available finite-element code. At present, our code can accommodate isotropic or cubic-crystalline media; additional material types may be easily added.

In this presentation we will discuss the underlying physics of the code. In addition, we shall present results of our work in modeling wavefront distortion in large-aperture solid-state lasers such as those envisioned for the National Ignition Facility.

Vibration-Based Structural Damage Identification With Linear Discriminant Operators (U)

Charles R. Farrar
Scott W. Doebling
David A. Nix
Los Alamos National Laboratory

Many aerospace, civil, and mechanical systems continue to be used despite aging and the associated potential for damage accumulation. Therefore, the ability to monitor the structural health of these systems is becoming increasingly important. A wide variety of highly effective local non-destructive evaluation tools are available. However, damage identification based upon changes in vibration characteristics is one of the few methods that monitor changes in the structure on a global basis. The material presented herein will first briefly summarize more recent developments in the field of global structural health monitoring. Vibration-based damage detection is a primary tool that is employed for this monitoring. Next, the process of vibration-based damage detection will be described as a problem in statistical pattern recognition. This process is composed of three portions: 1) data acquisition and cleansing; 2) feature selection and data compression, and 3) statistical model development. Current research regarding feature selection and statistical model development will be emphasized with the application of this technology to a large-scale laboratory structure.

A linear discriminant operator, "Fisher's Discriminant," is applied to the problem of identifying structural damage in a physical system. Accelerometer data in the form of time histories are recorded from sensors attached to a system of interest as that system is excited by either impulse-hammer or random excitation. Linear Prediction Coding (LPC, commonly referred to in the vibration literature as autoregressive moving-average models) coefficients are utilized to convert the accelerometer time-series data into multi-dimensional samples representing the resonances of the system during a brief segment of the time series. Fisher's discriminant is then used to find the linear projection of the LPC data distributions that best separates data from undamaged and damaged versions of the same system. The method was tested on data from concrete bridge support columns (flexure) as well as on an 8-DOF spring mass system (axial or membrane response). In both cases, the method captures a clear distinction between undamaged and damaged vibration profiles. Further, the method assigns a probability of damage that can be used to rank systems in order of priority for inspection.

This presentation will conclude with a discussion that shows how Fisher's Discriminant can be used to couple various data types (motion, environmental, operatioal, etc.) into the damage detection process.

Analysis of the B61 Common Radar Nose Axial Impacts (U)

Kenneth W. Gwinn
Sandia National Laboratories, Albuquerque, NM

The replacement of the B61 nose incorporating a common radar requires similar or better impact mitigating performance relative to the previous tube-type radar nose, even for greater impact velocities. As part of the ASCI/Revolution in Engineering and Manufacturing initiatives, much of the performance of this system is being defined via analysis. Validation of the analytical model has been performed with material, component, and full-scale testing, providing the basis for the extension into the complete design space. Working as part of the design team with the Advanced Weapon Projects Department 2167, this new common radar nose is currently undergoing qualification testing using the designs implemented within this concurrent engineering project.

Analysis results using the massively parallel version of Pronto3D will be detailed along with the design and validation philosophy of the project. Results from component actuator, rocket rail testing, and flash x-rays detailing the internal disposition of the various energy mitigating materials will be compared with the analytical model. These tests provide the validation of the analytical model. The use of the model to extend the performance into the untested regime will also be described, providing an understanding of the fundamental use and value of the analytical model.

Electromagnetics
Building 123 Conference Room A

Frequency Domain Analysis of Stratified Geometry Focusing on EUV Lithography (U)

Nathan J. Champagne
Robert M. Sharpe
Lawrence Livermore National Laboratory

The multi-layered Green's function that is present in EIGER may be used to model applications such as printed antennas and EUV lithography. EIGER contains a variety of spectral domain analysis methods that have been combined into a single integrated simulation suite. New software engineering methods, specifically object-oriented design, have been used to abstract the essential components of spectral analysis methods: elements, basis (expansion) functions, and operators. The benefit of this novel design is that the software may be easily modified and extended to treat new classes of problems without major changes to the entire code structure.

The multi-layered Green's function formulation in EIGER allows arbitrary structures to be simulated. However, this particular formulation involves computationally intensive operations that significantly increase the matrix fill time. There are several techniques to reduce the execution time, but these reduce the generality of the algorithm. An interpolation scheme has been developed that not only maintains the generality of the formulation, but also reduces the execution time. However, this approach also increases the amount of memory needed because of the storage needed for the interpolation table. The results presented will include printed antennas and EUV lithography examples with comparisons between the original and interpolation approach.

EIGER: Electromagnetic Interactions GEneRalized (U)

Robert M. Sharpe
Nathan J. Champagne
Lawrence Livermore National Laboratory

William A. Johnson
Roy E. Jorgenson
Sandia National Laboratories, Albuquerque, NM

The purpose of the EIGER (Electromagnetic Interactions GEneRalized) development effort is to combine a variety of spectral domain analysis methods into a single integrated simulation suite. New software engineering methods, specifically object-oriented design, are being used to abstract the essential components of spectral analysis methods: elements, basis (expansion) functions, and operators. The benefit of this novel design is that the software may be easily modified and extended to treat new classes of problems without major changes to the entire code structure. This is in contrast to standard design procedures where entire codes are developed around a single element with a specialized basis function for a specific operator (e.g., NEC and Patch). Although such tools can be effectively used to model large classes of problems, it is often very difficult to extend the tools beyond their initial design (e.g., modifying the Patch code to treat wires and wire-to-surface junctions within inhomogeneous media). Overcoming this limitation has been one of the most compelling goals of this project. Indeed, the applicability of EIGER is significantly broadened as a variety of analytic treatments (Green's functions) are cast into a form compatible with the numerical procedures in EIGER.

Efficient Spectral Domain Computations for Periodic Structures (U)

Robert M. Sharpe
Nathan J. Champagne
Lawrence Livermore National Laboratory

Efficient electromagnetic analyses of periodic structures are extremely important to such diverse application areas as antenna arrays, frequency selective surfaces and optical gratings. This paper describes a procedure for using analytical treatments by employing periodic Green's functions in conjunction with an integral equation solution of Maxwell's equations. The resulting periodic series are accelerated through a variety of transformations to improve efficiency. The boundary element solution can also be augmented by volumetric differential equation based finite elements to model complex or inhomogeneous problems. These hybrid formulations, as implemented in the EIGER electromagnetic analysis tool, will also be discussed. Representative results will be presented to demonstrate the solution process.

On the Calculation of Radar Cross Sections of Multilayered Spherical Targets (U)

Paul N. Demmie
Sandia National Laboratories, Albuquerque, NM

The numerical calculation of the radar cross section (RCS) of a spherical target with conductive or lossy materials can result in overflow during execution when real conductors or sufficiently lossy dielectrics are modeled. In this presentation, I discuss the source of this numerical problem, an algorithm to solve the problem, and the SPHERE computer program that implements this algorithm. SPHERE calculates the RCS of multilayered spherical targets using a corrected version of the formulation found in *Radar Cross Section Handbook* by Ruck, Barrick, Stuart, and Kritchbaum. The expressions in this formulation involve spherical Hankel functions. Overflow can result when calculating these functions since the exponential factor in a spherical Hankel function is unbounded as the conductivity or the imaginary part of the dielectric constant increases. The algorithm to calculate a spherical Hankel function scales the function by the reciprocal of this exponential factor. Then, the scaled function is evaluated using backward recursion for arguments with magnitude less than 0.2 and forward recursion for larger-magnitude arguments. After the expressions for a layer are evaluated using the scaled functions, the scale factors are returned in the final evaluation of the expressions for a layer. Furthermore, SPHERE evaluates these expressions using an ordering scheme that mitigates errors in predicted RCS due to roundoff. Such errors in calculated RCS are observed as the thickness of any layer approaches zero. The presentation includes examples of applications of SPHERE to thin metallic targets and RCS reduction.

Computer Modeling of the National Transparent Optical Network (NTON) (U)

Helena X. C. Feng
R. Lee Thombley
W. J. Lennon
Jonathan P. Heritage
Lawrence Livermore National Laboratory

The introduction of erbium-doped fiber amplifiers (EDFAs) in the late 80s and early 90s revolutionized optical fiber communications. Optical signals are attenuated as they propagate through optical fibers. Traditional power regeneration, which required opto-electro-optical conversion, had to be done every 80-100 km. This was expensive and could only boost power one channel at a time. In contrast, erbium-doped fiber amplifiers boost signal power in the optical domain. In addition, EDFAs have large gain bandwidths (35-100 nm), allowing amplification of multiple channels of signals simultaneously. The rapid deployment of wavelength-division multiplexing (WDM) technology is a direct consequence of the invention of the EDFA. With WDM technology tens of optical channels of Gb/s can be transmitted on a single strand of optical fiber for hundreds of kilometers without regeneration. The National Transparent Optical Network is a 2000 km 10-20 Gb/s WDM network deployed on the West Coast using in-place commercial fiber. One of the challenges in engineering such a large scale WDM optical network is to assess the physical layer impairments the transmitted signals accumulate as they propagate through cascades of optical fiber segments, EDFAs, and switching elements and to find effective methods to overcome them. Computer simulation is a very important and cost effective tool to do just that before expensive network components are installed. In this presentation the NTON will first be introduced, followed by computer simulation results of the network components and the network itself. Models of transmitters, EDFAs, optical filters, optical fiber, and receivers are developed using the characteristics of each component. These models are then verified against measurement. Simulations of optical signals propagating through optical links that are built with cascades of these components are carried out to estimate the bit-error-rate, which is an important measure of signal quality.

Validation and Verification
Building 132 Auditorium Room 1000

Validation of Finite Element Code Calculations of Shock Mitigation Through a Complex Joint (U)

Thomas A. Butler
Los Alamos National Laboratory

An important step in the development of large computer codes for simulating complex events is the validation of the code predictions. This paper addresses the validation of predictions made by the explicit finite element code PARADYN of the response of a complex joint to a high-level, short-duration pressure pulse. The joint studied includes most of the features present in the vicinity of the forward joint of a typical warhead. These features include gaps, sliding interfaces, preloaded components, tape joints, and threaded interfaces.

For the validation experiments the electronics and physics package were mocked with solid mass simulators. A titanium forward mount from an actual warhead was used to connect these mass simulators to cylindrical mockups of the outer shell of the weapon. The physics package mass simulator was attached to the forward mount with a tape joint.

PARADYN was used for pre-test predictions for designing the validation tests and for post-test analysis for the purpose of validating the computer code. Results from these analyses will be presented along with a description of the tests including the methods used to accurately determine the pressure loads and responses. Particular attention will be given to potential problems encountered when comparing measured data with analysis results.

Validation of the B61 Radar Nose Crush Model (U)

Terry D. Hinnerichs
John Pott
Kenneth W. Gwinn
Sandia National Laboratories, Albuquerque, NM

The Advanced Weapon Projects Department 2167 and its design team plan to qualify the new B61 Common Radar Nose crush performance by a combination of model-based simulations and by full-scale hardware testing on the Sandia-Albuquerque Rocket-Rail test facility. This presentation will focus on the validation process of the PRONTO3D finite element nose crush model that is being used for the qualification. The qualification testing is currently being performed at conditions thought to be the worst case based on past nose crush tests and relatively simple analyses. The purpose of this higher fidelity validated nose crush model will be to fully explore the design parameter space and make predictions on what are the most demanding impact angles for this new Radar Nose.

An overview of the validation process will be given that includes constitutive model, component model and full system model validation steps. Each step includes the construction of a Phenomena Identification and Ranking Table which will be presented. Also, through sensitivity analyses, the model parameters with significant uncertainties will be identified and the process for propagating these through the analyses will be described. Finally, the criteria for excepting the model as being validated will be discussed.

A Method for Configuration and Information Management of Analyses, Data, and Results (U)

Edward W. Russell
Edward J. Kansa
Lynn C. Lewis
Lawrence Livermore National Laboratory

This talk presents a method for tracking the quality assurance (QA) status of scientific and engineering analyses and models that meet the regulatory requirements of traceability, reproducibility, retrievability and transparency. The work reported is in support of the Yucca Mountain Project at LLNL. The main issue is to assure that an auditor or colleague has sufficient information to reconstruct very large models and results from certified analysis scenarios. To represent the process schematically, an object-orientated approach, Object Modeling Technique (OMT), was utilized to graphically depict the exchange of information through a large number of process elements. The OMT diagram approach allows a complex method to be viewed in terms of subsystems, model components and message flow, required for QA purposes.

Configuration and information management controls are defined in terms of configuration items (the items to be managed) and management authority hierarchy. The configuration identification scheme is employed throughout the analysis scenario. Also associated with configuration items are formal change control and approval mechanisms. Of principal concern is the qualification of the input data, which involves physical data as well as analyst-specified computational set-up parameters, such as mesh construction, time steps, convergence parameters and output controls. Work planning documents and technical implementing procedures provide a structure for documenting the pedigree traceability of the physical parameters, at the input level as well as throughout the analysis.

Validation of Probabilistic Finite Element Buckling Predictions for Spherical Shells (U)

Scott W. Doebling
Edward A. Rodriguez
Timothy S. Weeks
Los Alamos National Laboratory

Probabilistic analysis of structural response is becoming a more prominent part of engineering analysis research and applications. The ability to estimate statistical confidence intervals and probabilistic distributions for finite element model predictions introduces new possibilities for the quantification of confidence in simulations. These new capabilities also cause engineers to rethink the relationship between experiments and simulations. For example, model validation is no longer limited to the deterministic framework of "comparing one set of data to one prediction from the model." The new paradigm is "comparison of a model with quantified uncertainty to a set of data with quantified uncertainty." The tools of statistical hypothesis testing come into play, where distributions generated experimentally are compared statistically to those generated by simulation.

The project described in this presentation provides a framework for studying techniques to perform statistical model validation. A probabilistic prediction of the buckling behavior of a spherical shell is compared to the statistics of the measurements of experimental spherical shell buckling. Buckling is an ideal application for probabilistic structural analysis because of the high sensitivity to imperfections in the geometry and material properties. Spheres were selected because of the relative simplicity of modeling their buckling behavior versus that of a structural assembly.

Specifically, a sample drawn from a population of nominally "identical" spherical commercial marine floats is crushed in a testing machine to observe the buckling behavior. A distribution of load-deflection responses is obtained from the experiments. Another sample drawn from the same population is inspected using a number of nondestructive as well as destructive methods to establish distribution estimates of the geometric and material properties of the population. These estimates are then used as inputs for the probabilistic structural analysis code to predict the distribution in the load-deflection responses of the population. By comparing the measured distribution with the predicted distribution, the validity of the predictions can be assessed in probabilistic terms.

Neutron Diffraction as a Verification Method of a Finite Element Model: PIGMA-(Pressurized Inert Gas Metal Arc) Welded Beryllium Ring (U)

Ravi Varma
Donald W. Brown
Francisco M. Guerra
Mark Bourke
Paul Burgardt
R. F. Oleary
M. D. Garcia
Los Alamos National Laboratory.

The welding of beryllium has long been a problem of interest at LANL. Considerable effort has been expended in the modeling of such welds, with the intended outcome being the optimization of weld parameters, e.g., amount of preheat, for the manufacture of a superior bond. In this talk we present the preliminary results of a neutron diffraction study, undertaken to verify one such model, the details of which will also be presented at this conference. We will discuss, in some detail, the method of neutron diffraction as a tool for verification of finite element models.

The sample in question is a set of right cylindrical beryllium rings that was PIGMA welded using an Al-Si mixture as the weldment. Using the atomic lattice spacing as a strain gauge, strain measurements were taken along a line perpendicular to the weld, crossing the girth of the rings. For the purpose of verification of the model, the experimentally determined strains are compared to those generated by a finite element model of the same sample. Also, we will utilize strain determinations made along a circumference parallel to the weld to discuss the validity of an axi-symmetric model in this and similar cases.

Computational Fluid Dynamics 1
Building 132 Room 1102

Evaluation of a CFD Tool for RV Dynamics (U)

Robert M. Ferencz
Lawrence Livermore National Laboratory

The Methods Development Group has initiated an ASCI project to create methodologies and multi-physics software tools for simulating Reentry Vehicle Dynamics. Our goal is to create a capability to better assess the reentry flight load environment upon the RV and the resulting response of the NEP. Our approach is to enhance traditional MDG strengths in implicit solid and thermal mechanics with new physics and algorithms, while also leveraging complementary outside resources. In particular, we view our role to be that of "system integrator" with regards to the needed computational fluid dynamics capability. Thus an initial task has been to consider the requirements for such a CFD tool and to evaluate candidate codes. In this talk we provide an overview of our experience with the GASP (General Aerodynamic Simulation Program) product from AeroSoft, Inc. and our journey up the learning curve of hypersonic flow.

CFD Modeling and Experimental Investigation of Detrimental Heat Sources within the National Ignition Facility (U)

John D. Bernardin
Albert C. Owen
Kin L. Lam
Los Alamos National Laboratory

The National Ignition Facility (NIF) at Lawrence Livermore National Laboratory is being constructed as the latest in a series of high-power laser facilities to study inertial confinement fusion. In particular, NIF will generate and amplify 192 laser beams and focus them onto a fusion fuel capsule the size of a BB. The energy deposited by the laser beams will raise the core temperature of the target to 100,000,000 °C, which will ignite the fusion fuel and produce a fusion energy output that is several times greater than the energy input. The NIF's massive bays contain laser beam amplification, conditioning, and diagnostic equipment, large laser beam transport tubes, and a variety of optical shaping and alignment devices. The ability to generate, condition, and focus 192 laser beams onto a target the size of a BB, requires not only precision optical hardware and instrumentation, it also demands extreme environmental control measures. For example, small spatial and temporal excursions in the NIF environmental air temperature may cause minute distortions in beam alignment hardware as well as index of refraction gradients in the beam transport tubes, thereby degrading the operating performance and net energy yield of the NIF. To minimize the impact of thermal gradients, the NIF HVAC system has been designed to maintain a mean air temperature field of 20.00 ± 0.28 °C throughout the facility. Unfortunately, heat sources within the facility will create local hot spots in which air temperatures will exceed the upper limit of this range.

The purpose of this study was to assess the extent of spatial temperature excursions created by fluorescent lights, electronics racks, and pre-amplifier modules (PAMS) in the NIF laser bays, estimate their detrimental influence on the beam transport tubes, and offer design recommendations to minimize their impact on operating performance. To achieve this, experiments were performed to characterize the heat dissipation of both a fluorescent light fixture and an electronics rack and establish meaningful boundary conditions for computational fluid dynamics (CFD) models. Next, both CFD and analytical models were developed to investigate the magnitude and extent of thermal plumes and radiation heat transfer from the various heat sources. From the results of these studies, several design modifications were recommended. These included, reducing the size of all fluorescent lights in the NIF laser bays to single 32 W bulb fixtures, maintaining minimum separation distances between light fixtures/electronics racks and beam transport hardware, adding motion sensors in areas of the laser bay to control light fixture operation during maintenance procedures, properly cooling all electronics racks with air/water heat exchangers, and insulating the electronic bays and optical support structures on the PAMs.

LES Near-Wall Closure Using a One-Dimensional Unsteady Stochastic Simulation (U)

Rodney C. Schmidt
Scott E. Wunsch
Alan R. Kerstein
Sandia National Laboratories, Livermore, CA

It is increasingly recognized that Reynolds-averaged turbulence models omit effects of large-scale unsteadiness

that cannot be neglected in high-fidelity computational models of turbulent flow phenomena. Large eddy simulation (LES) can affordably capture these effects by filtering less important small-scale effects out of the governing equations. However, small-scale effects become important near solid surfaces. Wall treatments currently used in LES do not capture enough of the small-scale physics to achieve the model performance needed for multiphysics environments arising in engineering applications.

Here, a new near-wall model is proposed, involving a one-dimensional unsteady stochastic simulation implemented in each LES control volume that is adjacent to a solid surface. The simulation resolves the length and time scales of all relevant transport (mass, momentum, heat, species, etc.) and thermochemical processes in the boundary layer. Consistent with conventional (ensemble averaged) boundary-layer formulations, the one-dimensional spatial coordinate represents the local wall-normal direction.

The near-wall simulation is a variant of 'One-Dimensional Turbulence' (ODT). In ODT, turbulent advection is implemented in one dimension as a stochastic sequence of instantaneous mappings, representing turbulent eddies, applied to the spatial domain. The rules governing the mapping sequence reflect known turbulence phenomenology. These mappings, and molecular transport processes that are implemented deterministically, govern the evolution of velocity, enthalpy, and species profiles on the one-dimensional domain.

This formulation allows physically accurate wall boundary conditions to be applied. ODT evolution is driven by pressure gradients obtained from the LES-resolved bulk-flow solution. Control-volume averages of ODT properties transmit wall information (mass and momentum fluxes, etc.) to the LES solver. Thus, ODT mediates the coupling between the LES solver and the wall.

Anticipated applications include forced and natural convection heat transfer, flow separation and reattachment, and chemically reacting flows. Initial results and further details of model formulation and numerical implementation are presented in the talk.

Thermal Hydraulic Analysis of a Liquid-Metal-Cooled Spallation Target (U)

William S. Gregory
Richard A. Martin
Los Alamos National Laboratory

The Accelerator-driven Transmutation of Waste (ATW) concept has been proposed by the United States and other countries to essentially eliminate plutonium, higher actinides, and environmentally hazardous fission products. One of the key components in the ATW concept is a target, which, via spallations, produces neutrons to drive the burning of nuclear wastes. Since significant heat is generated during fissioning of the waste, an efficient heat removal system is necessary. It is believed that liquid lead-bismuth-eutectic (LBE) is an efficient coolant as well as a good spallation target for production of neutrons.

The spallation target consist of a cylindrical tube with flowing liquid LBE. The target window is made of a cone-spherical steel diaphragm with a thickness of 1.5 mm. Cooling of the target window is one of the major concerns of the design. The flow enters in an outer annulus and then is directed around the target window by an outer wall. The target has a diffuser plate with a large central opening placed immediately downstream (2.5 mm) from the hot window. The plate directs coolant flow towards the center of the target window to reduce the window temperature. However, this configuration also allows for possible flow separation and recirculation behind the plate. Recirculation of coolant in regions of intense energy deposition could lead to a hot region.

The International Science and Technology Center in Russia has performed a design study for a pilot target that will use the LBE concept. We have used a CFD code, CFX4.2, to study the thermal hydraulic behavior of this proposed design. The analysis consisted of determining maximum coolant temperatures and the temperature of the spallation target window when 1 MW of energy is deposited in the target from the Los Alamos Meson Physics Facility accelerator beam. The CFD study showed that the coolant temperatures and spallation target window temperatures were within acceptable limits.

Influence of CFD Analysis on the Design of Cooling Channels for the CCL Cavity for the Spallation Neutron (U)

Snezana Konecni
Nathan K. Bultman
Los Alamos National Laboratory

The Spallation Neutron Source (SNS) is an accelerator-based facility that produces pulsed beams of neutrons by bombarding a mercury target with intense beams of 1-GeV protons. Los Alamos National Laboratory is responsible for the design, fabrication, installation, and testing of the Linear Accelerator (linac) for the SNS project. The linac accepts beam from the front end system and accelerates it from 2.5 MeV to 1.0 GeV. The linac consists of a drift-tube linac (DTL), a coupled-cavity drift-tube linac (CCDTL), and a coupled-cavity linac (CCL). The DTL operates at an RF resonant frequency of 402.5 MHz, while the CCDTL and CCL operate at 805 MHz. Power dissipated in the linac due

to RF resonant frequency is removed by water circulating through the cooling channels of the cavities and the drift tubes. CCL cavities are figures of revolution about the beam axis. Several cooling passage schemes were looked at. The original scheme includes four main parallel annular paths around the cavity nose in the septum, fed and collected by internal plenums, and a circular path on the opposite face. The plenums are supplied by water from a manifold that feeds eight to ten cavities. In order to design the cooling system for the linac, pressure drop of the water flowing through the cooling channels was needed. Water flow in the cooling channels was simulated using the CFD code CFX4. Pressure drop in the cooling channels of the CCL cavity was calculated. The effects of the manifold on the pressure drop were studied also. Reducing the pressure drop was a primary goal of this exercise that led to changing the cooling channel entrance regions. Results of this analysis were used in sizing pumps required for the cooling system.

Session 6: Wednesday, November 3, 1999, 10:15 a.m.–12:00 p.m.

Mesh Generation and Visualization
Building 123 Auditorium

Graphical Programming Tools for Control System Development (U)

Gary W. Johnson
Lawrence Livermore National Laboratory

In the development of computer-based control systems, tighter integration between software tools for analysis and real-time execution can save time and improve results. A case study is presented, showing how commercial graphical programming software was applied to a DSP-based laser beam tracking loop. LabVIEW™ (National Instruments, Austin, TX) was used to characterize and simulate the system. Hyperception® (Dallas, TX) Hypersignal Block Diagram/RIDE™ was then used to implement the control algorithm, which ran on a single-board DSP computer. Graphical programming reduces programmer effort by providing high-level functionality in an intuitive block-diagram format, encapsulating low-level details, and eliminating many syntactical stumbling blocks. Limitations of the current packages will be discussed along with desires and expectations for future releases.

New Flexibility in Analysis Results from the MDG Code Family (U)

Douglas E.Speck
Lawrence Livermore National Laboratory

The family of finite element analysis codes developed and maintained by the Methods Development Group at LLNL, including DYNA, NIKE, and TOPAZ, has for years employed a fixed-format plot database. This database, the "Taurus" plotfile database, offers limited flexibility, mainly in that the mesh may be of arbitrary size (within the bounds of a single-precision specification). The development of a new I/O library, Mili, and its installation in DYNA3D/ParaDyn and MDG's GRIZ post processor, has initiated a significant increase in the flexibility of the data path between MDG analysis codes and GRIZ. Utilizing Mili, MDG analysis codes for the first time have the opportunity to tailor the set of state variables written to the plot database over arbitrary subsets of mesh objects. State variables specific to a material model can be output for just those elements applying the material model. Mesh definitions can be more finely resolved, explicitly distinguishing, for example, discrete elements from beams and thick shells from hexahedral elements. Mili even permits the analysis codes to define multiple output formats within a single simulation, opening the door to further tailor output data as a simulation evolves. Concomitant with the expanded variability in analysis outputs are major changes in the data handling capability of the GRIZ post-processor. GRIZ's underlying data structures for the storage and management of mesh and state data have been re-designed to support the flexibility required by a self-defining database. The necessity of making such wholesale changes provided opportunities for associated improvements to a number of GRIZ capabilities.

Three-Dimensional Geometry Reconstruction from Photogrammetry and Radiograph Data (U)

Jill Hefele
Richard D. Bolton
Kenneth B. Butterfield
David A. Fry
Ronald M. Dolin
Los Alamos National Laboratory

Reconstruction of geometry in a computer-aided-design (CAD) environment from computed tomography data has been well-researched and many software application tools exist for this purpose; especially for low density materials in the biomedical field. Reconstruction of geometry in a CAD environment from x-ray data has not had the same amount of effort applied until recently. Three-dimensional geometry reconstruction from two-dimensional x-ray projections provides essential information to the physics designer, assembly engineer, and engineering analyst that has not been available in the past. Los Alamos National Laboratory (LANL) is developing a process to recover geometric information from photogrammetry and x-ray data to create a computer model of a site reconstruction and a boundary representation CAD model of a radiographed unit. Commercial software is now available with these capabilities. Vexcel Corporation's FotoG® software allows site reconstruction from photogrammetric data. Simultaneous

execution of Vexcel Corporation's FotoG® and Parametric Technology Corporation's Pro/ENGINEER® software provides the boundary representation definition from x-ray data. Applications for this technology include as-built tooling design, as-built finite element and hydrodynamic analysis, assembly technique verification, and stockpile surveillance. The process was applied to a W80 Sled Test conducted at Los Alamos. Pre- and post-test photographs and radiographs were obtained and used to reconstruct both the test environment and the test unit.

Pandemonium: A New Tool for Glovebox Process Dose Modeling (U)

Drew E. Kornreich
David E. Dooley
Los Alamos National Laboratory

The nuclear weapons work at Los Alamos contains operations that require handling of nuclear materials. Los Alamos is dedicated to providing a safe workplace. Ensuring that personnel exposure to ionizing radiation is within acceptable limits is part of this dedication to safety. This work describes some new tools for estimating dose for a set of operations that occur in gloveboxes.

A model of a room containing gloveboxes has been constructed using the industry standard effective dose equivalent (EDE, dose) estimation tool MCNP. Such tools provide an excellent means for obtaining relatively reliable estimates of radiation transport in a complicated geometric structure. However, creating an input description of complex geometries equally complicated. Therefore, an alternative tool is desirable that provides reasonably accurate dose estimates in complicated geometries for use in engineering-scale dose analyses.

In the past, several tools that use the point-kernel model for estimating doses equivalent have been constructed. This new tool, the Photon And Neutron Dose Equivalent Model Of Nuclear materials Integrated with an Uncomplicated geometry Model (Pandemonium), combines point-kernel and diffusion theory calculation routines with a simple geometry construction tool. Pandemonium uses Visio™ to draw a glovebox array in the room, including hydrogenous shields, sources, and detectors. This simplification in geometric rendering limits the tool to two-dimensional geometries (and one-dimensional particle "transport" calculations). A Visual Basic™ macro is used to export the input data that feeds the dose calculation. The results can be used to evaluate the dose that people receive from nuclear materials throughout an array of gloveboxes.

Structural Dynamics 1
Building 123 Conference Room A

Seismic Analyses of NIF Structures (U)

Stanley C. Sommer, P.E.
David J. Trummer, P.E.
Michael A. Gerhard, P.E.
Lawrence Livermore National Laboratory

Paul B. MacCalden, Ph.D., P.E.,Vice President
The Ralph M. Parsons Company

The National Ignition Facility (NIF) is being constructed at the Lawrence Livermore National Laboratory (LLNL) as an international research center for inertial confinement fusion (ICF). Since LLNL is located in a seismically active region, considerable design and evaluation attention has been focused on seismic-induced effects. This paper will provide a brief overview of NIF, review NIF seismic criteria, and discuss seismic analyses of several representative NIF structures.

Using the provisions in DOE Standard 1020 (DOE-STD-1020), the Uniform Building Code (UBC), and LLNL Design Safety Standards, the NIF seismic design and evaluation criteria applies different levels of seismic requirements to structures, systems, and components (SSCs) based on their function. The highest level of requirements are defined for optical support structures and SSCs which could influence the performance of optical support structures, while the minimum level of requirements are consistent with DOE-STD-1020 Performance Category 2 specifications. Numerous structural finite element analyses have been performed by LLNL and the NIF Architect and Engineer, Parsons, to evaluate the responses of optical support structures and other SSCs to seismic-induced forces.

NIF is composed of two laser bays, two switchyards, a target building, an optics assembly building, an operations areas, and a central plant. Inside the two laser bays are hybrid support structures of reinforced concrete pedestals and steel frames or vessels as well as many utility systems. The switchyards contain large steel space frames connected to the corners of the switchyard building and the switchyard building is connected to a 100-foot diameter target building. Inside the target building are the target chamber and floors which support optical elements and diagnostic equipment. Seismic analyses have been performed on all the support structures, optical elements, foundations, building systems, utility systems, and mechanical equipment to demonstrate that these SSCs satisfy the NIF seismic design and evaluation criteria.

To Detail or Too Detailed, That Is the Modeling Question (U)

Michael A. Gerhard
Lawrence Livermore National Laboratory

In generating finite element models for the National Ignition Facility (NIF) laser support structures, I have been faced with the task of incorporating detailed models of relatively small components into large global models. I will discuss the processes I have used to approximate various detailed structural components in order to reduce overall model complexity and computation times.

Generally, the first step is to generate a detailed model of the desired component, including a detailed representation of the connection to the global model. Then, the connection detail is approximated using a simplified, reduced order model and the structural behavior of the two models are compared. Various properties in the simplified connection model are adjusted until the simplified model adequately represents the detailed model. This process generally converges to an adequate reduced order model in a few iterations. The iterations on the simplified model are very fast since the details of the global model have yet to be included. Once the simplified model is complete, it is incorporated in the global model.

I will show examples of mesh simplification which have maintained the overall behavior of the structure, such as using one-dimensional beam elements to model complex tube structures and brackets. I will also discuss modeling fundamentals which come into play when utilizing reduced order models in place of finely detailed models.

NIF Target Area Transport Mirror Wavefront Evaluations (U)

David J. Trummer
Robert B. Addis
Janice K. Lawson
Lawrence Livermore National Laboratory

The Target Area Building (TAB) of the National Ignition Facility (NIF) is 300 feet long, 100 feet wide, and 100 feet tall and is comprised of a cylindrical target building and two switchyard space frames. The reinforced concrete target building houses the target chamber, target positioner, transport mirrors, final optics assemblies, and diagnostics,

while the steel switchyard space frames support transport mirrors and diagnostic equipment. Within the TAB, the 192 independent laser beams of the NIF laser system must be positioned on target with a very high degree of accuracy while maintaining an acceptable focal spot size.

The optical focal spot size on NIF will be determined by many factors, chief among these is the combined wavefront distortions of every optical element in the beam chain. The spot size at target center is influenced by the cumulative effect of the mounting induced distortions on the transport mirrors. The transport mirrors will be mounted by attaching three lugs to the back of the optical substrate. The resulting mounting distortions that occur include the effect of lug placement, lug pressure, gravity deformation, and beam placement on the mirror.

Upon analysis, the initital transport mirror mounting design was found to produce unacceptably large mounting induced wavefront distortions. As a result, a considerable design, testing, and analysis effort was undertaken to redesign the mounting hardware. This presentation will discuss the process that was used to reduce the wavefront distortion to manageable levels.

Calculation of von Mises Stress in a Random Vibration Environment, Part I: An Efficient Method for Calculating RMS von Mises Stress (U)

Daniel J. Segalman
Clay W. G. Fulcher
Garth M. Reese
Richard V. Field, Jr.
Sandia National Laboratories, Albuquerque, NM

The von Mises stress is often used as the metric for evaluating design margins, particularly for structures made of ductile materials. For deterministic loads, both static and dynamic, the calculation of von Mises stress is straightforward, as is the resulting calculation of reliability. For loads modeled as random processes, the task is different; the response to such loads is itself a random process and its properties must be determined in terms of those of both the loads and the system. This has been done in the past by Monte Carlo sampling of numerical realizations that reproduce the second order statistics of the problem. Such an approach is impractical for problems involving large structural models.

A rigorous and efficient method is presented for calculation of RMS von Mises stresses for linear structures excited by stationary random loads. The RMS value is expressed in terms of the zero time-lag covariance matrix of the loads, which in most applications of structural analysis will be calculated from frequency-domain, stress-component transfer functions and the cross spectral density matrix of the applied loads. The key relation presented is one suggested in past literature, but that does not appear to have been exploited previously in this manner. The exact determination of RMS von Mises stress is used to demonstrate that the Miles' relation, commonly used in design, can be conservative or non-conservative. Finally, because of the efficiency with which the exact RMS von Mises stress can be calculated, the analyst can now perform surveys of von Mises stresses routinely, allowing a thorough investigation into the reliability of an engineering design.

Calculation of von Mises Stress in a Random Vibration Environment, Part II: Predicting the Probability Distribution for Cases of Gaussian Loads (U)

Richard V. Field, Jr.
Daniel J. Segalman
Clay W. G. Fulcher
Garth M. Reese
Richard V. Field, Jr.
Sandia National Laboratories, Albuquerque, NM

The von Mises stress is often used as the metric for evaluating design margins, particularly for structures made of ductile materials. For deterministic loads, both static and dynamic, the calculation of von Mises stress is straightforward, as is the resulting calculation of reliability. For loads modeled as random processes, the task is different; the response to such loads is itself a random process and its properties must be determined in terms of those of both the loads and the system. This has been done in the past by Monte Carlo sampling of numerical realizations that reproduce the second order statistics of the problem. Here, we present a method that provides analytic expressions for the probability distributions of von Mises stress which can be evaluated efficiently and with good precision numerically. Further, this new approach has the important advantage of providing the asymptotic properties of the probability distribution.

An example is presented to illustrate the method, where loads on a simple structure result in qualitatively different probability distributions of von Mises stress.

Classified 1
Building 132 Auditorium Room 1000

Amy N. Robertson
Thomas A. Butler
Ramsey C. Chun
Steven L. Creighton
Brian H. Aubert

Computational Fluid Dynamics 2
Building 132 Room 1102

Lattice Boltzmann Simulation of Particulate Media in Microfluidic Systems (U)

David S. Clague
Lawrence Livermore National Laboratory

Various numerical methods are used to explore the hydrodynamics of microfluidic systems. Here the lattice Boltzmann method is employed to calculate the hydrodynamic force and torque acting on a spherical particle that is confined between two parallel plates. Example particles include spores, polystyrene spheres, and proteins. The lattice Boltzmann method is benchmarked against known related hydrodynamic problems. The simulation results agree to within 5% of the expected values. Lattice Boltzmann results are then compared with the theoretical result of Wakiya (1957) for a stationary sphere confined between infinite parallel plates. Additional results are presented to demonstrate the utility of the method for simulating macromolecules in microfluidic systems.

Computation and Measurement of Turbulent Dispersion of Toxic Aerosols or Gases In Enclosures (U)

Richard A. Martin
Snezana Konecni
Lucie M. Parietti
Jeff J. Whicker
Los Alamos National Laboratory

Airborne toxins could occur in nuclear research facilities located at the National Labs in Livermore, Albuquerque (Sandia), or Los Alamos, and at other Department of Energy facilities. Contaminants can also occur in industrial facilities, in a subway system or building targeted by terrorists, on board an aircraft, or at home, and are generally recognized as serious potential hazards for human exposure.

Successful development and benchmarking of computational fluid dynamic (CFD) techniques using existing facilities and equipment at the Lab can lead to several benefits. The benefits include (1) reducing human exposure to toxic aerosols or gases in complex geometric environments, (2) improving the design of ventilated spaces including nuclear research laboratories, glove boxes, fabrication areas, storage areas, clean rooms, workspaces, homes, aircraft cabins, subways, military vehicles, etc., (3) optimizing the location of aerosol or gas safety monitoring sensors, and (4) accurately predicting spatial and temporal concentrations of contaminants.

In this study, the CFD code, CFX4, was used to simulate postulated aerosol release and transport in a large, ventilated workroom in the plutonium facility at Los Alamos. The workroom contained five rows of glove boxes and an overhead trolley. Four inlet air diffusers near the ceiling and four exhaust registers near the floor were modeled. Thermal anemometry equipment was used to measure the inlet and outlet conditions. The three-dimensional, steady-state flow field was computed using the κ–ε turbulence model. Ten short burst or "puff" releases of an idealized aerosol (scalar contaminant) were then simulated assuming dilute, monodisperse, neutrally buoyant particles. Transient calculations of the aerosol dispersion for seven minutes were performed, and aerosol concentration versus time recorded. This presentation includes results of CFD calculations and comparisons to measurements made in the same workroom using laser particle counters.

Homogeneous Charge Compresson Ignition Engine Combustion Modeling (U)

Daniel Flowers
Salvador Aceves
J. Ray Smith
Lawrence Livermore National Laboratory

Homogeneous charge compression ignition (HCCI) engines have the potential to achieve high efficiency with very low NO_x emissions. Heat release in HCCI combustion is a global process that depends on primarily on rate chemistry, not on flame propagation as is the case in conventional spark ignited or diesel engines. The combustion initiates simultaneously throughout the cylinder due to autoignition of the premixed charge. This autoignition process results in very rapid, near constant volume combustion. High compression ratios, near constant volume combustion, and very lean mixtures could yield an engine operating with very high efficiency and very low emissions.

Natural gas has been selected as a potential fuel for use in HCCI engines. The autoignition chemistry for natural gas is well characterized and has been extensively validated. A single-zone well-stirred-reactor model of the in-cylinder gas has been developed with HCT (Hydrodynamics, Chemistry, and Transport). This model includes volume change due to piston motion and an empirical engine heat transfer correlation.

The key to practical operation of HCCI engines is controlling the timing of the start of combustion. Studies have been conducted to assess the sensitivity of combustion timing to variations in fuel composition, compression ratio, intake temperature, intake pressure, and residual gas fraction.

Modeling Thermal Batteries using a Multi-Dimensional Stefan-Maxwell Framework (U)

Ken S. Chen
Sandia National Laboratories, Albuquerque, NM

Gregory H. Evans
Richard S. Larson
William G. Houf
Sandia National Laboratories, Livermore, CA

Thermal batteries are used as the primary power source in nuclear weapons because of inherent advantages such as long shelf life, fast activation, rugged construction, and high reliability; they are also widely employed in many military applications such as power sources for missiles and proximity fuzes in ordnance devices. Most applications use lithium alloys as anodes, metal-sulfides as cathodes, and molten salts as electrolytes. They are usually activated by melting the solid electrolytes using a pyrotechnic heat source based on Fe and KClO4. Phenomena in a thermal battery process are complex, involving 1) multi-physics (thermodynamics, multi-species diffusion, convection, energy transport, electrochemical reactions), 2) multi-dimensions, and 3) multiple length and time scales.

In this paper we present a general multi-dimensional framework for modeling thermal batteries with an arbitrary number of electrolytic species. Specifically, our framework utilizes the Stefan-Maxwell flux equations to describe multi-component diffusion of interacting species using composition-insensitive binary diffusion coefficients. In our model we take into account concentration gradients and electrical potential as driving forces for diffusion as well as the effects of nonideal solution behavior of the electrolytes. The unknowns (species mole fractions, electrical potentials in electrolyte and electrode, porosity, temperature, velocity, and pressure) are described by using the principles of mass, charge, energy, and momentum conservation, an electroneutrality constraint, and Ohm's law. We treat the porous electrodes as superposed continua without regard for the actual geometric details of the pores. We solve the resultant set of highly nonlinear and coupled equations using the GOMA platform, which employs the finite-element method and a fully coupled implicit solution scheme via Newton's method. Results from a case study of a LiAl/ LiCl-KCl/FeS thermal-battery cell are presented to illustrate the utility of the new multi-dimen-sional, multi-component framework.

Simulation of High Speed Gas Flow in a Reservoir-Receiver-Valve System (U)

Robert W. Meier
Los Alamos National Laboratory

Three-dimensional computational fluid dynamics (CFD) analyses and one-dimensional analytical solutions are obtained for gas flow in a reservoir-receiver-valve system. The objectives are to determine the pressure-time history within the valve and to determine the fill time and fill pressure of the reservoir. To develop a complete understanding of the flow processes, both analytical and computational approaches are employed. The analytical approach yields accurate predictions of reservoir fill time and final pressure. The computational model is developed to obtain detailed information about flow through the valve and is also applied to the reservoir-receiver system for model validation.

Analytical solutions are obtained by developing formulas for quasi-steady one-dimensional irreversible choked flow, but include the real gas effects of compressibility and variable isentropic exponent. The CFD models are developed with the FLUENT computer code and include the effects of three-dimensional flow of real gases. The CFD models yield predictions of pressures both within the valve and in the entire reservoir-receiver system. The FLUENT computer code is used to obtain computational solutions of the gas flow for various valve configurations and for several different gases.

Results from both the analytical solutions and the CFD modeling are compared with experimental pressure measurements in the valve, receiver, and reservoir.

Session 7: Wednesday, November 3, 1999, 1:15 p.m.–3:00 p.m.

Parallel Methods and Algorithms
Building 123 Auditorium

Moving NIKE3D Towards Parallelism: Exploratory Efforts with Sparse Direct Linear Solvers (U)

Robert M. Ferencz
Lawrence Livermore National Laboratory

ParaDyn, the parallel version of the explicit solid mechanics code DYNA3D, has reached sufficient maturity to be utilized as a production tool at LLNL and other DOE/DoD sites. This effort has created substantial experience in the Methods Development Group regarding parallelization of residual formations and contact algorithms. While ParaDyn development is ongoing, efforts are being initiated to parallelize the companion implicit solid mechanics code NIKE3D. In particular, parallel methods for solving the coupled linear system arising from implicit methods are an important consideration. Due to the numerical sensitivities of some of the algorithms in, and applications of, NIKE3D, we consider it essential to maintain a direct linear equation solving capability to complement iterative methodologies. As an exploratory exercise we have prototyped a master-slave version of NIKE3D that utilizes a parallel sparse direct solver package. We summarize this effort, some of the lessons learned along the way, and consider future development activities.

Zoltan: A Dynamic Load-Balancing Library for Parallel Applications (U)

Karen D. Devine
Bruce A. Hendrickson
Matthew M. St.John
Erik G. Boman
Sandia National Laboratories, Albuquerque, NM

Dynamic load balancing is a capability required by many parallel applications currently being developed at the DOE laboratories. Adaptive finite element methods and multiphase calculations (such as transient dynamics with contact detection) are examples of such applications, as the work per processor in these applications can change as the computations proceed. Dynamic load balancing has typically been implemented directly in applications, sharing the applications' data structures. Two disadvantages arise from this approach. First, the load-balancing code cannot be re-used in other applications since it relies heavily on the data structures of a particular application; each new application is forced to have its own load-balancing code. Second, application developers do not compare different load-balancing algorithms because of the work involved in implementing several approaches. The Zoltan Dynamic Load-Balancing Library addresses these issues by providing a general-purpose tool-kit of load-balancing algorithms. Its object-oriented interface is designed to separate the data structures of the load-balancing algorithms from those of the application, enabling a wide range of applications to use the library. The library contains a variety of algorithms, including geometric and graph-based algorithms, allowing an application to easily compare the performance and partition quality of different methods. Data-migration tools are also included to simplify the communication required to move data among processors in establishing new decompositions. We will describe the interface and performance of Zoltan, and give examples of its use in adaptive finite element applications.

Salinas—A Massively Parallel Sparse Eigensolver for Structural Dynamics Finite Element Analysis (U)

Brian J. Driessen
Garth M. Reese

Structural dynamics analysis is critical to applications in weapons, non-proliferation, space sensors, and computational manufacturing. Full body models that could not be solved using previous technology have been solved with a recently developed massively parallel eigensolver. Such capability allows for the vibration and shock analyses of full body models and also allows for timely optimization of smaller models.

The solver developed has been both theoretically and empirically demonstrated to have a complexity that is linear in the problem size, and very good parallel efficiencies have been demonstrated. Thus, with twice as many processors, a problem of twice the size requires roughly the same amount of time to solve. Both the CPU time per iteration,

and the number of iterations are independent of problem size. Moreover, memory requirements also scale linearly with size. So, the allowable problem size increases at the same rate as the number of processors. Scalability has been demonstrated on problems with more than 5 million degrees of freedom utilizing 1000 processors.

The MP structural dynamics software is designed to handle applications expected in the nuclear weapons program. In addition to capabilities for eigenanalysis, statics and implicit transient dynamics are supported. A rich selection of solid, shell and beam elements (including higher order elements) are available, together with support for multipoint constraints. An important part of this effort has been direct implementation of design sensitivities to assist in nondeterministic analysis and design optimization.

We will discuss the development of the finite element software and of the linear solvers and eigensolver.

Parallel Implicit Electromagnetics using the Vector Finite Element Method (U)

Daniel A. White
Joseph M. Koning
Lawrence Livermore National Laboratory

In this presentation we describe our approach for three-dimensional unstructured grid solution of Maxwell's equations. We will describe our semi-implicit and full-implicit approaches for time dependent problems as well as our approach for eigenvalue/eigenvector problems. Our discretization is based on the recently developed vector finite element method, which employs covariant vector finite elements as a basis for the electric field and contravariant vector finite elements as a basis for the magnetic flux density. There are several advantages to this method. First, this method maintains the proper continuity/discontinuity of fields and fluxes across material interfaces. Secondly, this method satisfies the divergence equations automatically, independent of any distortions in the grid. Thirdly, in the time domain this method is provably stable and energy conserving.

Our code is an eclectic combination of FORTRAN math libraries, C parallel communication libraries, C++ finite element classes, with an interpreted Python interface to top it off. We will report on preliminary parallel performance using the ASCI Blue machine, which we have used to analyze several linear accelerator components.

A Parallel Contact Algorithm with Dynamic Load Balancing for Explicit/Implicit Finite Element Methods and Applications in Solid and Structural Mechanics (U)

Anthony J. De Groot
Carol G. Hoover
Lawrence Livermore National Laboratory

The development of robust and efficient contact detection-enforcement methods for finite element discretizations of solid and structural mechanics applications is a multifaceted and challenging problem. Some examples of difficult contact detection problems are as follows: 1) folding-surface contact with thin shells where the inner and outer surface may be ambiguous, 2) tightly-toleranced, nested surfaces, 3) multiple materials interacting in localized regions, and 4) large deformation mechanics (or objects moving on the grid) where the surface motion becomes unpredictable and "arbitrary."

A new method has been developed and implemented in the DYNA3D program[1] to extend the capabilities and improve the performance of the "arbitrary contact algorithm." This new technique involves ideas using patch-on-patch contact as well as an improved technique for sorting contact surface nodes and patches. The new sorting method embeds a local sort within the global sort and improves the performance of the arbitrary contact algorithm on single-processor computers by a factor between five and ten. New capabilities in the arbitrary contact algorithm include a volume erosion method for the modeling of material damage and failure and the implementation of a LaGrange multiplier constraint method for contact.[2]

A parallel implementation of arbitrary contact is based on subdividing the mesh and interfaces on a finite element grid using graph tree methods. The partitioning methods couple a partition for the mesh with a separate partition for the contact interface. The partition for the contact interface allows dynamic load balancing of the contact calculations as material surfaces evolve on the grid.

We report on several recent developments and large-scale applications using parallel algorithms for arbitrary contact. Demonstration applications and performance will be presented.

1. Edward Zywicz, private communication.
2. Edward Zywicz and Michael Puso, "A General Conjugate Gradient-Based Predictor-Corrector Solver for Explicit Finite-Element Contact," Int. J. Numer. Meth. Engng. 44, pp. 439-459 (1999).

Structural Dynamics 2
Building 123 Conference Room A

Structural Dynamics Analysis of an Extreme Ultraviolet Lithography Optical System (U)

Clay Fulcher
Sandia National Laboratories, Albuquerque, NM

This is a placeholder.

Modal Survey of a Medium Energy Superconducting Radio Frequency Cavity for Accelerator Production of Tritium Project (U)

Gretchen W. Ellis
Brian G. Smith
Los Alamos National Laboratory

Small dynamic motions can adversely affect structures and equipment that perform precision operations. If significant vibration input to a structure corresponds with one of the structure's natural frequencies, resonance occurs which may result in unacceptable dynamic motion.

Some particle accelerators employ RF (radio frequency) cavities that resonate at particular electromagnetic frequencies to accelerate charged particles. Although elastic, cavity shape change as a result of dynamic motion can result in a shift in the RF resonant frequency and electromagnetic field, which can affect the acceleration and particle beam dynamics.

Predictions of natural mechanical frequencies, mode shapes and forced response behavior can be made fairly accurately using modern finite element software. However, it is often difficult to model boundary conditions and complicated aspects of a structure without introducing error. This error cannot be made inconsequential by introducing a large safety factor in the design of the structure, and may possibly result in the structure resonating at unpredicted frequencies.

To inspire more confidence in dynamic modeling results, a modal survey can be performed to validate numerical results. In a modal survey, all frequencies over a bandwidth of interest are excited in a structure and resonances are identified using spectrum analysis software. Frequency response functions, corresponding to excitation and response points, are used by modal analysis software to animate the mode shapes of the structure.

A modal survey of a medium energy superconducting RF cavity was performed to validate numerical results for natural frequencies and mode shapes obtained using Cosmos FEA software. The modal survey was performed by exciting the cavity using a shaker at a single excitation point and measuring the response with a triaxial accelerometer at many other points. The frequency response functions obtained from this test were then used by StarModal, a modal analysis software package, to animate the natural frequencies and mode shapes of the structure. Natural frequencies and mode shapes in the 1 to 1000 Hz range were of primary interest. Once all natural frequencies and mode shapes of interest were identified, the cavity structure was excited at several of its natural frequencies and the response motion at critical points was measured.

Design Parameter Sensitivity of the B61 Nose Structural Dynamics Model (U)

Howard P. Walther
James E. Freymiller
Sandia National Laboratories, Albuquerque, NM

A finite element model of the nose of the B61 lay-down bomb was developed for structural dynamics simulations. This model is part of a multi-year ASCI-funded effort at Sandia Labs (NM) to develop full-system models to simulate component structural response to various dynamic environments. A comprehensive suite of eigenanalyses and frequency response analyses was completed on this nose model to study the uncertainty in component response to changes in key design parameters. The major response of interest focused primarily on the acceleration of the radar. Critical parameters, such as the apparent stiffness of a compressed cellular silicone pad material, or the material or modal damping level, are difficult to determine without the benefit of testing. Moreover, many of the materials exhibit non-deterministic properties and we do not know apriori what the realized value of the variable is in the real system. The results of this study provide both qualitative insight on the structural behavior and quantitative data on the importance of key model variables on response. These results are vital in guiding decisions for a sub-system test program or for justifying specialized material property tests.

Seismic Fragility Models for Reinforced Concrete Moment Frames with Masonry Infill (U)

Michael W. Salmon
Lawrence K. Goen
Los Alamos National Laboratory

The paper presents work in progress for determining the seismic fragility of an existing reinforced concrete moment frame structure with masonry infill panels. Separate fragilities are developed for limit states which correspond to: 1) inability of the structure to provide confinement with loss of active ventilation, 2) onset of significant loss of structural strength, and 3) imminent collapse. Methodology and preliminary results are presented.

On the Use of Inverse Dynamic Analysis to Determine Hostile Shock Component Specifications for the MC4380 Neutron Generator (U)

Jeffrey L. Dohner
James P. Lauffer
Harold D. Radloff
Sandia National Laboratories, Albuquerque, NM

In this presentation, a methodology is presented to predict the transient responses and the shock response spectra used to define hostile shock component specifications for the MC4380 replacement neutron generator. In the past, these specifications were determined from data measured during numerous underground and full scale tests; however, with the present moratorium on underground testing and the present limitations on full scale testing, past methodologies for determining these specifications are no long applicable. In the future, these specifications will be determined using numerical analysis capabilities and codes developed as part of the Advanced Strategic Computing Initiative (ASCI). Nevertheless, at present, the level of validated ASCI capability required to determine these specifications, has not been fully developed. Thus, an interim methodology for determining hostile shock component specifications for the MC4380 needed to be developed.

This presentation summarizes the use of such an interim methodology. This methodology is not intended to be a long term solution since it requires a number of limiting assumptions, but is intended to produce interim solutions while ASCI capability is being developed and validated. The methodology is mathematically complex in that two inverse problems, and a forward problem, must be solved for permutations of model combinations representing possible variability's in generator dynamics.

Classified 2
Building 132 Auditorium Room 1000

Lara D. Daily
Allen G. Baca
Francisco M. Guerra
Francisco M. Guerra
Kin L. Lam
Susurla S. Murty