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Title: ASC Physics and Engineering Models (PEM) Program Overview

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Intended for: Various routine program update meetings at Los Alamos, LLNL, SNL, and HQ

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ASC Physics and Engineering Models (PEM) Program Overview

Mark Schraad, Manolo Sherrill, Scott Crockett, Tariq Aslam, Dean Preston, Rob Gore, Skip Kahler, Stephanie Frankle

June 8, 2015

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Introductions

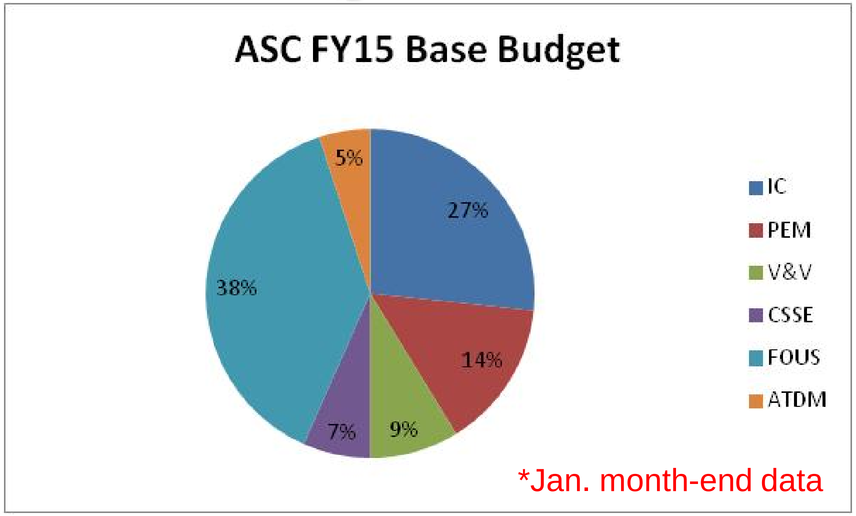
- Scott Crockett, PEM EOS Project Leader
- Dean Preston, PEM Materials Project Leader
- Stephanie Frankle
  - ASC PEM Threat Reduction/Global Security Project Leader
  - SC CNI Program Manager
- Abby Hunter, IC/PEM Staff Member Extraordinaire
- Aaron Koskelo, V&V Physics Validation Project Leader
- Gary Maskaly, W76 POC (@ Boost Fest, then LLNL)
- Marianne Francois (on foreign travel)
  - ASC Additive Manufacturing Team Lead
  - Deputy Group Leader, Fluid Dynamics and Solid Mechanics (T-3)
- Mark Schraad, PEM Program Manager

LANL Program Overview

Advanced Simulation and Computing (ASC)
Bill Archer, Program Director

Any guess what this was in 2004?

Integrated Codes (IC) Jerry Brock (XCP-DO)	$51.5M
Physics & Engineering Models (PEM) Mark Schraad (ADX)	$28.2M
Verification & Validation (V&V) Fred Wysocki (XCP-DO)	$17.0M
Comp. Science & Soft. Eng. (CSSE) Mike Lang (CCS-DO)	$12.8M
Facility Ops. & User Support (FOUS) Hal Armstrong (HPC-DO)	$74.1M
Adv. Tech. Dev. & Mitigation (ATDM) Mark Anderson (XCP-DO)	$9.7M
Platforms Manny Vigil (HCP-DO)	$106.1M
ASC Total	$299.3M
Base (w/o Platforms) Total	$193.2M
DAM (IC, PEM, & V&V) Total	$96.7M



*Jan. month-end data

The PEM portfolio represents 14% of the FY15 ASC Base Budget and 9.4% of the FY15 ASC Total Budget

Represents the majority of the theoretical physics and modeling capabilities maintained for the NW Program

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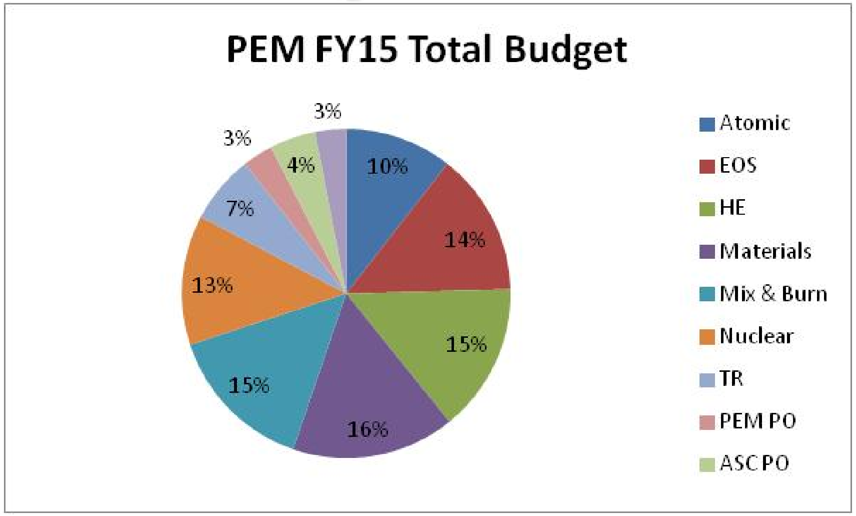
Physics and Engineering Models (PEM)
Mark Schraad, Program Manager

▪	Atomic Physics Manolo Sherrill (T-1)	$3.0M
▪	Equation of State Scott Crockett**** (T-1)	$4.0M
▪	High Explosives Tariq Aslam* (M-9)	$4.1M
▪	Materials Physics Dean Preston** (XCP-5)	$4.5M
▪	Mix & Burn Rob Gore*** (XTD-IDA)	$4.2M
▪	Nuclear Physics Skip Kahler (T-2)	$3.6M
▪	Threat Reduction Stephanie Frankle* (XTD-DO)	$1.9M
▪	PEM Program Office	$0.8M
▪	Work Package Total	$26.1M
▪	ASC Program Office	$1.3M
▪	Reserve	$0.9M
▪	PEM Total	$28.2M



*Effective 02/02/15
**Effective 03/02/15
*** Effective 04/15/15
****Effective 05/04/15
*Acting

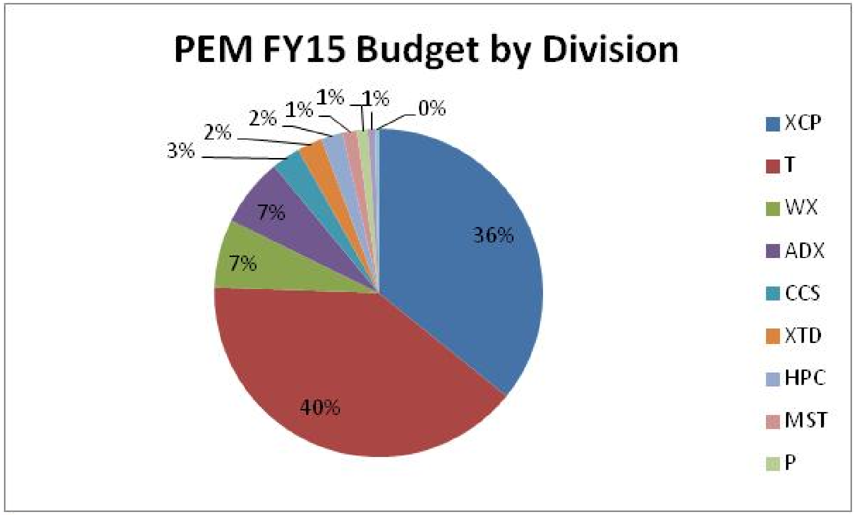
Mark Schraad
schraad@lanl.gov, 665-3946

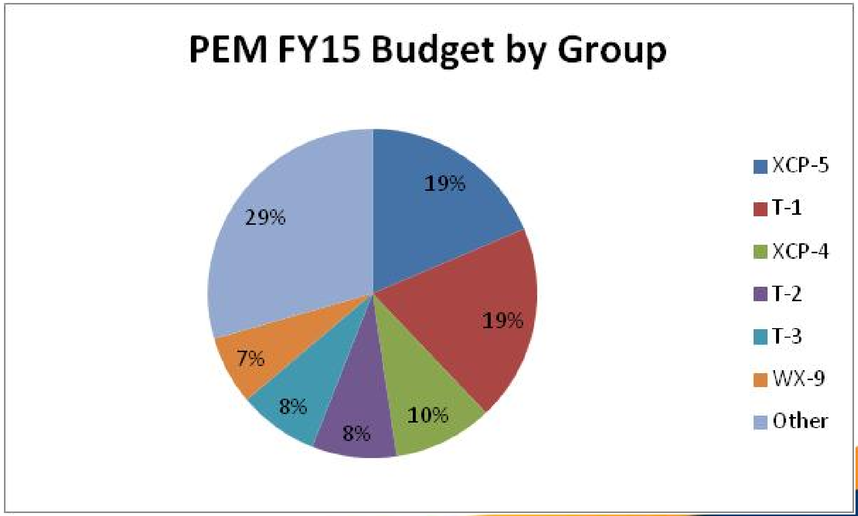
Contributing Line Organizations

- X-Computational Physics (**XCP**) $10.1M
- Theoretical (T) $11.2M
- Weapons Experiments (**WX**) $1.9M
- Weapons Physics (ADX) $1.9M
- **CCS**, **XTD**, HPC, **MST**, **P**, W, EES

- Materials and Physical Data (XCP-5) $5.2M
- Physics and Chemistry of Materials (T-1) $5.5M
- Methods and Algorithms (XCP-4) $2.8M
- Nuclear Physics, *et al*. (T-2) $2.3M
- Fluid Dynamics and Solid Mechanics (T-3) $2.2M
- Shock and Detonation Physics (WX-9) $1.9M
- Other $8.3M

Note overlap with PLs home orgs





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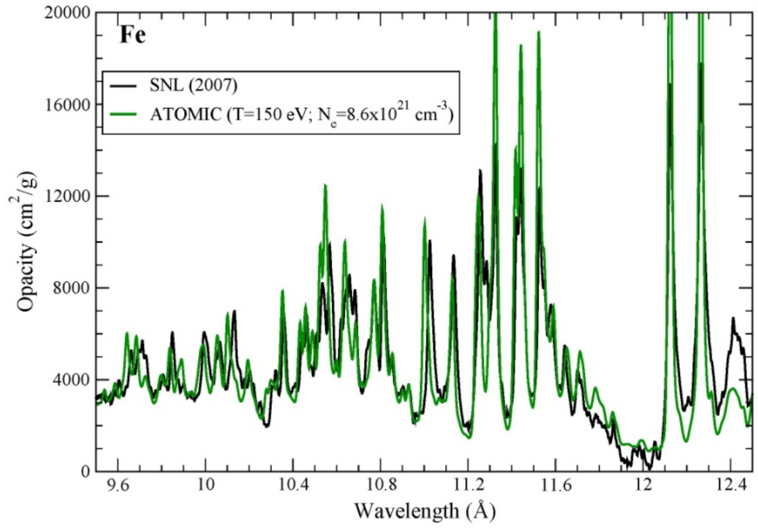
Atomic Physics
Manolo Sherrill (T-1)

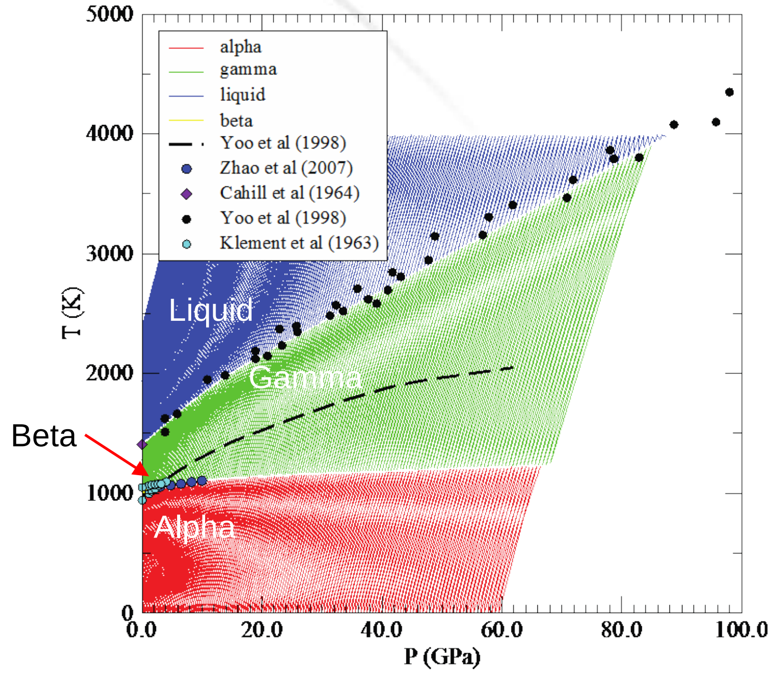
- Technical Scope
  - Atomic physics—structure and collisions
  - LTE (local thermodynamic equilibrium) and inline non-LTE opacities
  - Equations of state
  - Spectroscopic modeling
  - Data-FA activities
- Historic Delivery
  - OPLIB tables
  - Inline non-LTE models
  - Replacement of the legacy opacity code, LEDCOP, with the ATOMIC opacity code for production of new opacities (***FY15 L2***)
- Future Plans
  - Molecular opacity tables
  - FESTER, a spectral post-processing tool for synthetic spectral and image modeling, to be used in radiation-hydro simulations
  - Complete Linearizaiton (CL) model for opacity validation experiments
  - High-fidelity uranium opacity table, with converged atomic physics model



A comparison of the SNL Z-machine measurement of Fe versus an ATOMIC calculation

Equation of State (EOS)
Scott Crockett (T-1)

- Technical Scope
  - Equation of state physics and production
  - Multi-phase EOS theory and modeling (kinetics)
  - Fluid phase theory and modeling
  - QMD modeling of melt lines and shear moduli
  - DFT & DMFT calculations for EOS
  - Data-FA activities (e.g., EOSPAC)
  - Modeling support for dynamic experiments
- Historic Delivery
  - Sesame tables, shear* and melt tables
  - EOSPac
  - Multi-phase EOS (***FY14 L2***)
- Future Plans
  - Thread-safe EOSPac
  - Fluid EOS table from Pseudo-Atom Molecular Dynamics and fluid EOS tables for mixtures
  - Multi-phase EOS improvements/extensions
  - Delivery of Improved Materials Models Supporting FY18 PCF Peg Post (***FY17 L2***)



PEM is moving from a material-focused perspective to a phase-focused perspective—this begins with multi-phase equations of state

Scott Crockett (T-1)

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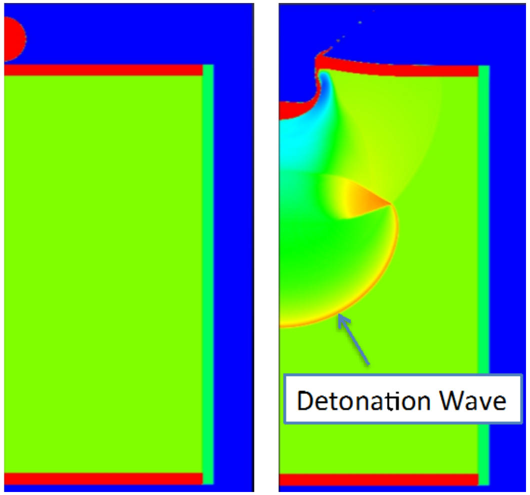
High Explosives
Tariq Aslam (M-9)

- Technical Scope
  - Reactive burn model development
  - Equation of state physics and EOS production (for HE reactants & products)
  - Meso-scale modeling (phys. & chem.)
  - HE safety
- Historic Delivery
  - Detonation Shock Dynamics/Psuedo Reactive Zone Model (DSD/PRZ)
  - WSD, SURF, *et al*.
  - Visco-SCRAM/MATCH
- Future Plans
  - Parameterization and Implementation of the Pseudo-Reaction-Zone High Explosive Model (***FY15 L2***)
  - Comprehensive evaluation of reactive flow models, including resolution requirements
  - Magpie
  - Higher fidelity reactive flow models
  - Delivery of Improved Materials Models Supporting FY18 PCF Peg (***FY17 L2***)

Fragment Impact of PBX 9501 using SURF in Pagosa



A Pagosa simulation of a steel ball moving at 1.65 km/s, impacting a steel-enclosed cylinder of PBX 9501. The burn model used in this simulation is SURF. A shock-to-detonation transition occurred and the detonation wave is shown in the figure.

X. Ma (T-3), B. Clements (T-1), and R. Menikoff (T-1)

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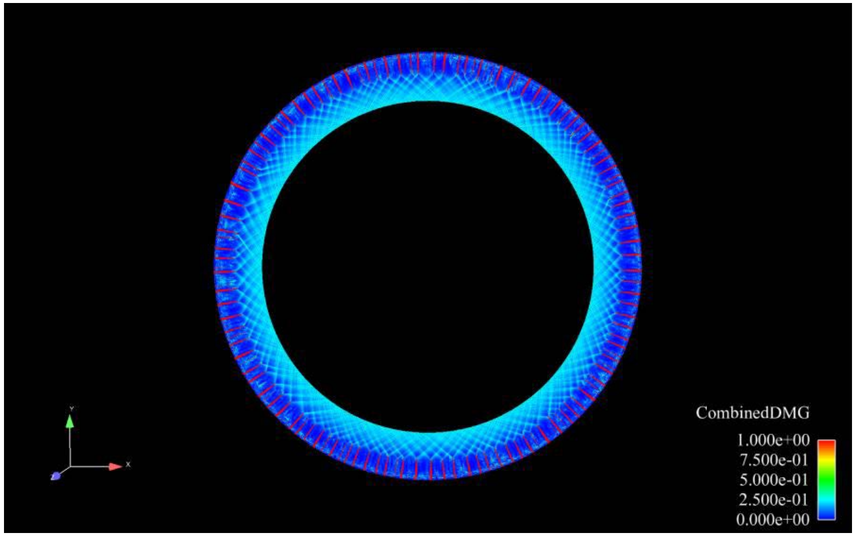
Materials Physics
Dean Preston (XCP-5)

- Technical Scope
  - Plasticity, strength, and phase transformations
  - Damage and failure
  - Supporting science: interatomic potentials, grain boundary physics, crystal plasticity, sub-grid models, non-local theories, etc.
  - Integration with ASC, SC, and DSW
  - Additive manufacturing
- Historic Delivery
  - PTW (strength model)
  - Ductile damage models
  - Multi-phase strength model (kinetics)
- Future Plans
  - PTW re-calibration for multi-phase EOS consistency (***FY14 L2***)
  - Multi-scale strength (dislocation dynamics based)
  - Dynamic fracture model for brittle metal phases (***FY16 L2***)
  - Delivery of Improved Materials Models Supporting FY18 PCF Peg Post (***FY17 L2***)

FLAG – Brittle Fracture Modeling



A thick-walled cylinder subject to a constant internal pressure of 4.0 GPa. The color scheme corresponds to a combination of tensile and compressive brittle damage.

Abigail Hunter (XCP-1) and Esteban Rougier (EES-17)

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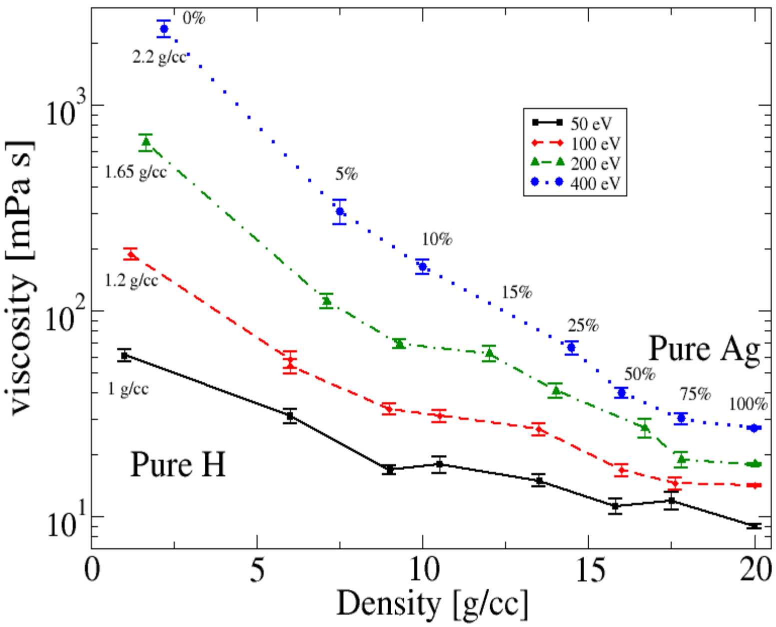
Mix & Burn
Rob Gore (XTD-IDA)

- Technical Scope
  - Mix model development
  - Ejecta modeling
  - Spectral modeling
  - Burn formula for non-pre-mixed reactions
  - Modeling support for sub-crit experiments
- Historic Delivery
  - BHR (inclusion of plasma properties)
  - Ejecta model (***FY14 L2***)
- Future Plans
  - Modal model (strength dependence); BHR initialization
  - A Feature Rich Model for Initial Mix Deposition (***FY17 L2***)
  - Ejecta model improvements
  - Delivery of Improved Materials Models Supporting FY18 PCF Peg Post (***FY17 L2***)
  - Multi-species mix model

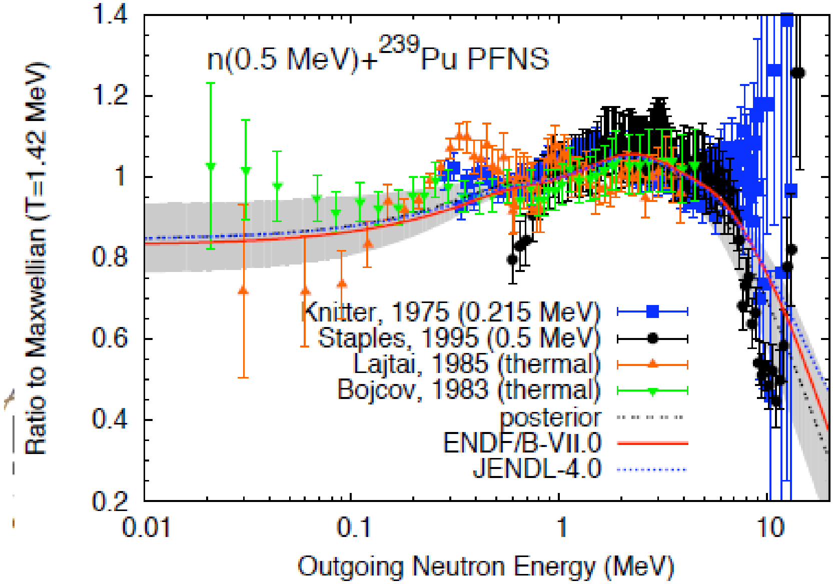


This plot shows the variation of viscosity as a function of density (concentration) on an isobar for several temperatures. The viscosity of the gas (H) is much higher than the metal (Ag) and the gas viscosity significantly varies with small amounts of metal. These simulations are run on Cielo and are first principle microscopic simulations.

Chris Ticknor (T-1)

Nuclear Physics
Skip Kahler (T-2)

- Technical Scope
  - Refined fission and reaction theory development
  - Nuclear structure model development
  - General purpose and application specific evaluated nuclear data files (ENDF)
  - Data-FA activities
- Deliverables
  - Nuclear data libraries
  - Nuclear data evaluations to ENDF/B
- Milestones
  - Thread-safe Nuclear Data Interface (NDI)
  - Delivery of Improved Materials Models Supporting FY18 PCF Peg Post (***FY17 L2***)
  - Next-generation nuclear data processing code, NJOY21
  - Continuous improvement to the nuclear cross-section library



Obtaining new PFNS data, with emphasis on reduced uncertainty in both low-energy and high-energy regimes, is a LANL priority

Threat Reduction
Stephanie Frankle (XTD-DO)

See Stephanie's Slides Under Integration

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What is Success? Year-One Results

Focus: Leadership, Near-Term Delivery, Integration

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- **Leadership**: EOS, HE, Materials, Mix & Burn, and TR Projects may all require new leadership—challenge and opportunity!!!
- **Delivery**
  - HE: Successful completion of the FY15 L2 Milestone on Implementation of a Pseudo-Reactive Zone (PRZ) HE Model
  - PEM: Successful completion of the FY15 L1 Milestone
  - Mix & Burn: First ejecta model tested and validated
  - EOS: Complete multi-phase EOS implementation, testing, and validation
  - Materials: Ensure strength models are thermodynamically consistent with multi-phase EOS
  - Atomic: Successful completion of the FY15 L2 Milestone Replacing the Legacy Opacity Code
  - Nuclear: New multi-temperature cross-section library based on national data base
  - Threat Reduction: Improved modeling capabilities for Deflagration-to-Detonation Transition (DDT)
- Integration Strategy—On day one, new dialogues will begin with:
  - ASC PO, *et al*.: To determine what is working well and what is not
  - Immediate/near-term needs from others:
    - Science Campaigns: physical insight, calibration and validation data, etc.
    - ASC IC: implementation; ASC V&V: testing and validation; ASC ADTM: setting the stage now for future M&S capabilities
    - DSW: How can PEM make the designers' jobs easier, more productive, more interesting, and how can we work together (and with IC, ADTM, and V&V) to establish future capability needs and approaches for meeting them?
    - All of the Above: To ensure the above list and other near-term goals are met, and to begin establishing stronger partnerships for our evolving longer-term program strategy
  - ADX, ADTSC, ADW, ADEPS: To begin establishing optimal use of capabilities and leveraging opportunities, and to communicate the evolving program strategy and expected changes
  - PEM PLs and staff: To communicate the evolving program strategy and expected changes …
  - LLNL, SNL, HQ: To ensure program coordination and to help establish a relationship with HQ

Future PEM success will depend on more fully establishing **partnerships** across NW

Integration Activities

Program Overview Audiences

Tail System P.O.C.'s Meeting	03/18
Secondary V&V Project Meeting	04/14
C2 Program Meeting	04/16
XCP Division Technical Topics Meeting	04/16
Theoretical Division Staff Meeting	04/30
	06/04
XTD-Nuc. Threat Ass. Group Meeting	05/07
LANL ASC All Hands Meeting	06/15
PEM Project Meetings	Ongoing

PEM Responsibilities

- Develop more accurate and/or more complete understanding of relevant physical processes ⇒ PEM-SC
- Ensure this accuracy and understanding are represented in our physics models ⇒ PEM
- Partner to provide models that are implemented, validated, and working robustly in ASC codes ⇒ PEM-IC,V&V
- Engage to see that requested/need modeling capabilities are put in the hands of, used by, and valued by, the design community ⇒ PEM-DSW,GS
- Balance near-term delivery with long-term physics theory and modeling capability development ⇒ PEM-Univ.

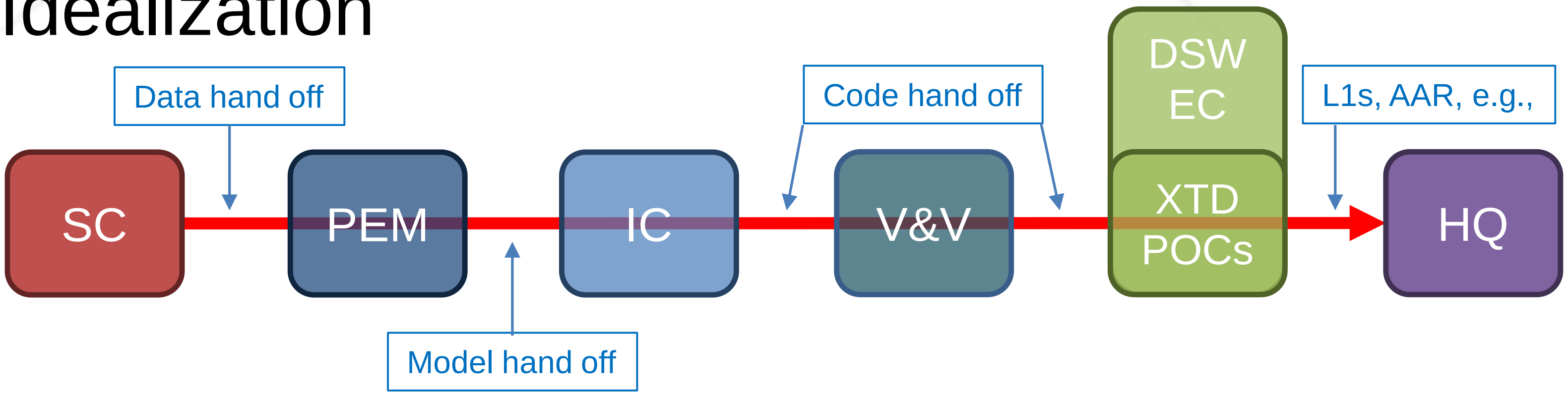
I see very few problems in the Nuclear Weapons Program that can be solved by one organization, program, or scientific community

Questions to Answer …
… Before Taking the First Modeling Step

- Who is asking for the capability? ⇒ PEM-DSW,GS
- Who is going to generate the data that you will need to calibrate and test your model? ⇒ PEM-SC
- What is the target (IC code, continuum scale model, discovery physics question, etc.)? ⇒ PEM-IC
- Who are you going to partner with to ensure proper implementation? ⇒ PEM-IC
- Who are you going to partner with to ensure proper testing, validation, and verification? ⇒ PEM-V&V

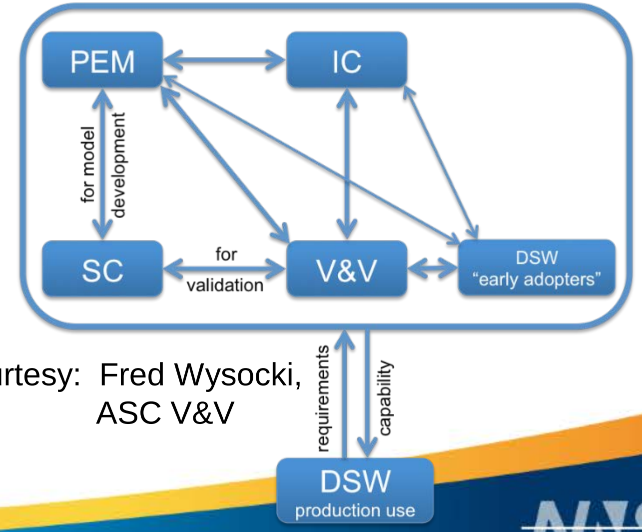
Line of Sight
Model of Integration

- Idealization



- Reality

Fundamentally, hand offs don't work as well as partnerships, and partnerships require common goals and priorities



Courtesy: Fred Wysocki, ASC V&V

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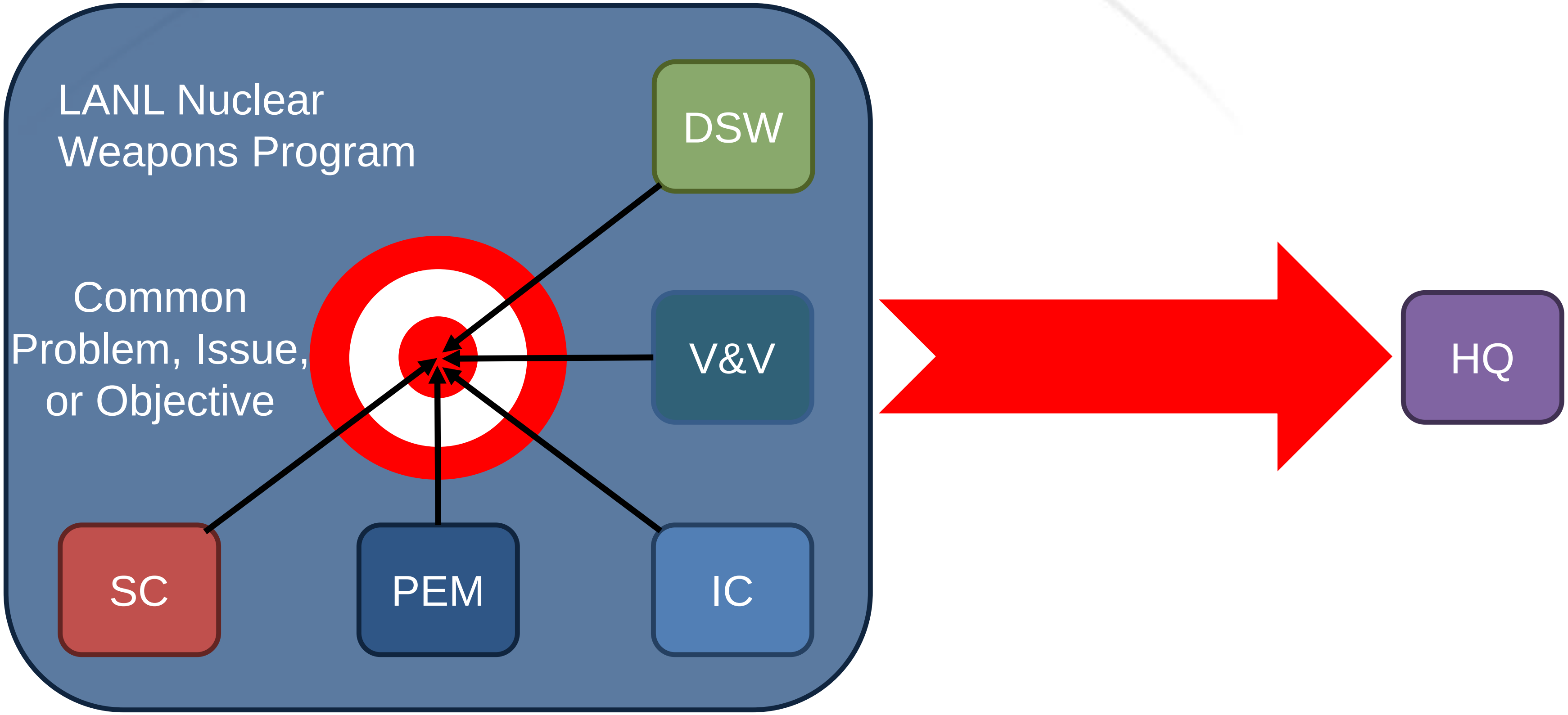
Common Problem/Shared Fate Model of Integration



I see very few problems in the Nuclear Weapons Program that can be solved by one organization, program, or scientific community ⇒ ***integration!***

An Example: PTW Calibration

- Team
  - PEM: Dean Preston (Materials), Scott Crockett (EOS), Sky Sjue, *et al*.
  - DSW: Gary Maskaly (W76), David Jablonski (B61), John Vandenkieboom, Von Whitley
  - SC: Bill Blumenthal (C2), Rusty Gray (C2)
  - V&V: Aaron Koskelo (Phyics Validation), Karlene Maskaly, Bob Chrien
  - IC LAP: Ted Carney, Abby Hunter
  - IC EAP: Gary Dilts, Rick Rauenzahn
- Tasking
  - Generate prioritized list of relevant material phases of interest (DSW-PEM)
  - Identify gaps in data needed to calibrate all prioritized phases (PEM-SC)
  - Develop experimental plans to fill these data gaps (SC)
  - Form 3 teams to focus on first 3 phases and associated PTW calibration (PEM)
  - Calibrate first 3 phases (highest priority for which data exists) (PEM)
  - Validation of new parameters sets (PEM-V&V-DSW)
  - Ensure coordination with IC (PEM-IC-V&V)
  - Release of parameter sets for first 3 phases and documentation (All)
  - Go to calibration step and repeat for next 3 phases

PEM Program Goals and Priorities

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Critical Delivery Now + Short-Term Successes = Long-Term Research Viability

- PEM Top Ten
  1.) ATOMIC L2 and low Z opacity tables
  2.) DSD/PRZ L2: Detonation shock dynamics for HE
  3.) Phase-dependent strength model (PTW) calibration
  4.) Comprehensive reactive burn model evaluation
  5.) Ductile damage model robustness optimization
  6.) EOSPAC: Thread safety and optimization
  7.) Next-generation code activities
  8.) Atomic, EOS, and Nuclear Data-FA activities
  9.) Future ejecta modeling capabilities
  10.) TR/GS portfolio evolution
  …

Select **Examples of PEM Integration**

- PEM Integration
  - EOS-HE: HE product and reactant EOS, Magpie development
  - EOS-Materials: thermodynamic consistency between EOS and strength
  - TR/GS-Nuclear Physics: see below
- Science Campaigns
  - PEM-C1: material aging, boost
  - PEM-C2: many topics across EOS, HE, Materials, and Mix & Burn
  - PEM-C4: energy balance, PEM Materials overseeing C4.2 modeling efforts
- ASC Integration
  - PEM-IC: forming dual points-of-contact for implementation issues
  - PEM-V&V: multiphase EOS, PTW calibration, HE, …
- DSW Integration
  - Weekly meetings with System Team Leads for B61, W76, W78, W88
  - Peer review of Annual Assessment Review (AAR)
- GS Integration
  - See below

Integration with Global Security

See Stephanie’s Slides

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Questions from HQ
(To be Elaborated on During the Discussion)

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- How Can PEM Improve Its Integration?
  - Common problems/shared fate approach to program integration
  - Cross-program teams (blurred program lines)
  - All of the PLs and the majority of staff have to be engaged
- Can We Better Delineate the Role of PEM Outside ASC?
  - Broader Nuclear Weapons Program
  - Global Security
  - Office of Science
  - DoD
  - LDRD

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Mission Impact

Historic PEM Delivery

- OPLIB Tables
- SESAME Database
- Reactive Burn Models and Detonation Shock Dynamics
- PTW Strength Model
- BHR and Ejecta Models
- Nuclear Data Libraries
- EOS, Nuclear Data, etc. for GS Applications

And let's not forget about relevant historic physics discovery impacting the Nuclear Weapons Program (e.g., history dependence through phase changes)!

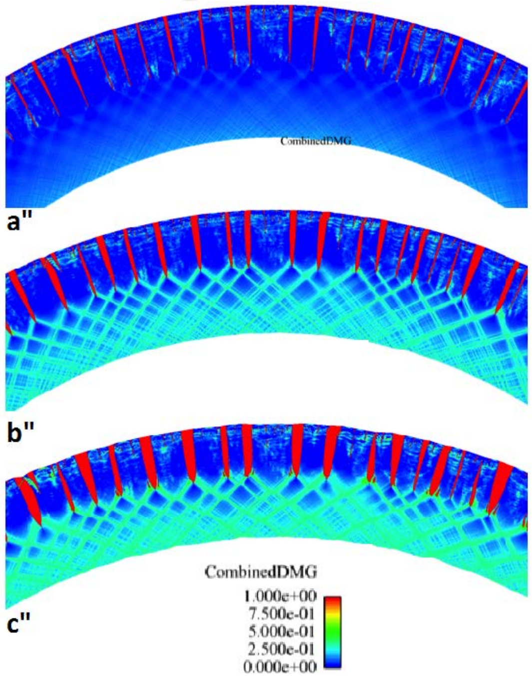
Recent Accomplishments

- Several new Equations of State have been developed, including several new multi-phase equations of state for relevant materials and associated alloys. These multi-phase equations of state are being used, in part, to satisfy an upcoming L1 Milestone.
- A full ejecta source model has been developed, implemented, and delivered to the V&V community for testing and validation. This model is being used, in part, to satisfy an upcoming L1 Milestone.
- Our legacy opacity code has been replaced with an advanced code with higher fidelity physics, and which produces more refined opacity tables. This new code has been used to produce opacity tables for 30 light elements as part of an FY15 L2 Milestone
- Development of a new Detonation Shock Dynamics (DSD) solver is being completed and coupled with an advanced Pseudo-Reactive Zone (PRZ) model for High Explosives (HE), as part of an FY15 L2 Milestone
- Developed a new multi-temperature, multi-group neutron cross-section library based upon ENDF/B-VII.1 in response to LANL DSW user needs
- Development of our next generation strength model, based on dislocation dynamics, completed with implementation underway

Numerous significant accomplishments in the longer-term science that supports the shorter-term mission delivery outlined above!

Upcoming L1 Milestone Contributions

- Mix & Burn
  - First ejecta model implemented, tested and validated
- EOS
  - Multiphase EOS implemented, tested, and validated
- Materials
  - PTW strength model re-calibrated for thermo-dynamic consistency with multi-phase EOS
  - Continuum-scale damage model for brittle-to-ductile transitions in metals demonstrated



The damage evolution in a thick-walled cylinder subjected to internal pressure and the resulting complex pattern of shear bands.

PEM Involvement in Out-Year Milestones

- Level 1
  - FY15 Primary Reuse Capability
  - FY16 Secondary Life Extension Program Capability
  - FY16 Advanced Safety Baseline Capability
  - FY18 Primary Performance - Nominal
- Level 2
  - FY15 Replacement of the Legacy Opacity Code LEDCOP with the ATOMIC Opacity Code for Production of New Opacities
  - FY15 Parameterization and Implementation of the Pseudo-Reaction-Zone High Explosive Model
  - FY16 Dynamic Fracture Model for Brittle Metal Phases
  - FY17 A Feature Rich Model for Initial Mix Deposition
  - FY17 Delivery of Improved Materials Models Supporting FY18 PCF Peg Post
- Level 3s and Level 4s
  - Part of LANL's internal 5-year planning process
  - Points more toward program integration rather than impact

Questions From HQ (To be Elaborated on During the Discussion)

- How Can PEM Improve Its Impact?
  - PM, PL, staff engagement with the broader design community
  - Developing stronger partnerships with the IC and V&V communities
- How Should Long-Lead-Time Research Be Balanced With Near-Term Impact?
  - By integrating more formally with programs outside of the NW Program (e.g., Office of Science, DoD, LDRD, etc.)
- Does PEM Need To Be More Agile?
  - To do all of the above, yes

Challenges

Challenges

- Budget versus Scope
- Personnel Shortage
- Implementation
  - Path-dependent mechanics in Eulerian and ALE frameworks
  - Coupled physics and understanding physics package interdependencies
- The Disparate Needs of the User Community

Questions From HQ (For Discussion)

- What Are Some Common Challenges?
- What Can We Do to Better Coordinate and Address Major Challenges?

Questions?