



FY06 Progress

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

My current job description is to “Interact” w/ Ideas, Projects, People

- High Energy Density Physics (HEDP)
- QMU
- PSP
- V&V
- ASC Program

**ASC – All my funding is in
one Project/Task from
Pilch**

- Work w/ Laura McNamara
- Work w/ John Shadid

Unfunded

HEDP – Growth built on success?

Pilch, Mehlhorn

Key FY05 Validation Milestone Completed

Flyers were the focus of a successful FY05 V&V milestone

Validation Plan

- Demonstrate code suitability for the validation activities
- Characterize and validate material models
- Perform laboratory-scale validation (one or more experiments)
- Perform Z-pinch validation (one or more experiments)
- Archive available documentation
 - This form has been used for externally reviewed milestones and is appropriate for this milestone.

May 7, 2006 HEDP IPT Kickoff Meeting 17

FY07+ - ASC “Focus Area”/Integrated Product Team

HEDP IPT: Mission Driven Capability Development

ASC Focus Area Management Team (AMT):
 AMT Champion: Marty Pilch
 Lab stakeholder POC: Tom Mehlhorn
 HEDP IPT PI: Christopher Garasi
 Analysis POC: Ray Lemke

PE Reps: Summers Collis? Pilch Aidun/Lash? Paviakos?
 Apps Algorithms V&V Material Modeling Pre-/Post-process
 IPT Tech Reps: Drake Shadid Knupp/Trucano Desjarlais Rogers

HEDP IPT Mission & Vision

- Predictive design and analysis capability to effectively use SNL Z-pinch capability
- Generate design for next generation pulsed power facility (ZXP) capable
- Contribute to the National Predictive Science Program
- Have SNL ASC participate in a more permanent role in HEDP

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Large \$ request in FY07

Foundation for FY08 Validation Milestone Foundation for ASC HEDP Focus Area

- “A collaboration between LLNL and SNL resulted in improved capabilities for both organizations.” (PSP FY06 Final Report)

Impact: I helped guide the delivery of this milestone at a high-level.

My current role: representing the V&V program; consulting on V&V and HEDP to 1674 and 1431; writing. (I also consult on HEDP too.)

QMU – A Very Important Goal

Pilch, Novotny

- The ASC strategic goal of credible predictive capability impacting the Stockpile requires QMU (Quantitative Margins and Uncertainty).
- SNL V&V program is defining methodology for QMU that centers on new application of old ideas (RIDA) as well as new ideas (rigorous V&V).

QMU = Information + Decision Process

The information has the form: **Best Estimate + Uncertainty**

The decision process is decision-making under uncertainty (**RIDA**)

SNL DP has now acknowledged the importance of QMU.

V&V Program Concepts (in progress).

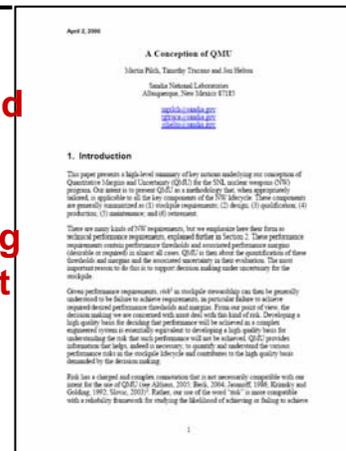
Rottler QMUWG:

- Novotny, Paulsen, Pilch, Diegert, Klenke
- SNL conception

SNL attended last QMU working group meeting (Feb/LANL)



Impact: I am the lead writer for V&V program QMU documents (building on my broad insight and technical knowledge).



Others docs in progress:

- Technical Specs
- Resource material

Predictive Science Panel – FY06

Kusnezov, Cornwall, Hale

FY06 review cycle completed May 2006;
report out ~ May 9

Key sections include:

ASC Strategy/Roadmap*; Validation*, UQ/QMU*; Verification*, code development*, algs*; Physics processes* (TBI); EOS*, strength*, aging*; Misc (RRW, “Retribution,” etc)

**Impact: my particular expertise in V&V and UQ;
and that I can speak substantively on all of
the asterisked topics.**

Kusnezov –

- “PSP reports have great value.”
- Specifically liked the V&V/UQ/QMU discussion
- “V&V should be more empowered by the program”
- “Program does a disservice in simplistic representations of computation – experiment comparisons.”
- “Measuring progress in predictive capability is critical for the program.”

Executive Summary—Report of the ASC Predictive Science Panel

Los Alamos, October 12—14, 2005
Livermore, April 4–6, 2006

Submitted by John M. Cornwall, Chairman
May 5, 2006

1 General remarks

The ASC Predictive Science Panel (PSP) met at Los Alamos on October 12–14, 2005, and again at Livermore on April 4–6, 2006. This report covers both meetings.

A two-sentence summary of the Panel's findings:

The ASC Program of the future has numerous superb accomplishments in machine acquisition, code development, and progress in modeling and validation. But this Program will very soon be under considerable pressure from new threats to transform the complex and reduce its budget, including the Reliable Replacement Workload (RRW) and transformation of the plants and the ASC Program can no longer delay proactive planning for facing the transformation threats.

Before taking up the substance of these issues we briefly discuss some other matters.

1.1 Membership and attendance

In the year after the 2005 Livermore meeting until now, there have been several membership changes. For various reasons, Bill Dahlborg, Paul Drazich, Ray Jankita, and Vic Reib have left the Panel, and we have three new members: Bill Chandler (from code, ex-LANL), Elaine Chandler (national sciences, Stanford University), and David Doocho (statistics, Sandia University). Bill Chandler and David Doocho joined after the LANL meeting, and Elaine Chandler attended the LANL meeting. Elaine Chandler was able to come to both meetings. At the LANL meeting,

Dahlborg, Drazich, Goodman, Meiron, and Weinberger were unable to attend, and at the LLNL meeting Jim Axy, Dan Reed, and Doocho were unable to attend. The present membership roster and meeting agenda are attached to this report. It is likely that a new member or two will be added before the next LANL meeting this fall.

1.2 Meeting structure

The PSP is relatively new, and the best format for our meetings has been discussed in previous reports and with the laboratories. We are pleased that they have been very responsive to our suggestions, both at LANL and at LLNL, and have made serious efforts to find the best format.

At the LANL meeting, Mark Chadwick and other organizers, in response to PSP suggestions, included participation of a LLNL leader at the LANL meeting.

At LLNL, Lynn Kinsel and his fellow organizers reciprocated by having a LANL leader. Both meetings provided a number of occasions for participation by NNSA personnel, including the ASC Program Director Dimitri Kozminov.

A somewhat unplanned happening at LLNL unexpectedly led to a meeting modality that the PSP feels could become a permanent feature of our reviews. LLNL had, in part because of our suggestion, planned an hour for a site tour. However, most PSP members had already had such a tour, and we felt that a better use of the hour would be to hear from NNSA about some issues going beyond the ASC sci-

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**SNL has planned to establish
a “Predictive Engineering
Science Panel.”**

ASC Program – Alliance V&V Whitepaper

Kusnezov, Hale

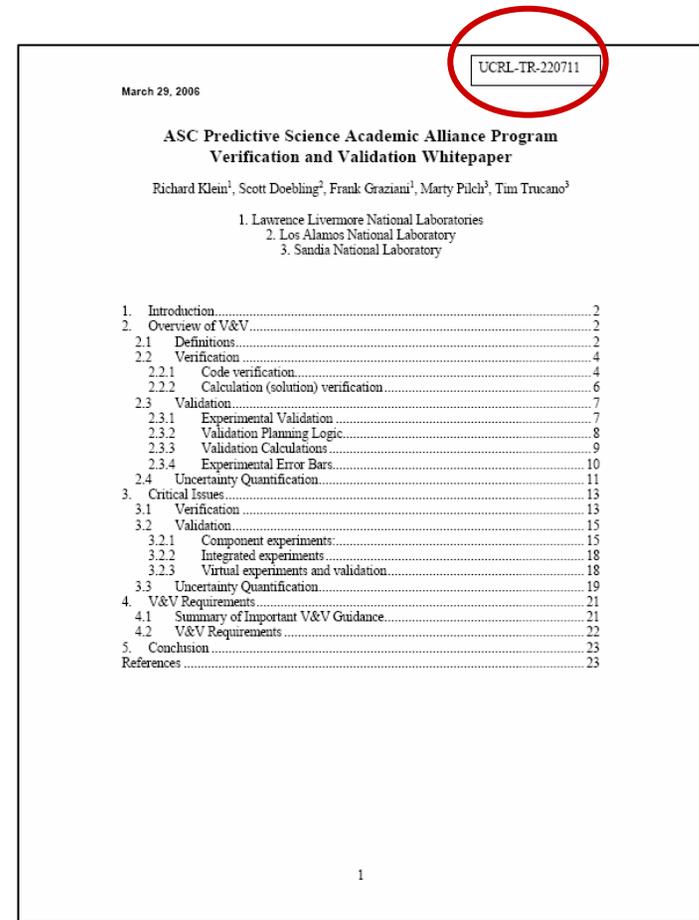
The strongest public statement on V&V yet by the ASC Program!

“It is mandatory that proposals address the following two topics:

- 1. Predictability in science & engineering.**
- 2. Verification & validation strategies for large-scale simulations, including quantification of uncertainty and numerical convergence.”**

Example quotes:

- **“No experimental data = No validation”**
- **“The first question that must be asked in any validation calculation that is compared with experimental data is: “Does the numerical error fatally corrupt the comparison with experimental data?” There are only three qualitative options for relevant answers to this question: (a) Yes; (b) No; (c) I don’t know.”**
- **“Don’t do validation if you aren’t willing to assess the consequences.”**
- **“Good enough for a journal does not imply good validation.”**

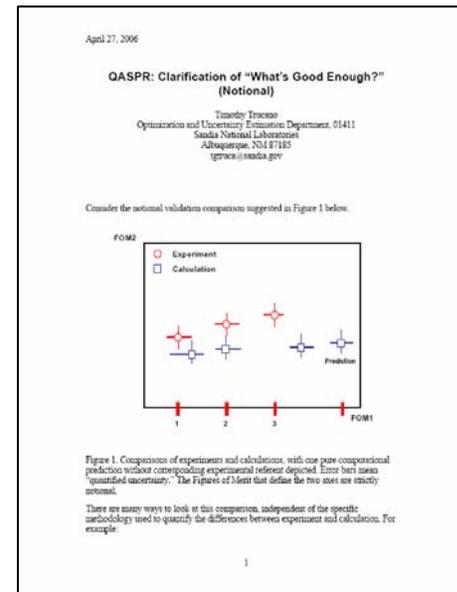
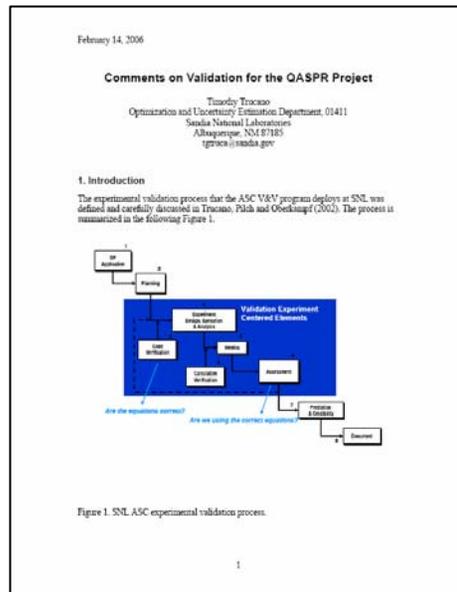


Impact: I wrote >50% of the White Paper.

ASC Program - QASPR

Pilch, Wohl, Hutchinson

- My engagement with QASPR is mirroring my engagement with HEDP (w/ less subject-matter knowledge): consultation, advice, some written contributions.
- I'm primarily focusing on "system-level" V&V/UQ issues.
- In progress; **my current impact is advice and writing.**

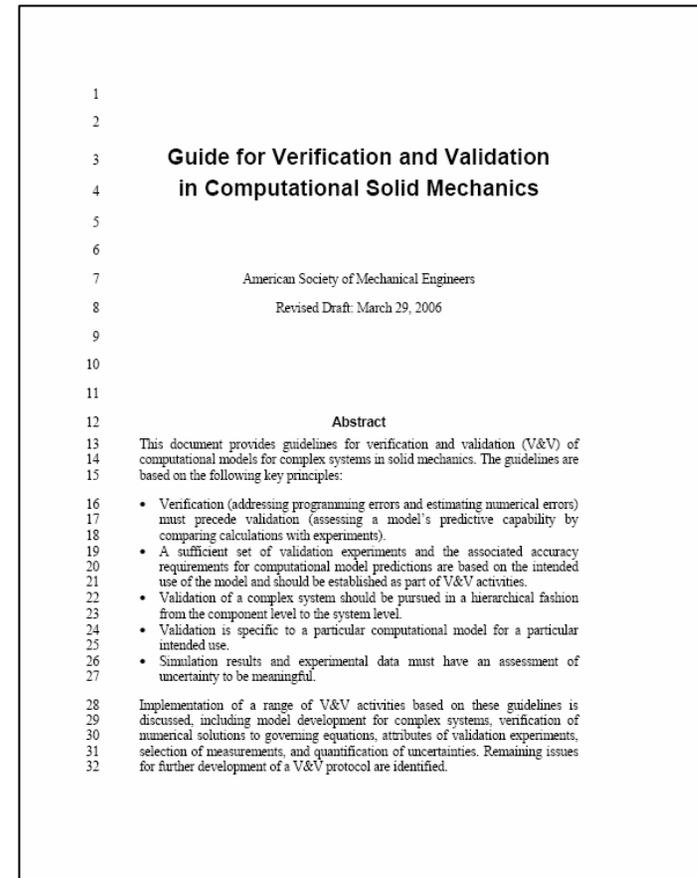


ASC Program – Misc.

- **ASC Roadmaps: (Hale, Yarrington, Pilch)**
 - I've been part of the group of lab reps (about 35) who have contributed to the ASC Roadmap document that is still in progress.
 - The SNL internal “roadmap” planning emphasizes needs and strengths in V&V, UQ, and QMU, especially in focus areas, so I have been engaged in significant internal planning around these issues for most of the past year.
- **SNL ASC Technology Readiness Level (TRL) Study: (Hale, Pilch Yarrington)**
 - I am a member of the “ModSim (TRL) Steering Committee” that is charged with developing TRLs for SNL ASC.
 - I provided the first concrete analysis of this issue.
- **ASC V&V: (Pilch)**
 - Up to about 6 weeks ago I was the prime lab rep working with Jamileh Soudah (HQ) on writing the Tri-Lab V&V Strategy document; the V&V program leads are now pushing the completion of the document and my role is critical input into the final versions.
 - I have been aggressively pushing the relationship between ASC V&V, M&S “Predictive Capability” and SBET.
 - Presently negotiating with Carl Peterson to perform a modification of work proposed in a Late Start LDRD proposal.
 - The Predictive Capability Maturity Model (PCMM) was proposed by Pilch in the wake of last year's JASON study, and is being elaborated in our ongoing QMU writing.
 - I'm currently developing our position on its relevance to TRLs and its use in graded V&V approaches and definitions of “sufficiency” for V&V.

ASC V&V Program – Misc. Pilch

- The ASME PTC-60 Committee “Guide for Verification and Validation in Computational Solid Mechanics” has been completed.
- Final steps completing approval of the document are happening in May 2006.
- It will be (hopefully) published by ASME prior to 2007.
- Such documents are essential measures of our national V&V impact.
- **Impact: I’ve been a member of the group working on this since 1999. Significant amounts of SNL writing on V&V have been used in the document.**



CUD – Cognition and Uncertainty in Decisions w/ McNamara

CUD Notes Volume 1; 231 pp



ASC ↔ QMU ↔ CUD



“Societal Evolution Simulations for Long-Term National Security Insight”

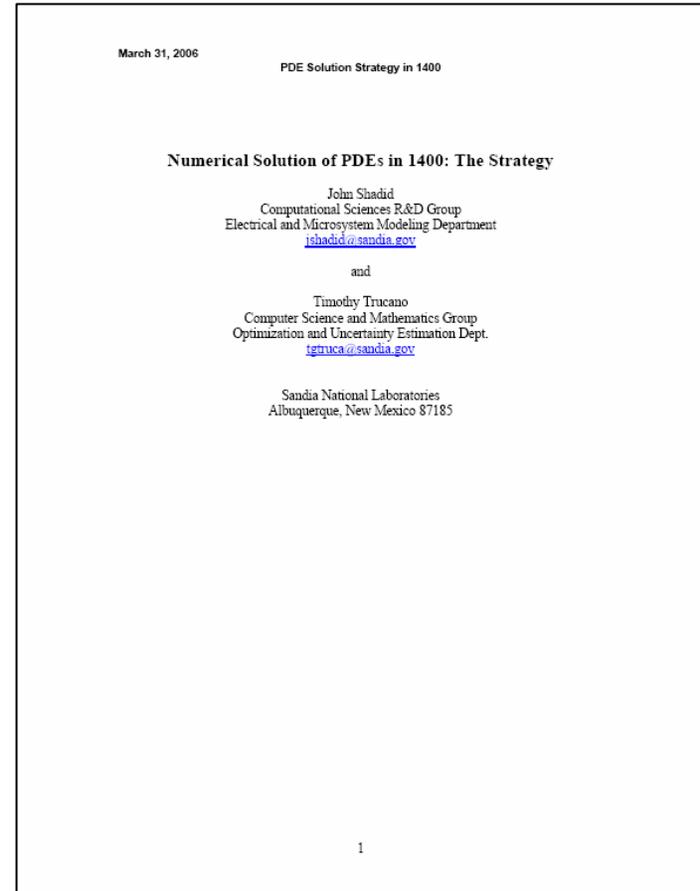


“Computational Modeling and Uncertainty Quantification in the Epistemic Culture of Intelligence Analysis”

- We are trying to get funding to pursue the following research:
 - UQ, especially in the IC
 - V&V (“evaluation”) of social models
 - Social & organizational issues in stockpile stewardship
 - E.g. “Community of Practice” factors in V&V
- UQ/V&V are critical for proper use of social models in areas like IA.

PDEs in 1400 w/ Shadid

- Started in Q1 FY06; requested by Camp/Womble.
- **Goal:** The goal of this study is to provide a useful categorization, assessment, and analysis of the current and long term strategic alignment of algorithmic R&D support for PDE-based applications in CCIM.
- Interviews completed; analysis in progress.
- Way behind schedule – sorry!
- **Impact - TBD**



Data summarized in 66 page document



Conclusion:

- I'm not sure where I'm going...
- But my real mission, as stated last year, is:

**Advocate high-quality, high-impact
computational science intelligently
and constantly.**