FY04 Progress

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Outline – Everything is in progress

- **FY05 ALEGRA-HEDP Z-Pinch Level II Validation Milestone**
- **Prediction**
- **Service**
- **I am struggling with over commitment**

Current workload: all in progress

- Validation Metrics → work on Level II milestones
  - Hostile environments validation; FY04; Kensek and Scrivner
  - Z-pinch validation; FY05; see below; (many links)
- PRIDE LDRD (Greybearding)
  - Links to CUU; V&V; Voth's AD project
- Calibration Under Uncertainty (MICS) – collaboration with Laura Swiler
  - Link to predictability
    - Link to Tak Igusa (John's Hopkins – "Role of Computational Learning Theory in Calibration and Prediction) → paper needed
    - SAMO 2004 Talk → two requested papers
      - V&V Foundations 2004 Invitation → requested paper
- Four other documents in progress for V&V:
  - Using single experiments for validation (link to HDBT/Shawn Burns)
  - Stockpile computing concepts
  - "QMU" concepts (link to DHS whitepaper/Jennifer Nelson)
  - Invited paper on V&V for Edinburgh CS meeting (link to Post)

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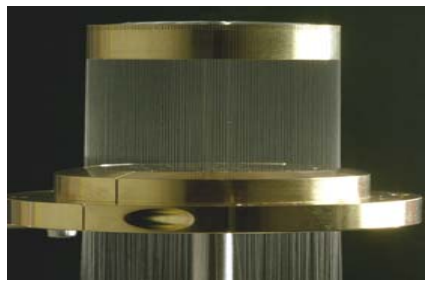
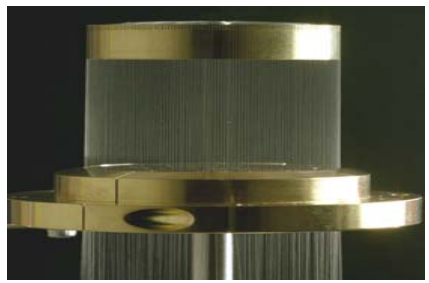
FY05 Level II Milestone: "Z-Machine Modeling Validation"

- This means: Building confidence in ZR predictions using ALEGRA-HEDP
  - $ start in FY04
- Great opportunity – thanks to Bob Thomas
- Specific S&T focus: (Breaks the "Tyranny of the LEPs" in some minds.)
- Partnership between 1600, 9200, V&V program
- I think this is a high-impact milestone: success may lead to future V&V funding for FY07 milestone pointing at ZX.



To Do: High Level

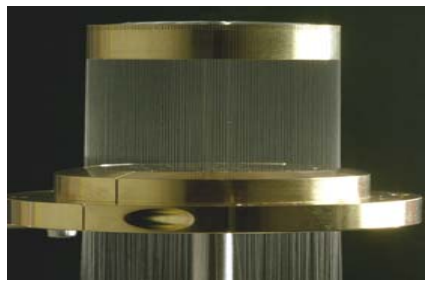
- Long-term planning (~2010) aiming at ZX
- Specific validation tests centered on:
  - External, less-integral experiments (choice in progress)
  - Z-machine integral experiments
    - Magnetic flyers
    - “Bare” pinch implosions
    - Dynamic hohlraum implosions
- FY05 will culminate (hopefully) with ZR predictions
  - ZR only starts operation in FY06
- Followed by FY07 milestone funded by V&V (hopefully)



My role:

- Greybeard for V&V methods to the team
  - Information gathering exercise in progress
  - V&V plan (aiming at ZX) by end of Q3
  - Code suitability information by end of Q4
- Rad-hydro expertise as needed
  - Mainly consulting
- Represent Pilch

This is all new (i.e. in addition to my existing work) as of February.



Prediction: Current Thinking

(Mainly arising out of our MICS project)

- Emulators – Baby Steps to Prediction
  - Approximations to “real” models (?)
- Understood basis for doing UQ, sensitivity analysis, optimization
- How selected?
- How applied?
- What are the limits on prediction with these things?

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Case 1: Approximating the real model

- **Model (Code):** $M\left(\vec{p}\right)$ **Emulator:** $M_E\left(\vec{p}_E\right)$
- **"Data" – benchmarks (V&V)**
- **Emulator chosen to optimally mimic performance of code on the data.**
- **One goal is to have an emulator that evaluates rapidly. This facilitates multi-evaluation applications (sensitivity analysis, optimization, uncertainty quantification)**
- **Straightforward calibration neglects model uncertainty, calibration under uncertainty doesn't.**
- **Gaussian process view: select emulator from a parameterized class via a stochastic process methodology. Bayesian updating improves the choice (Laura Swiler discusses her current work on this).**
  - **Why update? Reduce variance (for example) of emulator calibration;**
  - **Variance is measure of uncertainty; reduced variance implies increased "predictive confidence" (smaller confidence intervals for instance).**

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Case 1: Approximating the real model Cont

- **“Good Emulator” facilitates UQ because of probabilistic fidelity (WE HOPE!).**
- **“Emulator” – the word “surrogate” is typically used in optimization.**
  - **“Prediction” is then associated with “multi-fidelity” optimization.**
- **“Emulator” can be a regularization of an ill-posed inverse problem.**
  - **Use of Bayesian methods mentioned in Sabatier (2000), for example.**
  - **E.g. potential link to the source inversion problems of current interest to us.**

Case 2: Approximate the error in the real model

- Evaluating $M\left(\vec{p}\right)$ on benchmarks provides an "error field" $D\left(\vec{p}\right)$
- An interesting approach is to emulate the error field instead of the code: $D_E\left(\vec{p}_E\right)$
  - Provides a ***prediction*** of error
    - E.g. mesh dependence (if people would study it)
    - E.g. Validation domain extrapolation
  - Notice mechanistic requirements of emulation still hold – it is expensive, maybe impossible, to evaluate error of the code over an application domain.
  - Opportunities for advanced mathematical type thinking (Igusa and learning theory)
  - Note if code is "appropriate" we should expect the error field to be rather featureless compared to the code; this provides some basis for accepting the strong assumptions made in the CUU literature we have been studying.

Case 2: Approximate the error in the real model Cont

- Necessary condition for extension of reliability theory to quantifying model quality .
  - Existence proof – temporal reliability theory for software (Poisson process prediction of “bug” statistics).
  - But “faults” are different for scientific software; assumed stochastic process should also be spatial.
  - How to characterize “faults” is a big issue
    - Legal requirements in NRC and WIPP
    - Physics labs – designers specify
    - Sandia – less information from DP about accuracy requirements for models – we are different. ☹
    - Z-pinch milestone offers rich laboratory for investigating this.

Case 2: Approximate the error in the real model Cont

- Baby steps in the W80-3 validation milestone (maybe other milestones) provide opportunities too:
  - Error field summarized by simple analysis and statistics.
  - No real construction of emulators (but need is evident in my opinion)
    - Possible application of Laura's current work…
  - Some success in thermal.
  - Some success in mechanical.
- LANL trying to deal with this on their FY04 Level II milestone.
- The world is moving in this direction.

Case 3: Reduced Order Models – Pure Speculation

- Exciting – but just starting to think about this (and learning from Scott Collis)
- Opportunity: where does the "uncertainty" enter in?
  - Existence proof: Chorin's methodology for selecting "optimal" (reduced order) models using Gaussian processes and maximum likelihood (?) in turbulence theories.
  - Example question: how is Chorin's methodology related to a technique like Variational Multiscale Method (?)
- The world is moving in this direction.

Service:

- DOE Physics Lab reviews
  - FY03 Burn Code Review – Wrap Up ("We don't need no stinking reviews.")
  - FY04 Level II milestone review team for LANL ESA validation milestone
  - Invitation to participate on new "Predictive Science" (?) review panel for LANL and LLNL; details in progress.
- Wrapped up SEPR SEG duty:
  - Resource analysis process completed and published (being used as model in current DOE exercise)
  - Software lifecycle analysis no longer my concern!
- Giving high priority to requests for help in 9200 (MICS; planning; brainstorming; proposals)
- Guest editor chores almost complete (continuation from last year)