

Code Validation as a Reliability Problem

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A Bayesian definition of code Validation?

The process of increasing our subjective degree of belief in the results of a single calculation, or of a set of calculations.

- “Subjective” does not mean “arbitrary”
- “Belief” does not equal “imagination”

Compare this to how the ASCI V&V program actually defined code Validation.

The process of determining the degree to which a computer calculation is an accurate representation of the real world.

•The V&V “vision” was stated as follows:

“Establish confidence in the simulations supporting the Stockpile Stewardship Program through systematic demonstration and documentation of the predictive capability of the codes and their underlying models.”

Following a thought of Easterling, consider the scheme:

My degree of belief goes way up if the following quantity is “small”:

$$\mathbf{e} = \mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3$$

$$\mathbf{e}_1 = \langle \mathbf{y}_{\text{nature}} - \mathbf{y}_{\text{experiment}} \rangle$$

$$\mathbf{e}_2 = \langle \mathbf{y}_{\text{experiment}} - \mathbf{y}_{\text{calc}} \rangle$$

$$\mathbf{e}_3 = \langle \mathbf{y}_{\text{calc}} - \mathbf{y}_{\text{exact}} \rangle$$

$\mathbf{y}_{\text{nature}}$ is “reality”;

$\mathbf{y}_{\text{experiment}}$ is what we “measure”;

$\mathbf{y}_{\text{exact}}$ is the exact solution of the model;

\mathbf{y}_{calc} is the code solution of the model;

The terms suggest a general norm used to assess differences

Making e_3 “small enough” is the verification problem:

- **Relying upon the mathematicians to tell us what the exact solution is probably won't work.**
- **Relying upon numerical analysis to tell us exactly what the normed difference is probably won't work.**
- **Uncertainty quantification is part of the solution of this problem.**

Making e_2 “small enough” is the “practical” validation problem:

- **The ideal validation problem is to compare the experimental data with the exact model result. We can't do that in any case anybody care's about.**
- **The “practical” approach looks like it really works as long as you have also done the verification problem.**
- **Ergo, verification and validation are strongly coupled. This is not exactly a revelation.**
- **Uncertainty quantification is part of the solution of this problem.**

Making e_1 small enough is beyond our scope.

- The problem is real. Think about the enhanced surveillance program.
- We know that a high quality interaction between codes and experiments can lead to reduction in the size of the difference between “reality” and “experiment.”
- Uncertainty quantification is part of this problem. It is highly subjective in frontier experimental sciences (high energy physics, for example).

The obvious conclusion is -

**Uncertainty quantification
is important for validation.**

We seek to validate multi-physics codes.

Multi-physics often implies general purpose.

General purpose implies that users are a huge component in “correct” application of the code. Code validation does not address user error per se, but we still need to worry about it.

Multi-physics also often implies research models are present.

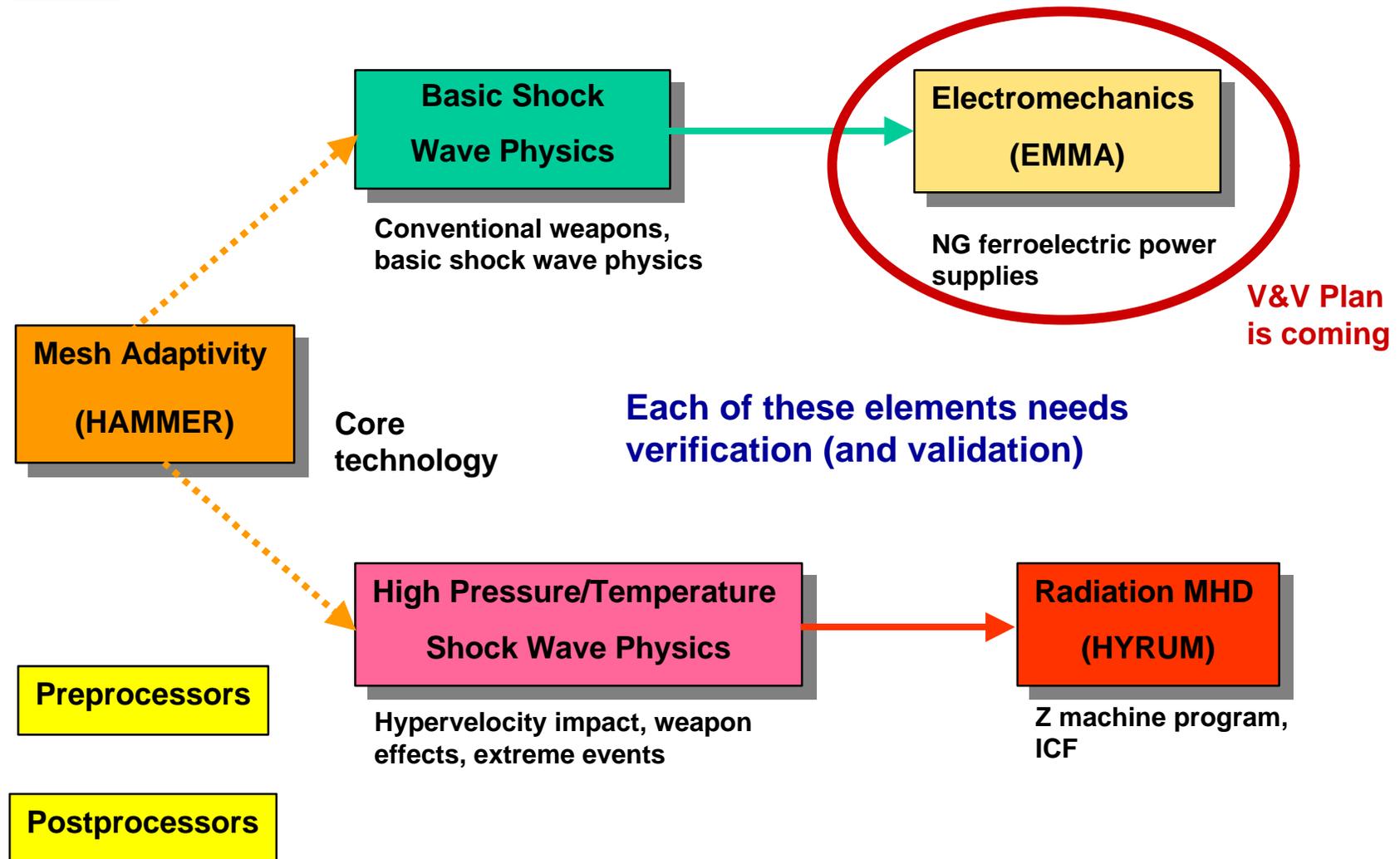
An example is the Sandia code ALEGRA:

3-D multi-material Arbitrary Lagrangian Eulerian Radiation-MHD shock wave physics code

C++ (150000 lines) + MPI + C + Fortran, etc. (1,000,000 total including special libraries)

Under development

Example: ALEGRA is a multi-physics code.



Do we need validation “science”?

"...we never (least of all in science) draw inferences from mere observational experience to the prediction of future events. Rather, each such inference is based upon observational experience...plus some universal theories..."

Karl Popper, Objective Knowledge

What is “uncertainty quantification” and why do I care?

Uncertainty quantification: an anti-reductionist measure of “error”.

The forward prediction problem:

Characterize the “input” uncertainty (stochastic, fuzzy, etc)

Propagate this uncertainty through the code

Characterize the resulting output uncertainty

Refine this characterization via comparison with data

Develop “code reliability” metrics and statements (need requirements)

(Most of this is not rocket science for an initial implementation.)

Now follow it with backward prediction:

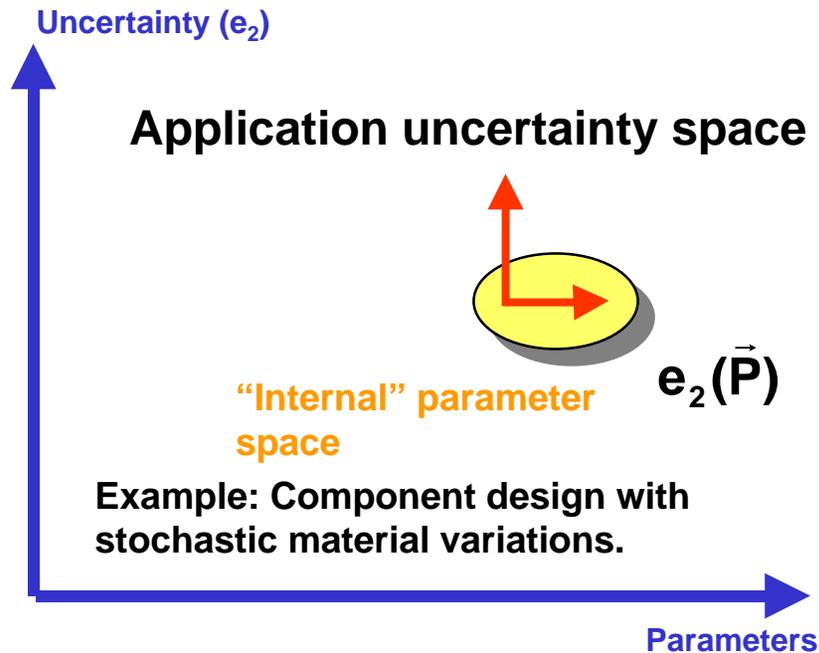
Reduce the code uncertainty via the output uncertainty characterization (Bayesian?).

(This IS rocket science.)

Now optimize:

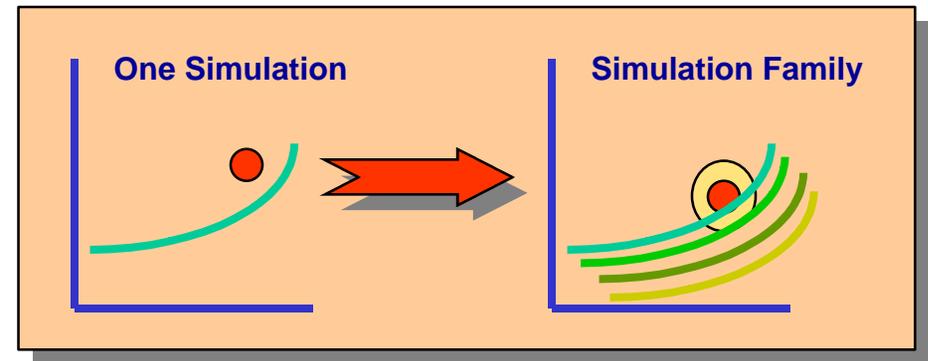
Perform forward/backward prediction sweeps to increase “code reliability” and guide new experiments.

Local validation begins with local uncertainty quantification, a high dimensional problem.



Local uncertainty quantification performs systematic studies of code uncertainty from stochastic treatments of parameter uncertainty. U is a random variable, P is a random vector.

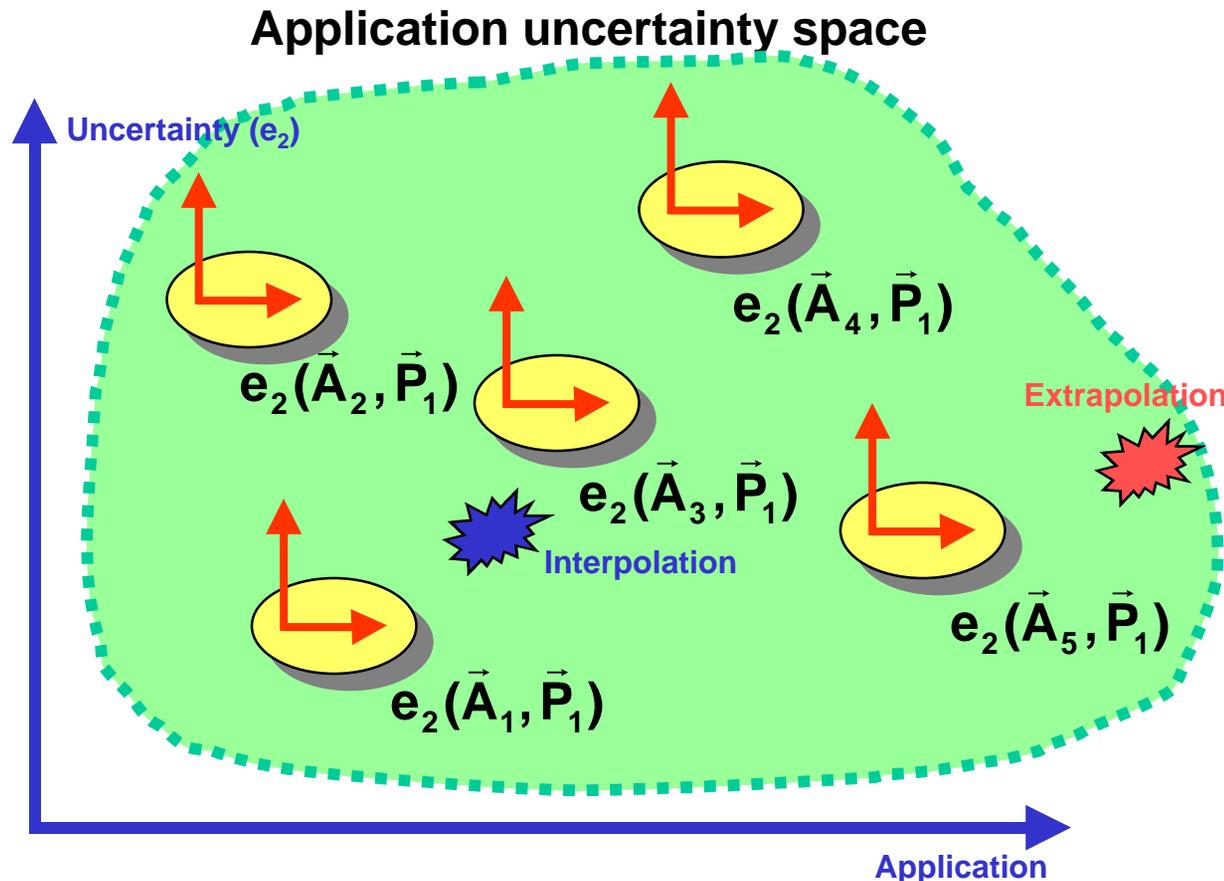
Notice that how uncertainty U is defined is an issue.



Alternatively, think of results being replaced by probability distributions of results. Then, do response surface methods, or other things, to characterize the result family stochastically. The most important issue is this characterization.

The number of parameters can be enormous - *parsimony* is hoped for (but unlikely?).

“Global” validation leads to global uncertainty quantification, an even higher dimensional problem with “internal” and “applications” parameters.



Uncertainty has two components:

“Local” - uncertainty quantification and local data comparisons.

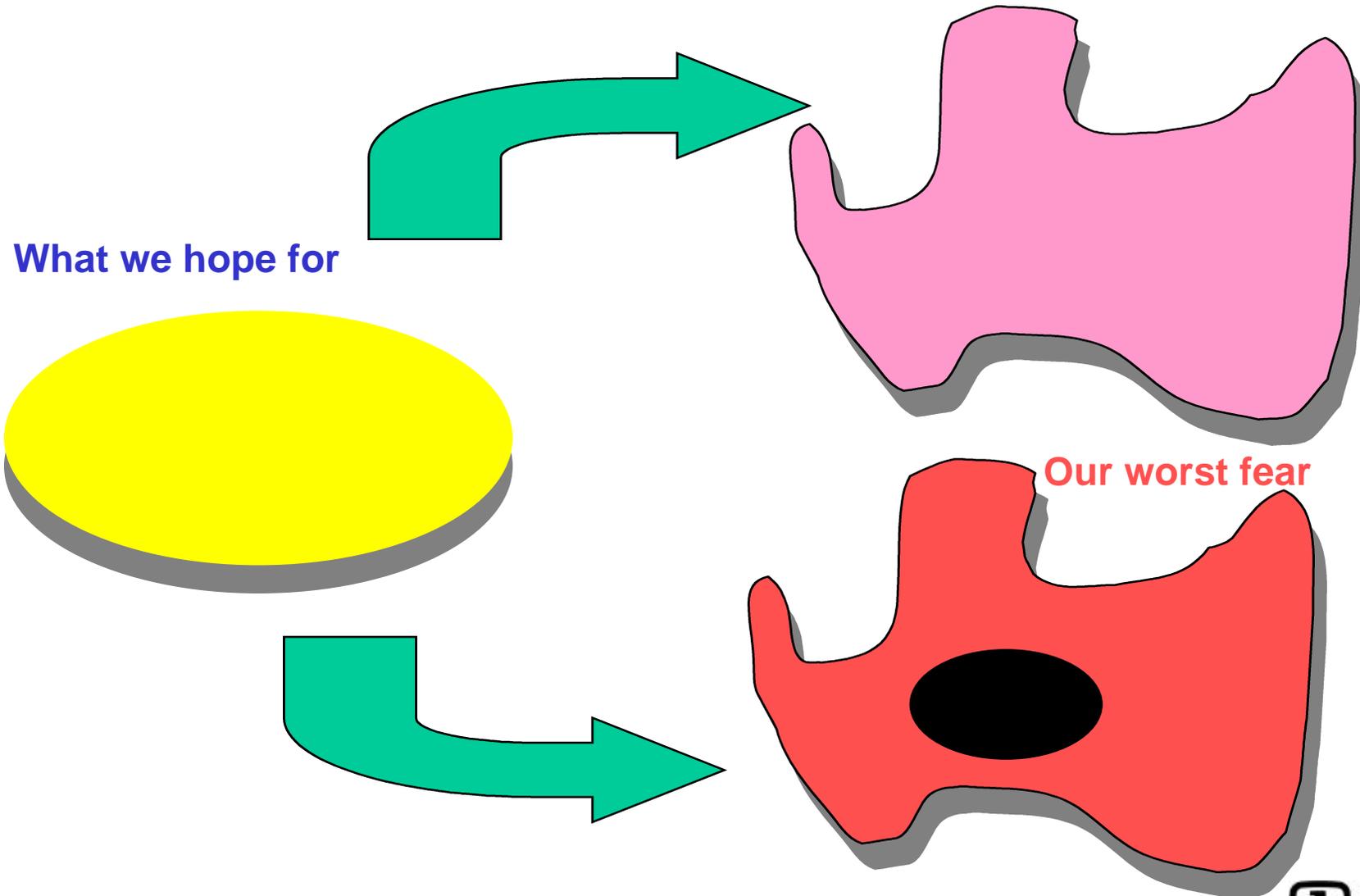
“Global” - system scale uncertainty quantification and global data comparisons.

Can we use spatial statistics methods (like kriging) to characterize $e_2(A,P)$?

Note that we have simplified the problem by assuming that the internal parameter functional dependence is constant over application space. Is this true?

Example: NIF ignition capsule design confidence levels based on uncertainty quantified NOVA design calculation experience.

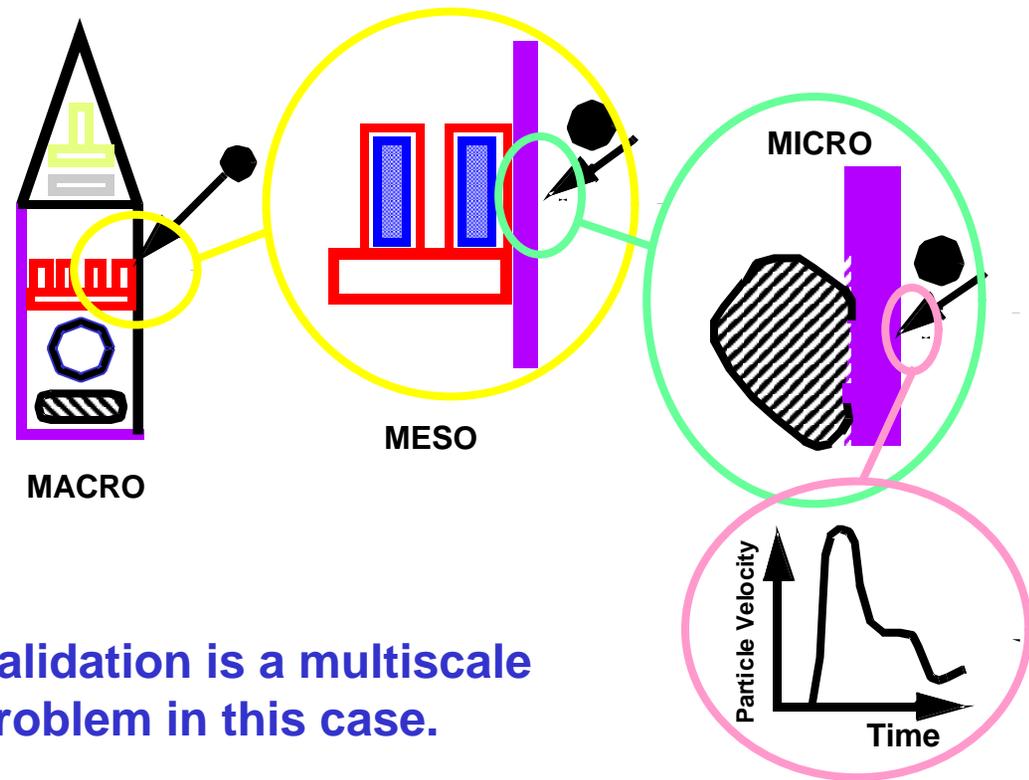
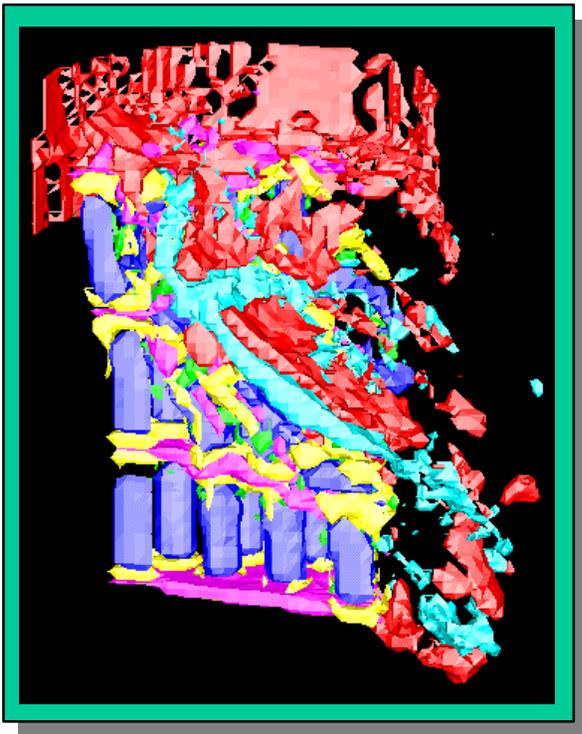
“Uncertainty” probably looks a lot more complex than suggested by the previous figures.



Example - Hypervelocity Impact

Missile defense simulations provide an excellent application for studying predictive complexity.

There are at least six stochastic parameters to begin with: the hit point and the engagement velocity

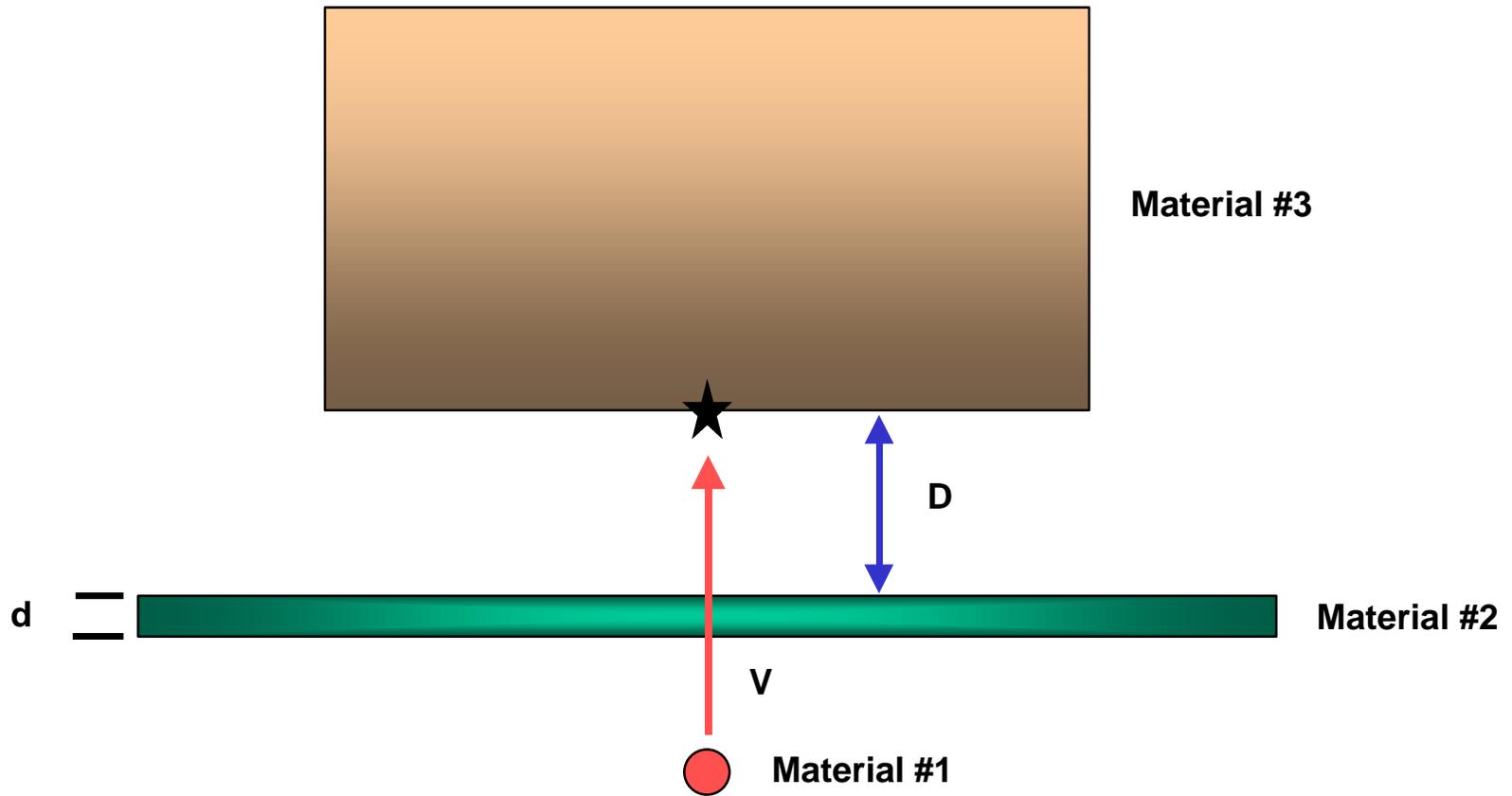


Validation is a multiscale problem in this case.

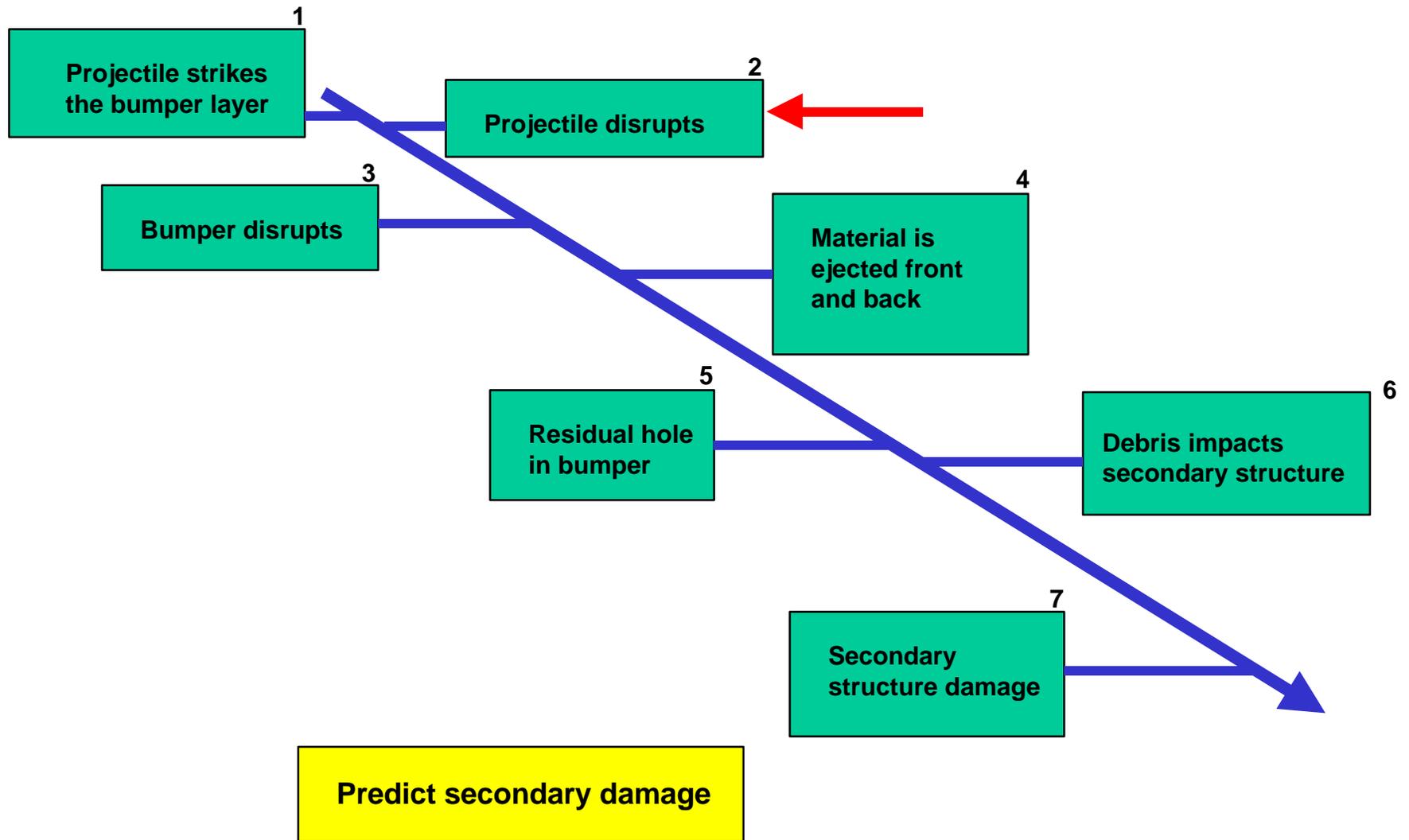
The necessary information is a mix of qualitative and quantitative.

“Validation data”.

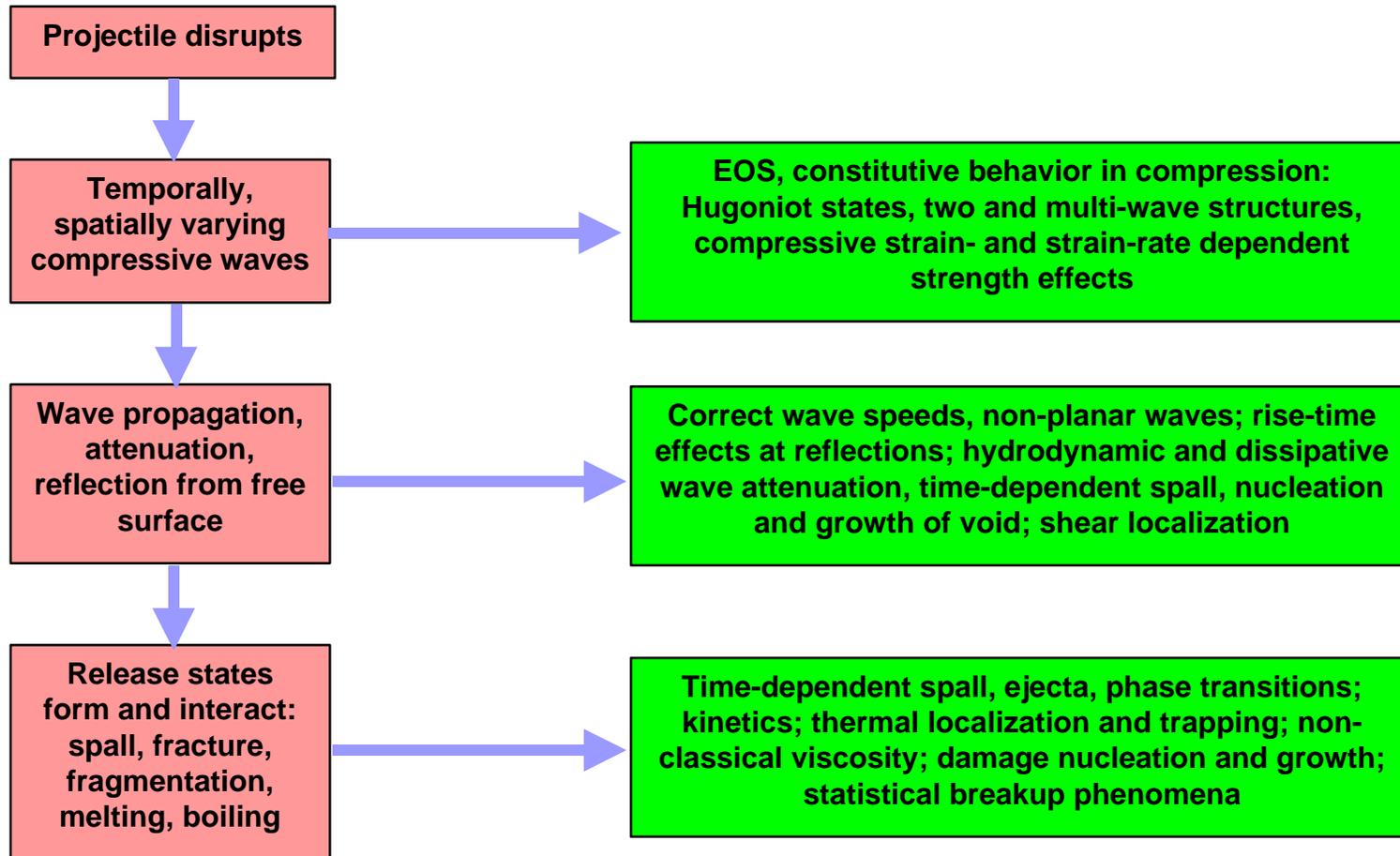
Consider validating the microscale with laboratory hypervelocity impact experiments.



Levels of phenomenology at the microscale:



Further levels of phenomenology in this experiment:



The parameter space for these experiments:

“Experimental” parameters:

- Impact location (2)
- Velocity vector (3)
- D, d (2)
- Projectile geometry (1)
- Materials (none)

Total = 8

“Internal” parameters:

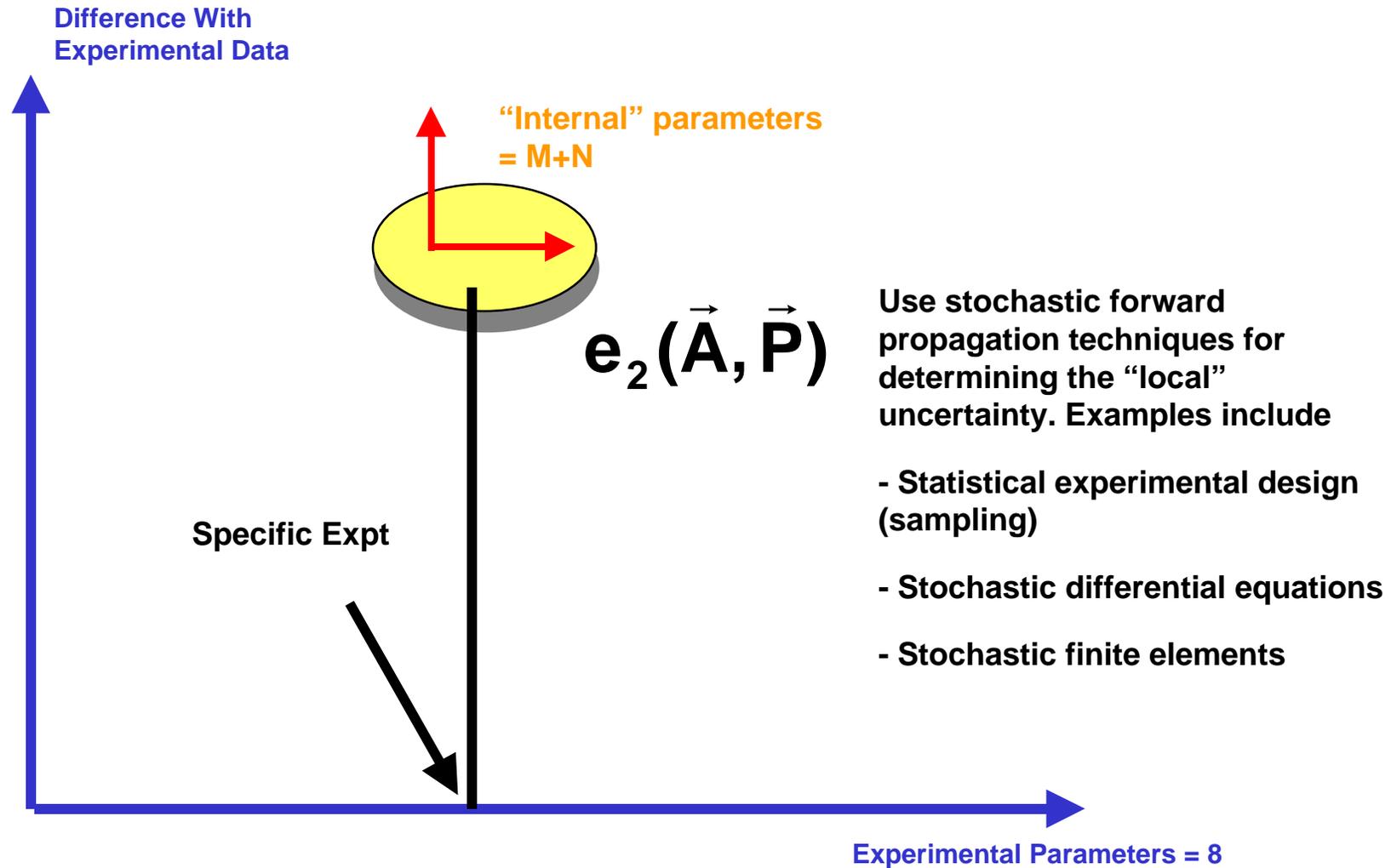
- Hydrodynamic parameters (H)
- Material Models (M)

Total = H+M

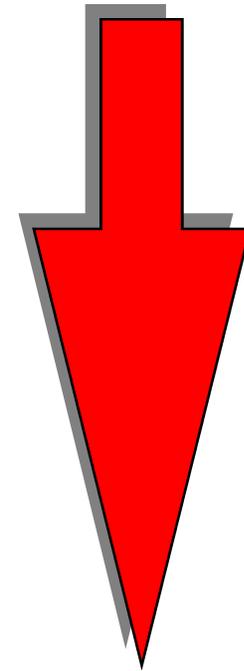
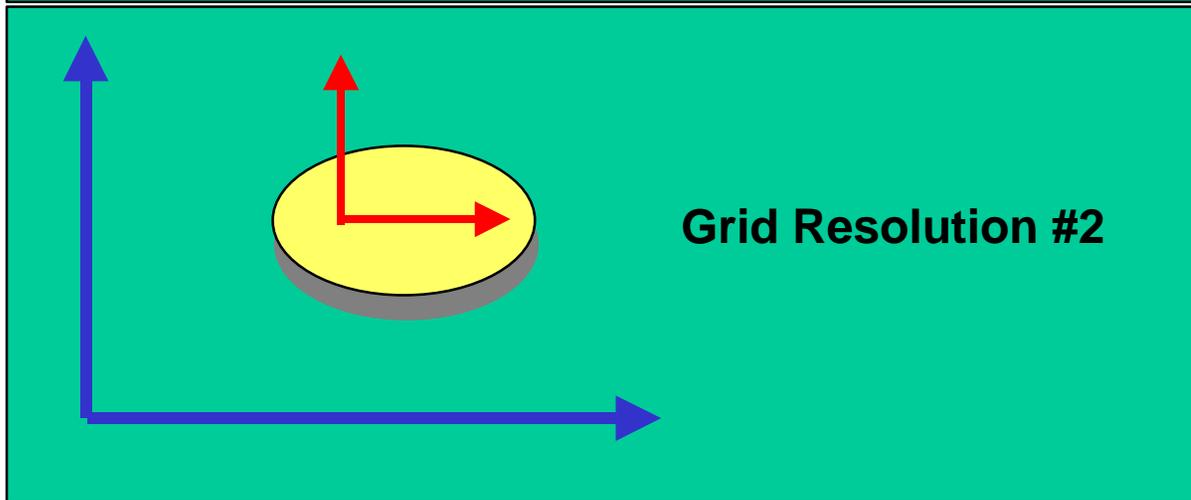
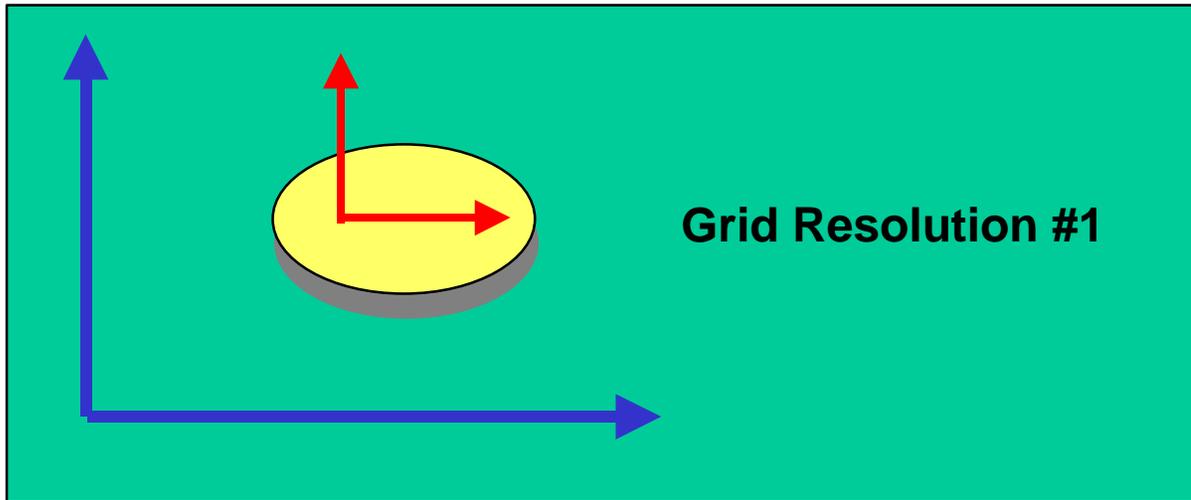
“Uncertainty” Metrics:

- Time-resolved data in witness material (PVF gauges)
- Time- and spatially-resolved debris cloud data (radiography)
- Target recovery and inspection

Parameter versus uncertainty space



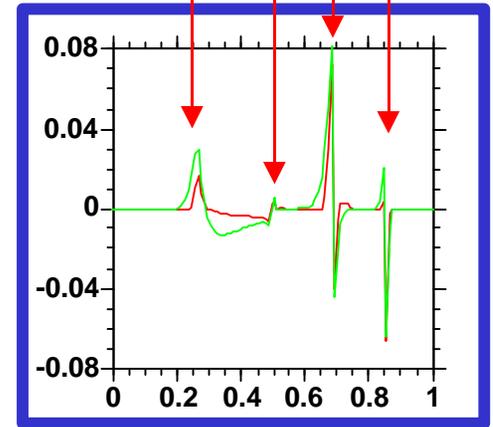
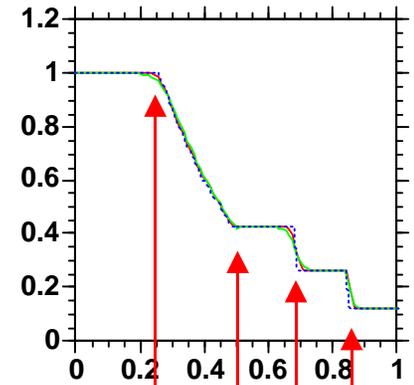
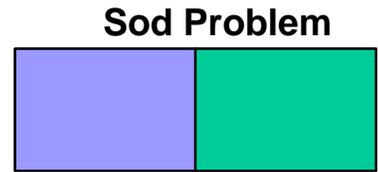
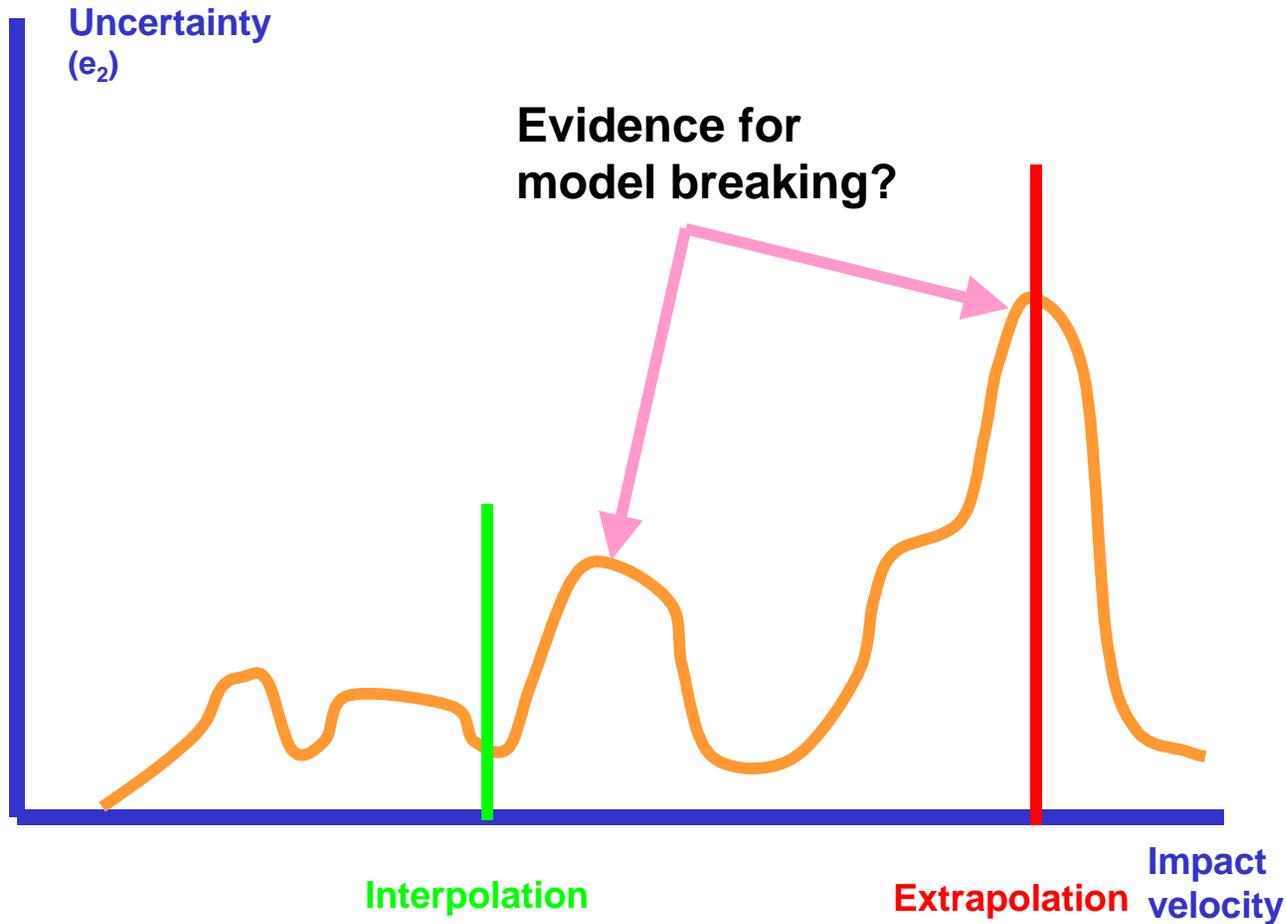
One way to worry about grid resolution:



Increasing grid resolution

Increasing grid resolution does not mean uniform refinement (ALE, adaptivity, geometry constraints). Algorithm parameters controlling dynamic grid resolution are included in the internal parameters.

A thought experiment: projecting the uncertainty



Thanks to Kamm and Rider

Some speculation and reasonable opportunities for research: Uncertainty as a spatial random field

I. Let the uncertainty be represented by a $(M+H+8)$ dimensional spatial stochastic process

For example, we end up worrying about properties of something like the variogram:

$$\text{var}[e_2(\vec{A}_j, \vec{P}_j) - e_2(\vec{A}_i, \vec{P}_i)] = 2\gamma((\vec{A}_j, \vec{P}_j) - (\vec{A}_i, \vec{P}_i))$$

Then, we can develop predictors for U at other points, such as the BLUP (**Best Linear Unbiased Predictor**):

$$\hat{e}_2(\vec{A}_0, \vec{P}_0) = \sum_{i=1}^n \lambda_i \hat{e}_2(\vec{A}_i, \vec{P}_i)$$

Or (μ = mean of random field, S = fine structure, and ε = “measurement error”):

$$\tilde{e}_2(\vec{A}, \vec{P}) = \mu(\vec{A}, \vec{P}) + S(\vec{A}, \vec{P}) + \varepsilon(\vec{A})$$

Comments:

See J. Sacks, W. J. Welch, T. J. Mitchell and H. P. Wynn (1989), “Design and Analysis of Computer Experiments,” Statistical Science, Vol. 4, No. 4, 409-435; N. Cressie (1988), “Spatial Prediction and Ordinary Kriging,” Mathematical Geology, Vol. 20, No. 4, 405-421.

Do we need another framework other than probability to do this?

What is the appropriate way to partition this random field among the experimental parameters and the internal parameters? Does this question even make sense?

What structure do we require on the projected random field $U(A,P)$ to facilitate piecing together the various uncertainties?

Speculation: Sensitivity coefficients

II. Sensitivity studies define which of the H+M+8 parameters is most important. Probabilistic evaluation of the sensitivities is of interest.

Is parsimony really true?

Does the sensitivity structure projected onto the internal parameter space remain invariant as the experimental parameters alone vary? If no, does this imply model invalidity?

Does the sensitivity structure remain invariant over grid variations?

Don't assume that the parameters are all uncorrelated. Then we need "interaction" coefficients.

The literature on sensitivity analysis is huge. See M. D. McKay (1995), "Evaluating Prediction Uncertainty," Los Alamos Report, LA-12915-MS for one important approach.

Speculation: Model calibration

III. Some understanding of U should lead to improvement in the model. “Calibration” reduces U locally in the application space by optimizing the internal parameters.

How does the calibration vary with the experimental parameters?

Comments:

A Bayesian approach can be applied to the formal study of improving model uncertainty in the presence of parameters derived via comparison with experimental data. See, for example, K. M. Hanson (1998), “A Framework for Assessing Uncertainties in Simulation Predictions,” Los Alamos preprint.

Statistically rigorous comparisons between uncertain calculations and uncertain data with the intent of providing code validation are the subject of a recent tutorial report by R. G. Hills (1998), “Statistical Validation of Engineering and Scientific Models: Background,” Sandia National Laboratories Contract Report.

This question also leads to the use of “surrogates” for studying parameter calibration, as well as other optimization questions associated with code uncertainty. Consider the important work A. J. Booker, et al (1998), “A Rigorous Framework for Optimization of Expensive Functions by Surrogates,” Boeing Shared Services Group Report, SSGTECH-98-005.

Other papers that the reader might find of interest are D. D. Cox, J. Park, and C. E. Singer (1996), “A Statistical Method for Tuning a Computer Code to a Data Base,” Rice University Department of Statistics Report 96-3 and M. B. Beck (1987), “Water Quality Modeling: A Review of the Analysis of Uncertainty,” Water Resources Journal, Vol. 23, No. 8, 1393-1442.

Speculation: Structural (Model) uncertainty

IV. Is there anyway to deal with “structural” uncertainty?

A Bayesian structure can be developed for considering structural uncertainty. See D. Draper (1995), “Assessment and Propagation of Model Uncertainty,” J. R. Statist. Soc. B, Vol. 57, No. 1, 45-97.

This involves developing posteriors via conditioning over the space of models, a rather hopeless endeavor on the face of it. Additional structure might make this more feasible.

Model uncertainty is often treated in multi-physics code through the introduction of tuning parameters. If a code (sub)model is built out of sub-submodels:

$$M = \sum_j M_j$$

Uncertainty about the overall model is then treated by modifying this equation to:

$$M = \sum_j \alpha_j M_j$$

Add $(\alpha_1, \dots, \alpha_m)$ to the parameter list and proceed as before.

Speculation: Is probability appropriate for this discussion?

How do we treat “variability” in the assumed distributions on the parameters to do experimental design, sensitivity analysis, and forward propagation?

Is probability the canonical way to capture “uncertainty?”

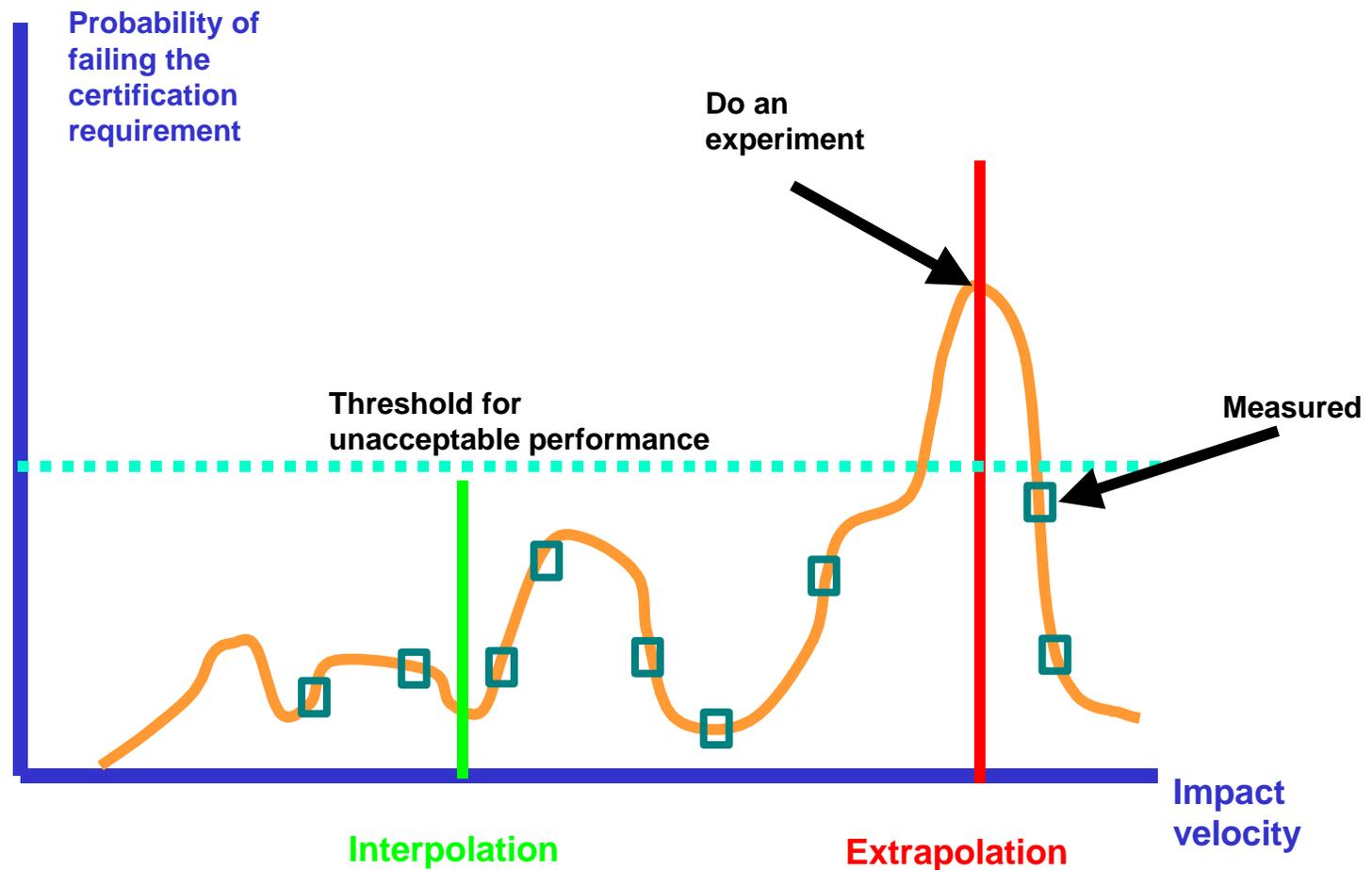
Is saying “I don’t know what the value of a parameter is” the same as placing a probability distribution on it?

We need to design validation processes to attack the weak points of codes.

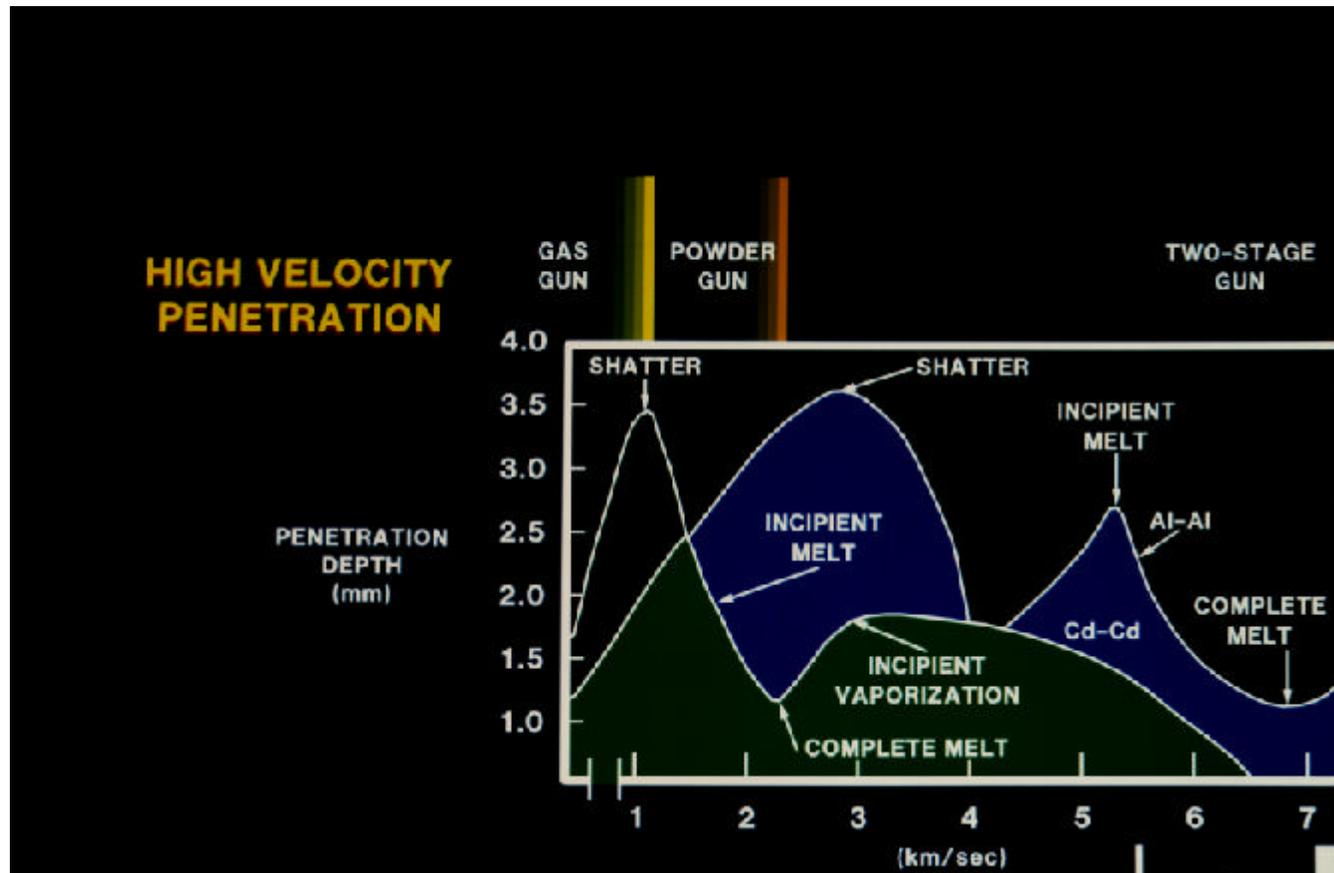
"...the theorist is interested in explanation as such, that is to say, in testable explanatory theories: applications and predictions interest him only for theoretical reasons - because they can be used as tests of theories..."

Karl Popper, The Logic of Scientific Discovery

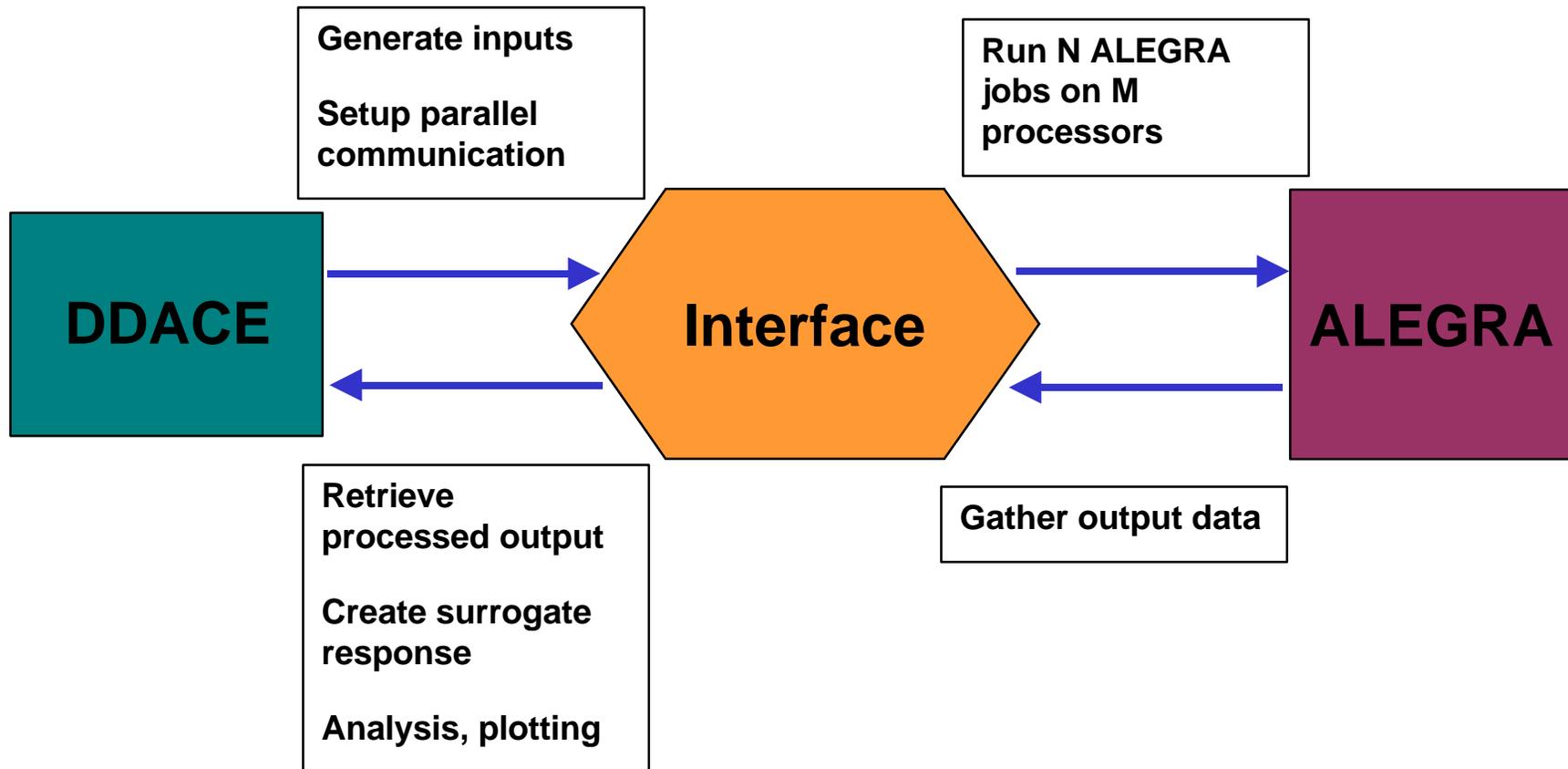
Speculation: “Certification” leads to quantitative “reliability” analysis.



There is some connection to reality here.



DOOMSDACE: Distributed Object-Oriented Software With Multiple Samplings for the Design and Analysis of Computer Experiments



DDACE - Who's doing the work (8950):

Juan Meza - manager

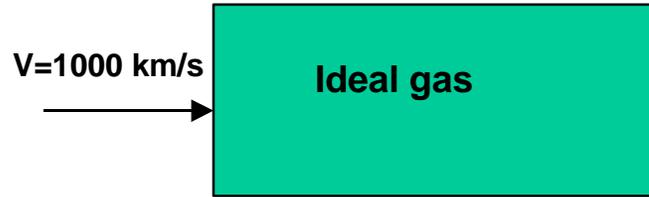
Charles Tong - project lead; DDACE development

Kevin Long - ALEGRA link and DDACE development;

Leslea Lehoucq - in ABQ; ALEGRA link and DDACE development

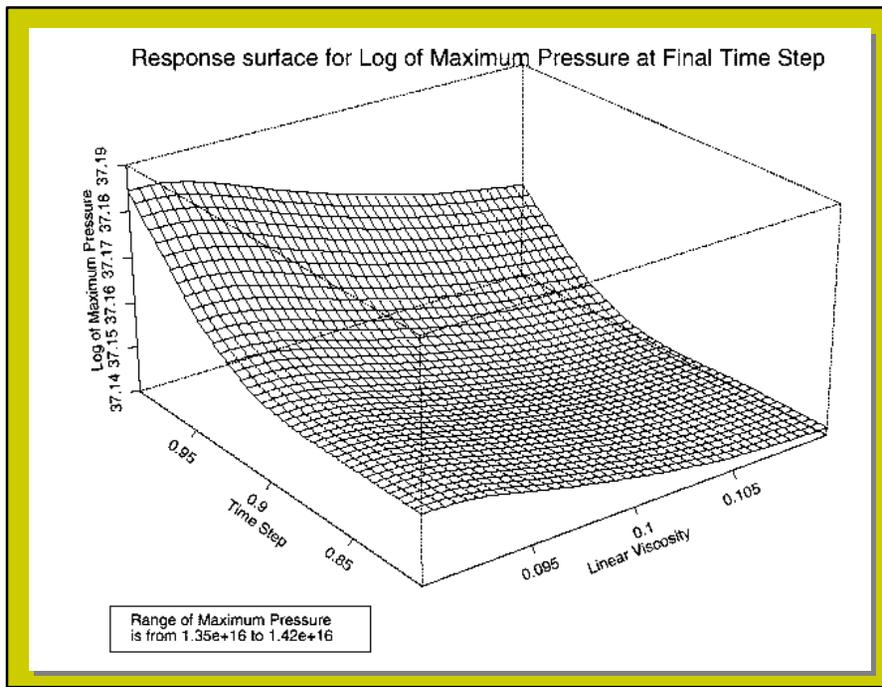
Todd Plantegenet - JAVA GUI development

Illustration of past work: 1-D “Saltzman” problem

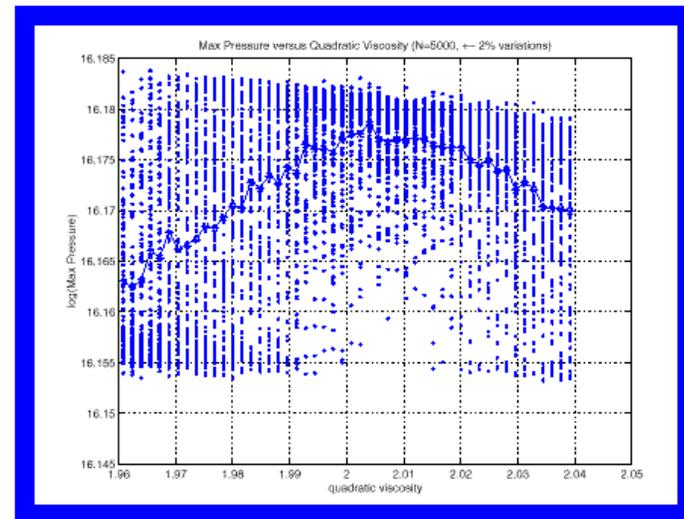


McKay “correlation ratio” analysis

Linear Viscosity	0.36
Quadratic viscosity	0.04
Hourglassing	0.02
Courant Limit	0.3

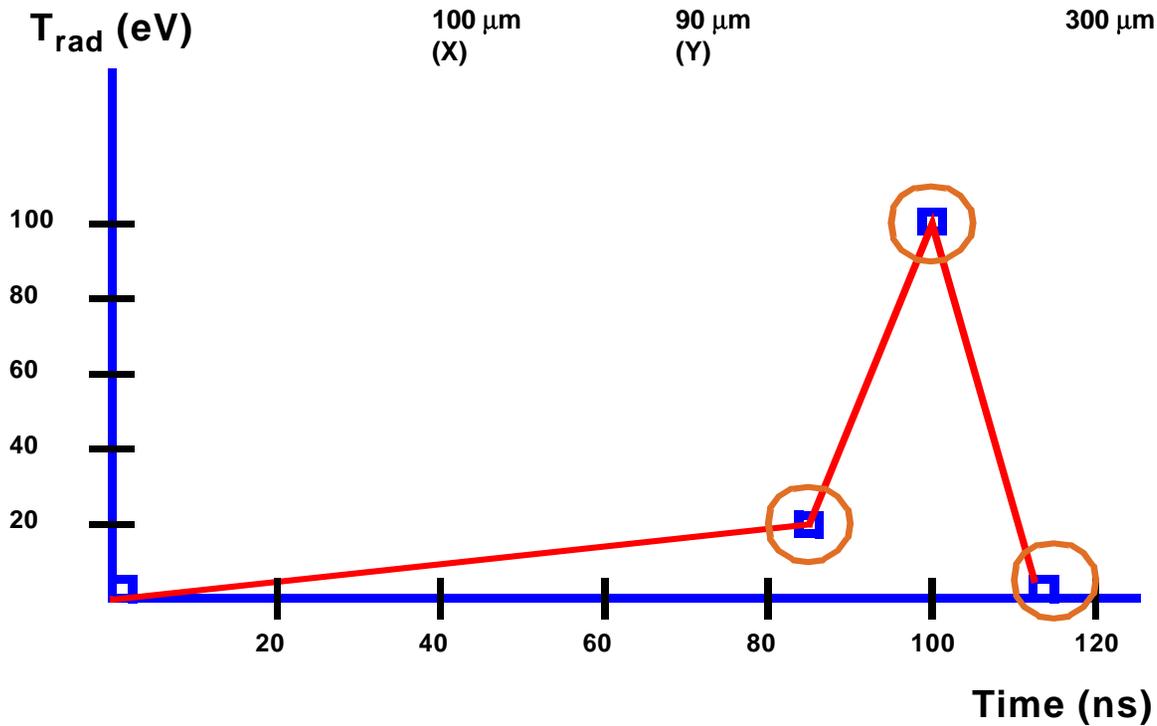
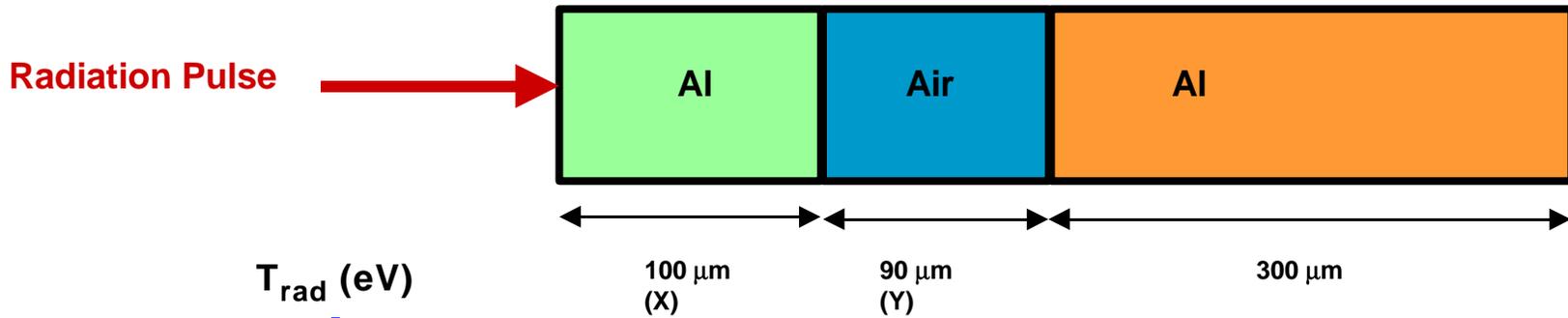


P_{max} vs quad viscosity



Response surface for log P_{max} vs linear viscosity vs Δt Courant limiting

Example: A 1-D rad-hydro calculation



Variability parameters:

Initial phase:

<u>Parameters</u>	<u>#</u>
Numerical parameters (as before): timestep, artificial viscosity (5% variations)	3
Geometry parameters: x (50-200 μm) and y (50-200 μm) (Most important parameters)	2
Material parameters: gas density (variation to be determined)	1
Radiation pulse parameters: $(t_i, T_{\text{rad},i})$, $i=1,2,3$ (10% variations)	6
Radiation algorithm parameters: ?? (to be determined)	2

Second phase - additional parameters:

<u>Parameters</u>	<u>#</u>
XSN opacity parameters: ?? (to be determined)	2-4

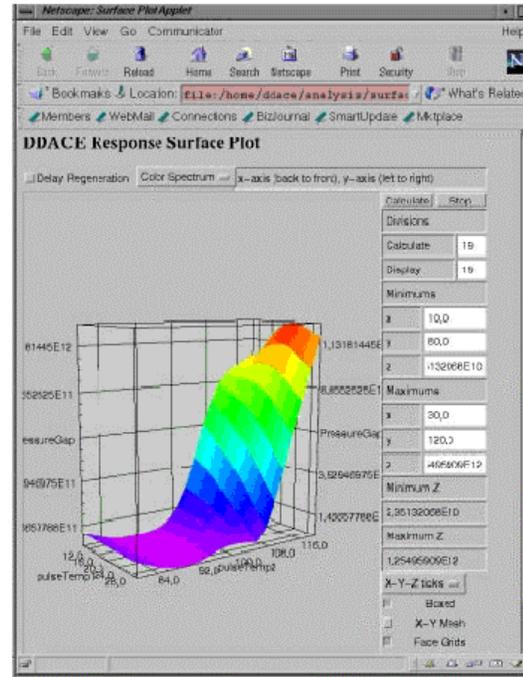
A recent design study shows what is on our mind.

Work performed by Kevin Long.

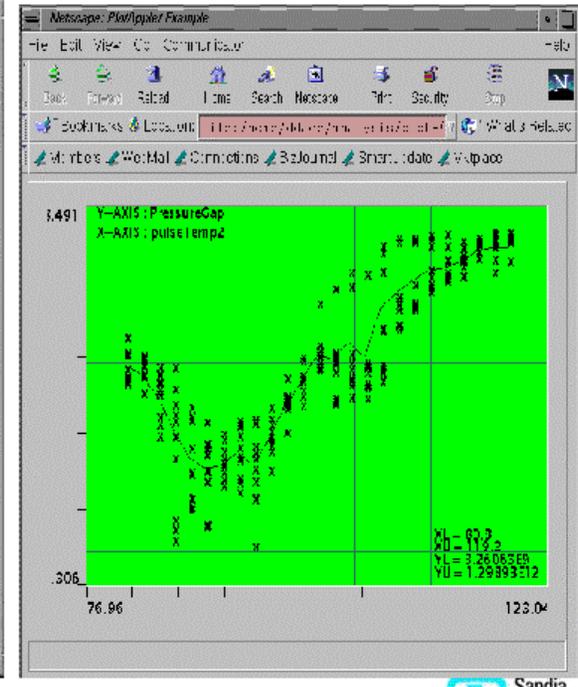
Experimental Design - 250 design points (LHS?).

Run on 32 processors of Elmo (a California SGI). Each function evaluation takes about 1/2 hour or more on the Ultra 2 in my office. You do the arithmetic related to serial running of this. Think about the scaling to 2000 processors on ASCI Red.

Six hours wall clock time for the total experiment.



Response surface construction for “quality metric” vs two pulse parameters.



“Quality metric” vs most sensitive pulse parameter.

Where we are going with DDACE?

This work is exploratory.

Aiming at exploring some “real” problems:

- Rad-hydro shock wave experimental design problems
- Neutron generator power supply problems

Test bed activities:

- Link up with Brian Rutherford’s DOE work
- Link up with Rich Hill’s work

Big questions:

- How do we make this stuff payoff for strong shock wave problems?
- How far can we push a “black-box” approach to UQ for a code like **ALEGRA**

In conclusion:

"Summary: Computers Are Here To Stay. They Endanger Thought, Language, Science, and the Survival of Man. Like Any Other Dangerous Tool, They Should Be Put Under Strict Controls."

Clifford Truesdell, "The Computer: Ruin of Science, Threat to Man" in An Idiot's Fugitive Essays on Science