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LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Uncertainty Quantification system for EOS

Ann E. Mattsson, John H. Carpenter, Allen C. Robinson, William J. Rider, Richard D. Drake
Computational Shock and Multiphysics
Sandia National Laboratories
Albuquerque, NM 87185

Bert Debusschere
Reacting Flow Research
Sandia National Laboratories
Livermore, CA 94551

E-mail: aematts@sandia.gov
Web: http://www.cs.sandia.gov/~aematts/
http://dft.sandia.gov

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NNSA National Nuclear Security Administration

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Bridges between Fundamental Law of Nature and Engineering: Science based engineering.

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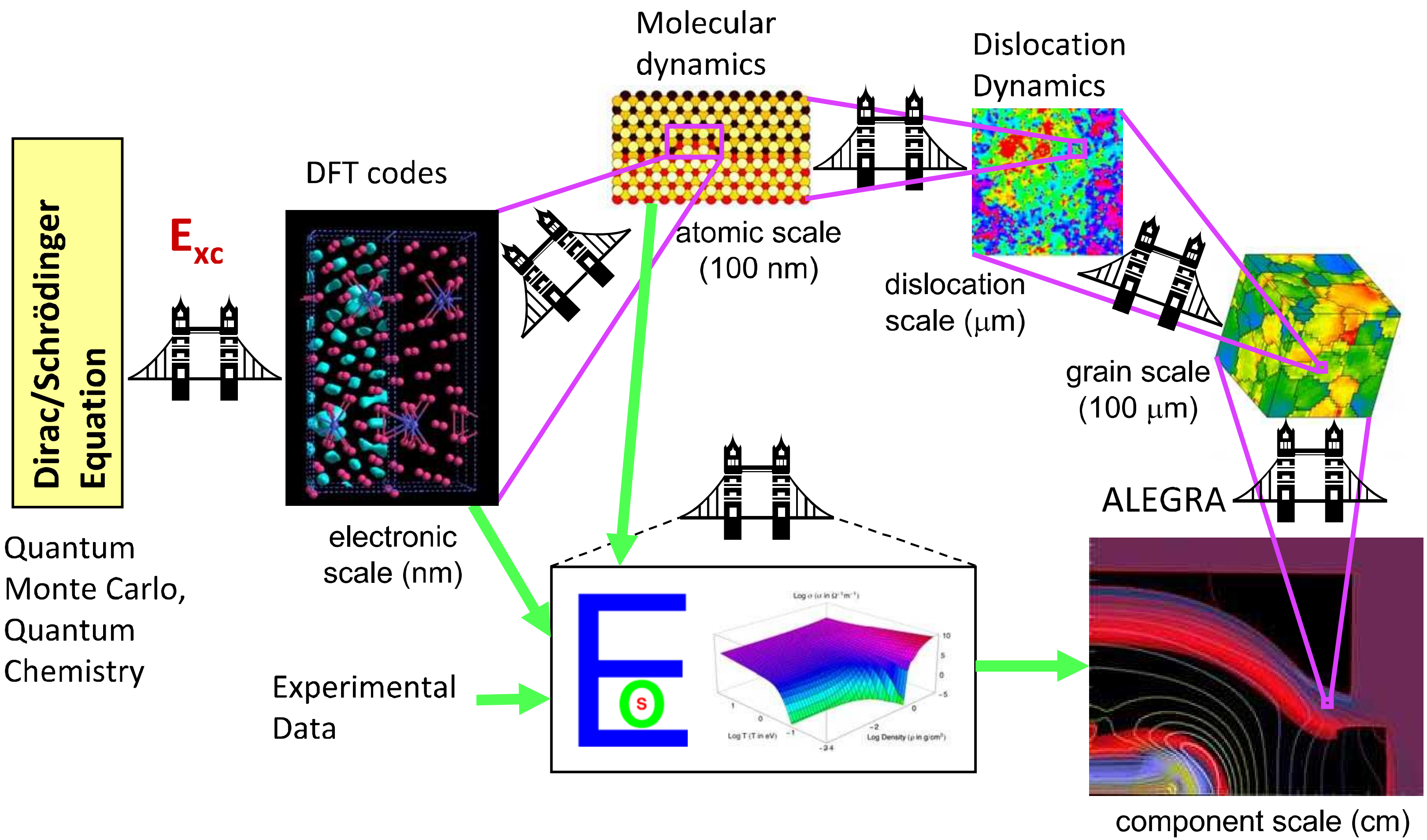

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Example: UQ in Modeling and simulation of Nuclear Energy related systems

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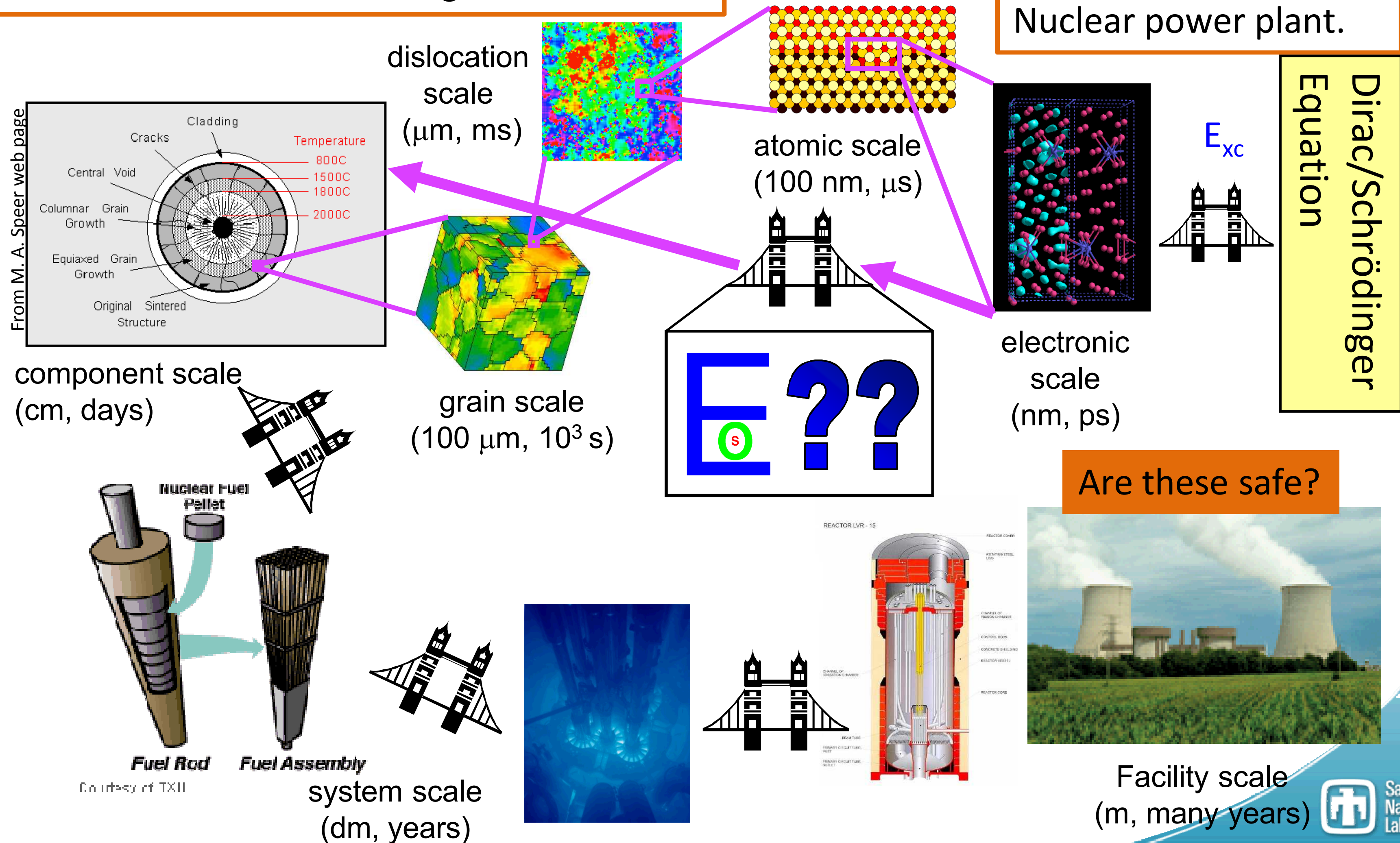
Upscaling needed. In each step, reality that cannot be modeled is resulting in error bars.

We cannot solve the Dirac Equation for the Nuclear power plant.



Uncertainty Quantification

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Will it rain tomorrow morning?
Will it be too windy?

Time	Conditions	Temp	FEELS LIKE:	HUMIDITY:	PRECIP:	WIND:
4 am	Partly Cloudy	12°	11°	72%	20%	ESE at 11 km/h
5 am	Few Showers	12°	11°	74%	30%	ESE at 11 km/h
6 am	Few Showers	12°	11°	77%	30%	SE at 11 km/h
7 am	Few Showers	12°	11°	80%	40%	SE at 11 km/h
Sunrise at 7:10 am | Upload Your Sunrise Images						
8 am	Showers	12°	11°	8[illegible]%	50%	SE at 11 km/h
9 am	Showers	13°	12°	74%	60%	SE at 11 km/h
10 am	Showers	15°	14°	67%	60%	SSE at 16 km/h
11 am	Scattered T-Storms	17°	16°	58%	60%	SSE at 21 km/h

Provide data to decision makers so that they can make good decisions.

Bridges between Fundamental Law of Nature and Engineering: UQ4Up

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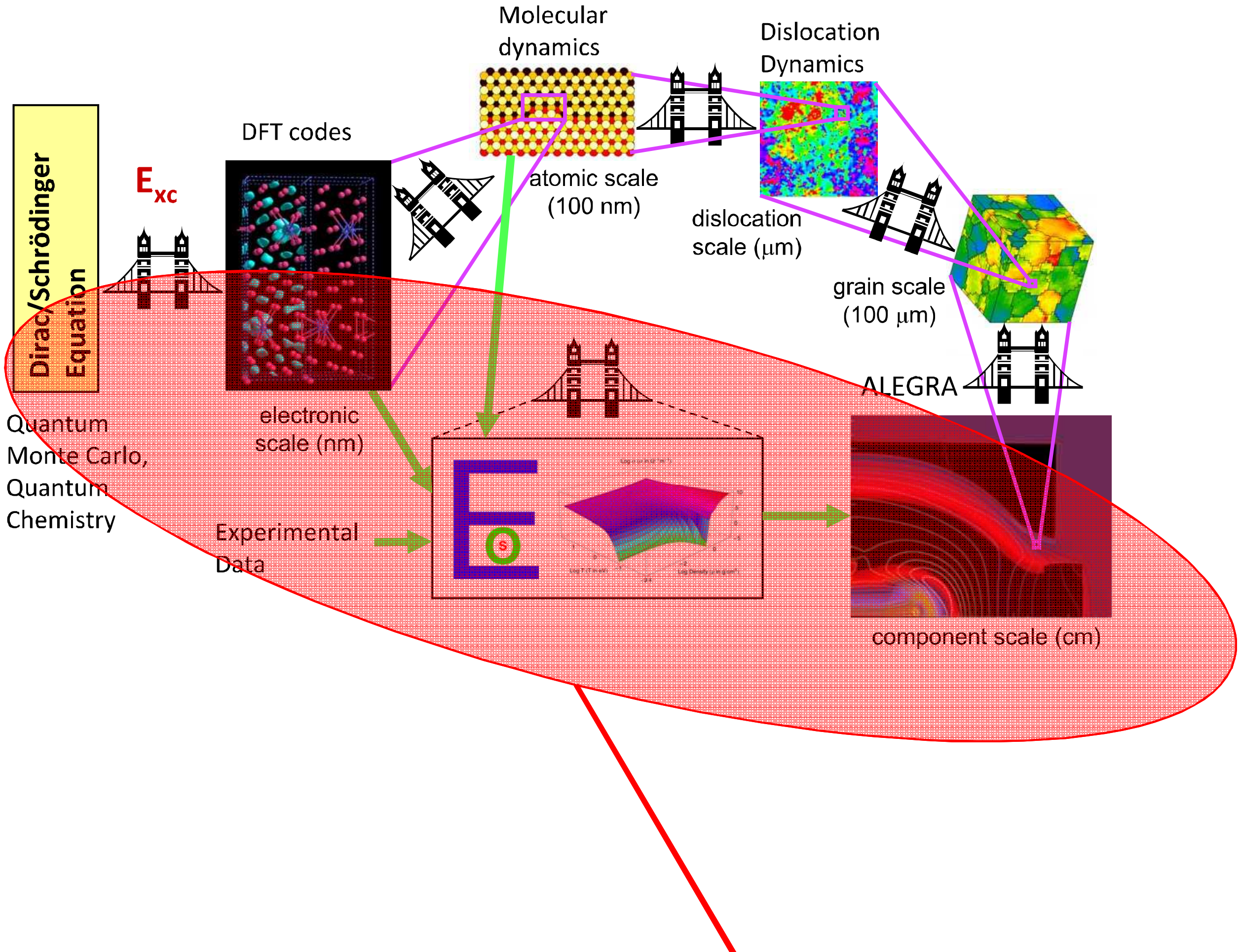

Propagating uncertainty in experimental and DFT data to the analyst using the continuum code.

Bridges between Fundamental Law of Nature and Engineering: UQ4Up

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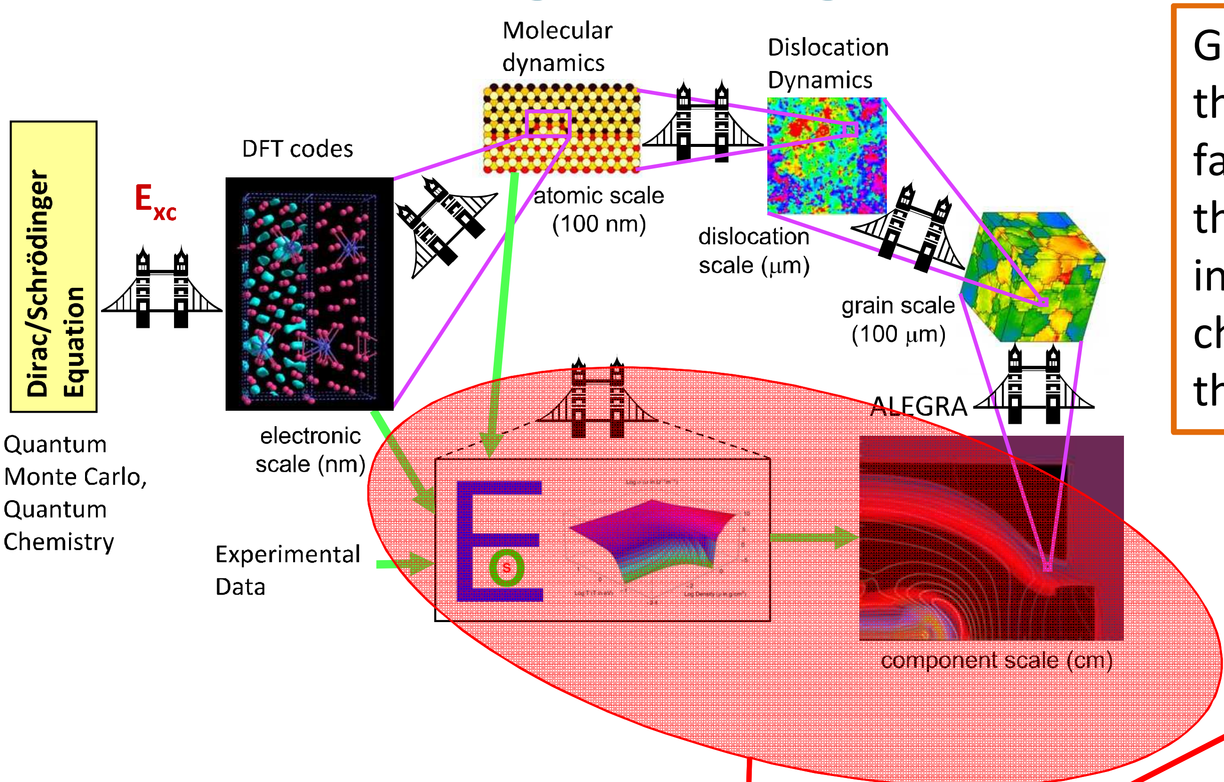
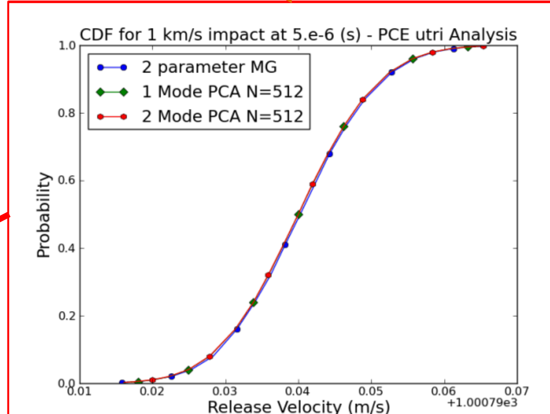


Goal: The analyst running the continuum code should fairly easily get results out that can be transformed into the equivalent of "50% chance of rain" to give to the decision maker.



First focus: Propagate uncertainty due to statistically equivalent possible EOS fits to same experimental data, to the analyst.

From data to EOS table input to hydro code

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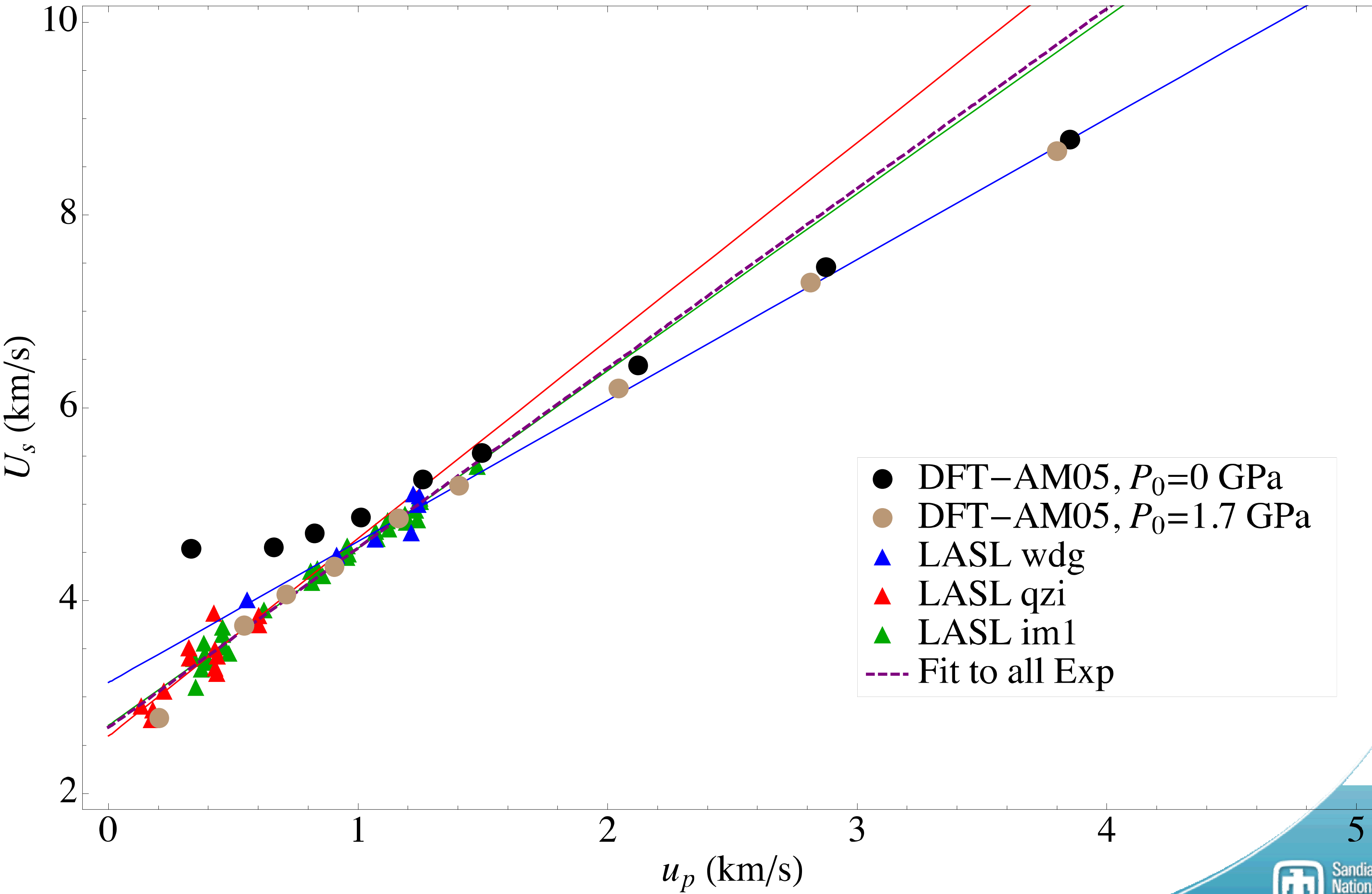
We want to build a framework that is working for the modern complex multi-phase tabular EOS input to multi-physics codes. Thus some of our solutions might look more complicated than needed for simple test problems.

Data: Experimental and calculated, with or without explicit error bars.

EOS model: ranging from single formula, such as Mie-Grüneissen, to many different models each used in one part of the parameter space (density-temperature). Number of parameters to determine by fitting to data are ranging from 1-2 to several tens.

EOS table: Is actually a set of tables. At least $P(\rho,T)$ and $E(\rho,T)$. Usually P and E from the EOS model are given on a rectangular grid of ρ and T. John Carpenter will talk much more about this later.

Data and EOS models: PETN U_s-u_p



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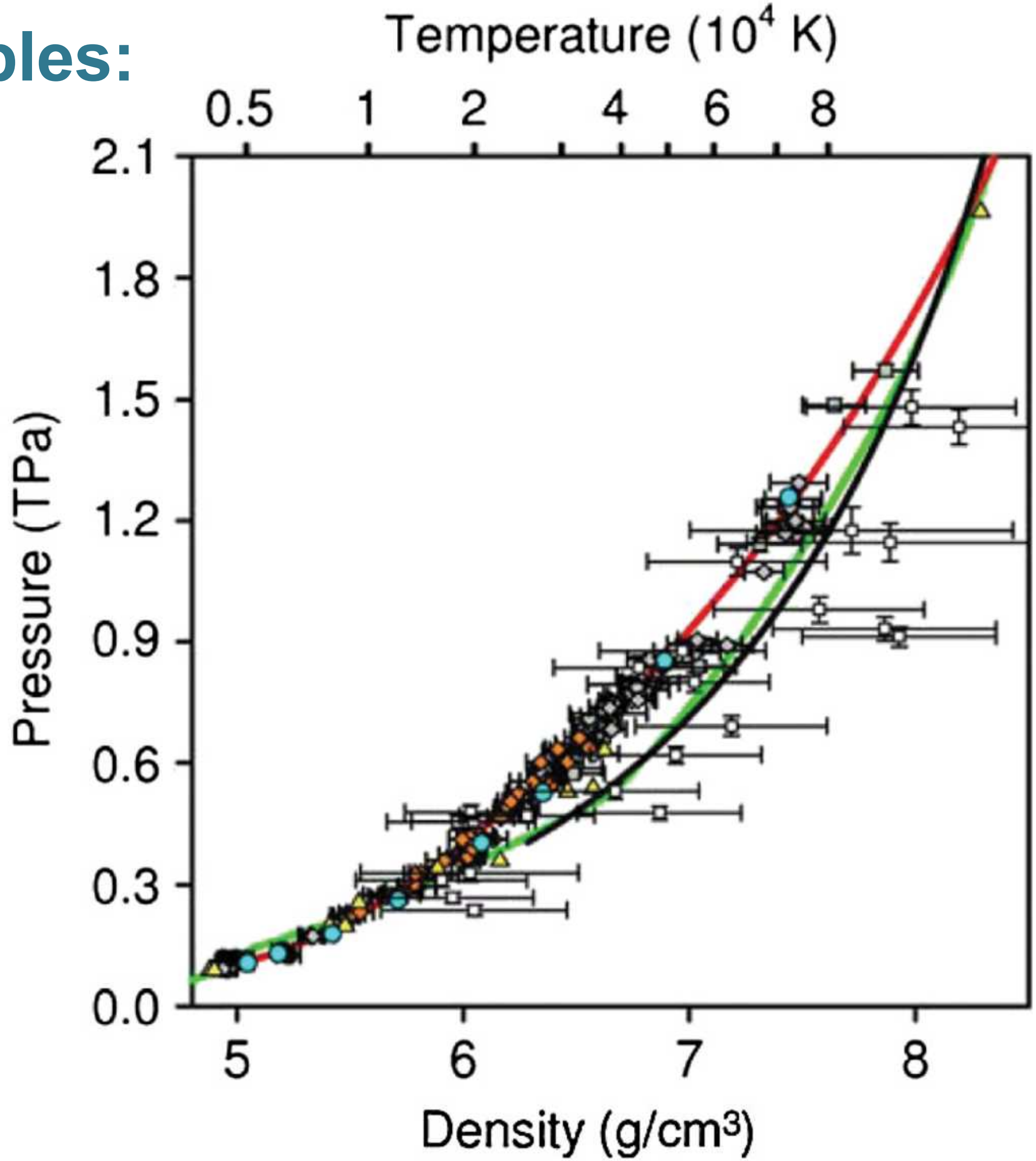
Data and EOS tables: Quartz

Quartz:

DFT AM05 (turquoise) and Z experimental data (orange and grey, small error bars) give the red line. Green line is SESAME 7360 and black line is based on LLNL data (white squares, large error bars).

What does a new Quartz standard give?



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Data and EOS tables: Deuterium experiments with the new Quartz standard

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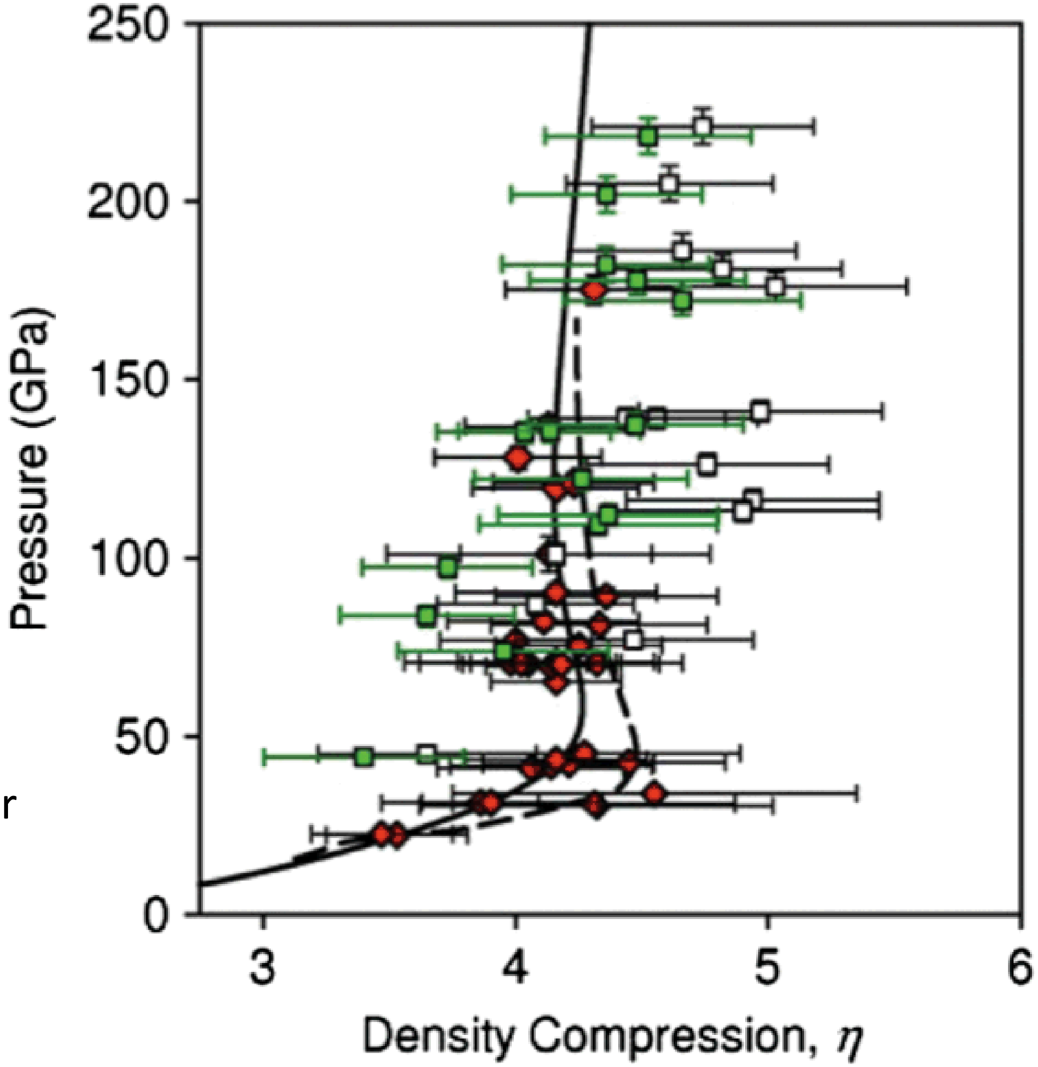
Deuterium:

White squares are LLNL laser data, which corrected with new quartz standard give green squares, much closer to red Z data and Sandia developed DFT based EOS (black dashed line). Black line is 2003 Kerley EOS.

Solves decade long controversy on why laser data was too soft.



From data to continuum output

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1) Data has error bars.

2) These error bars determine the probability that sets of specific values for the parameters in the EOS model is representing the data.

3) This joint distribution of the EOS model parameters is used to generate samples to run through the continuum code to give a distribution of outputs.

Several questions and problems to deal with in each step.

Data has error bars

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We assume statistical noise in experimental data (we do not yet deal directly with explicit experimental or calculational error bars).

Data+EOS model => Parameter distribution (Posterior distribution function, PDF)

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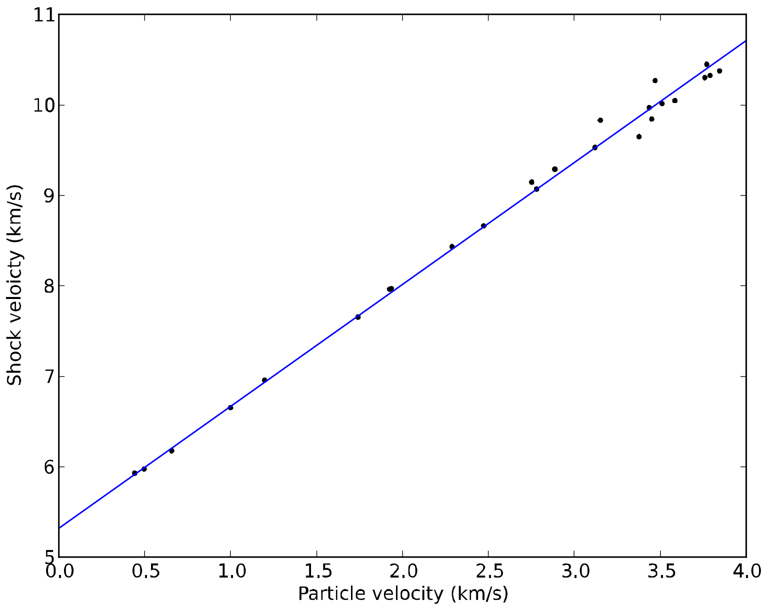
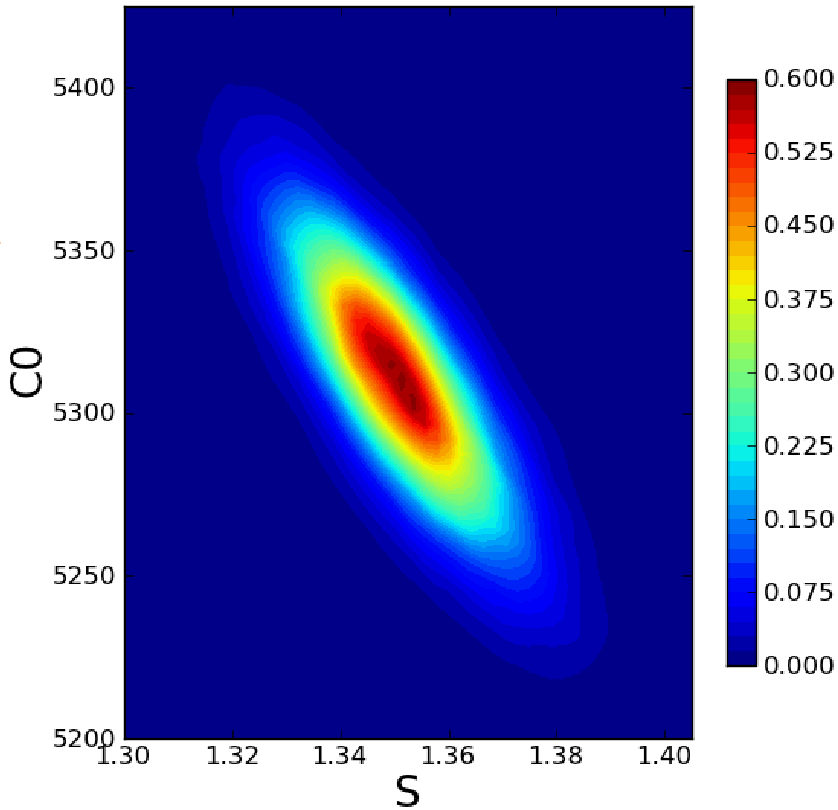


Black points are Marsh handbook Al data

$$U_s = C_0 + S\,u_p$$

The point in the middle of the red is the most likely value of C_0 (m/s) and S, given the data. But there is some likelihood that other (C_0,S) values are correct.



Note the correlation between C_0 and S.

Representing the PDF

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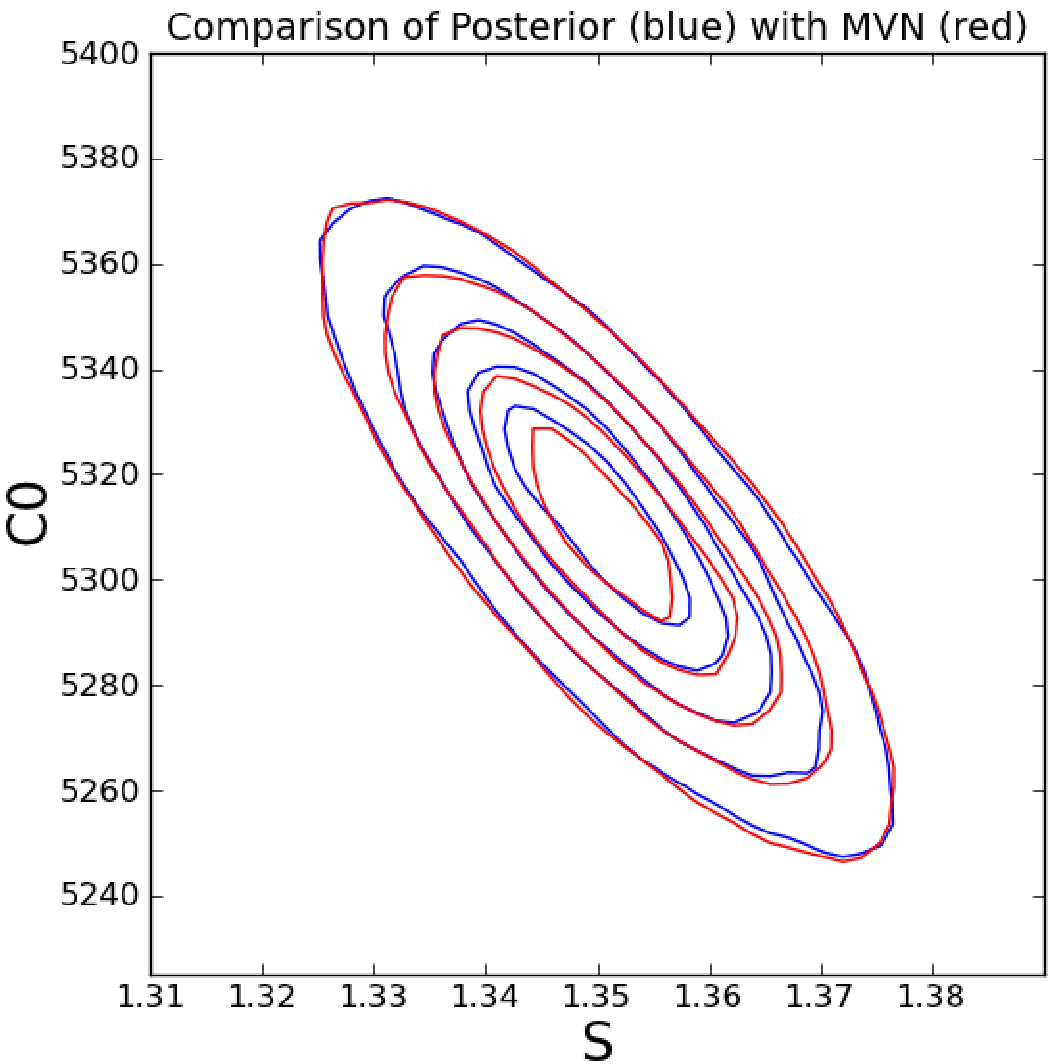

The Posterior distribution is typically a set of a large number of points. We need a more compact form.

Example: Multi-variate normal (MVN) approximation.

$$C_0 = 5310 - 26.25\xi_1 + 20.25\xi_2$$
$$S = 1.351 + 0.01367\xi_1$$

ξ_i : Independent identically distributed Gaussian random variables. (Mean zero).

Analytical EOS model => ALEGRA output

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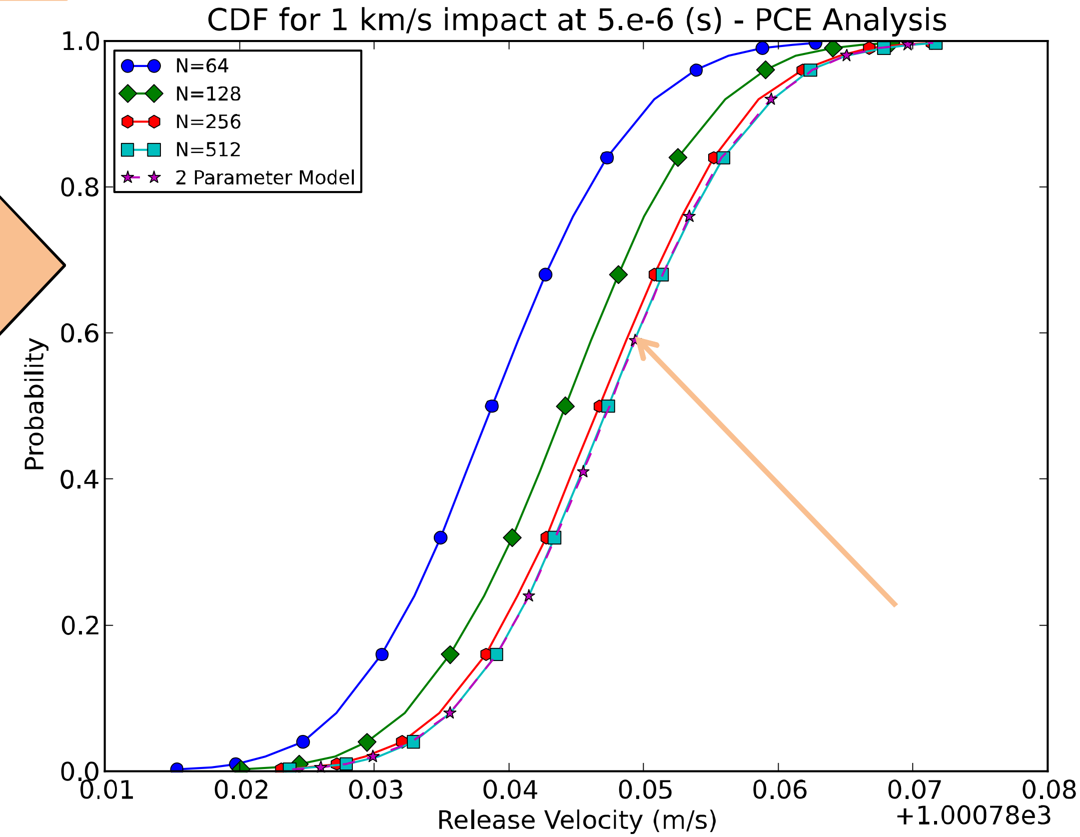
$$C_0 = 5310 - 26.25\xi_1 + 20.25\xi_2$$
$$S = 1.351 + 0.01367\xi_1$$

Note: On this slide we do not use a table but use C_0 and S as the inline analytical EOS model in ALEGRA.

Use some sampling technique to choose a limited set of samples of (C_0,S) to send through ALEGRA to obtain a distribution of results. In this example we used the Polynomial Chaos Expansion (PCE) technique.



For this example, the PCE requires only 9 (C_0,S) samples, thus only 9 ALEGRA runs.

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Now: EOS Tables => ALEGRA output
1) Table resolution

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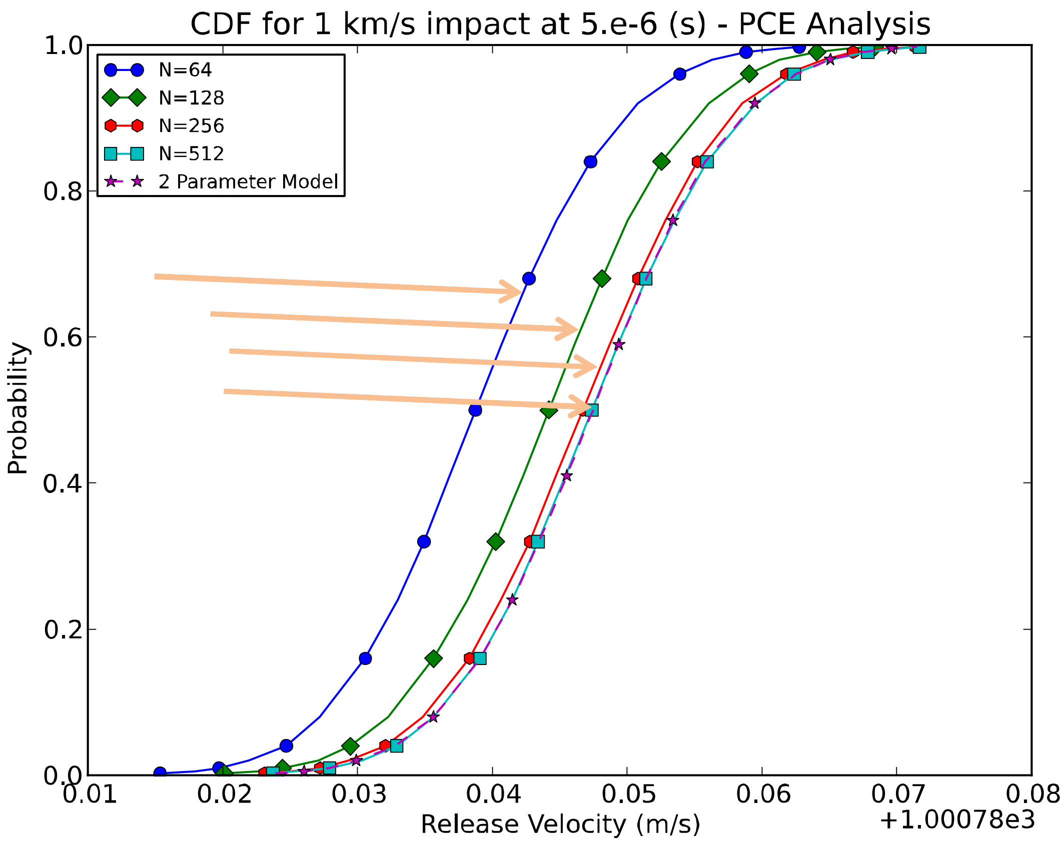
Making tables with different grid sizes from the chosen (C_0,S) samples and send these through ALEGRA gives the other lines.



We need really good resolution in the tables to not introduce artificial errors.

9 tables required for every curve.

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Now: EOS Tables => ALEGRA output
2) Number of tables and ALEGRA runs

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In our example we had two statistical variables to sample over, 3 samples in each variable gave $3^2=9$ samples. If we have 20 statistical variables to sample over: $3^{20}=$ (far to much).

Every statistical sample needs its own table for its own ALEGRA run.

Strategy: Generate tables for samples but use them to do a Principal Components Analysis (PCA) resulting in:

$$T = \overline{T} + \xi_1 T_1 + \xi_2 T_2 + \xi_3 T_3 + \cdots$$

(we reserve space in our tables for 9 modes).

Now the analyst can chose how many ALEGRA runs he/she can afford and generate tables only for these.

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Principal Components Analysis

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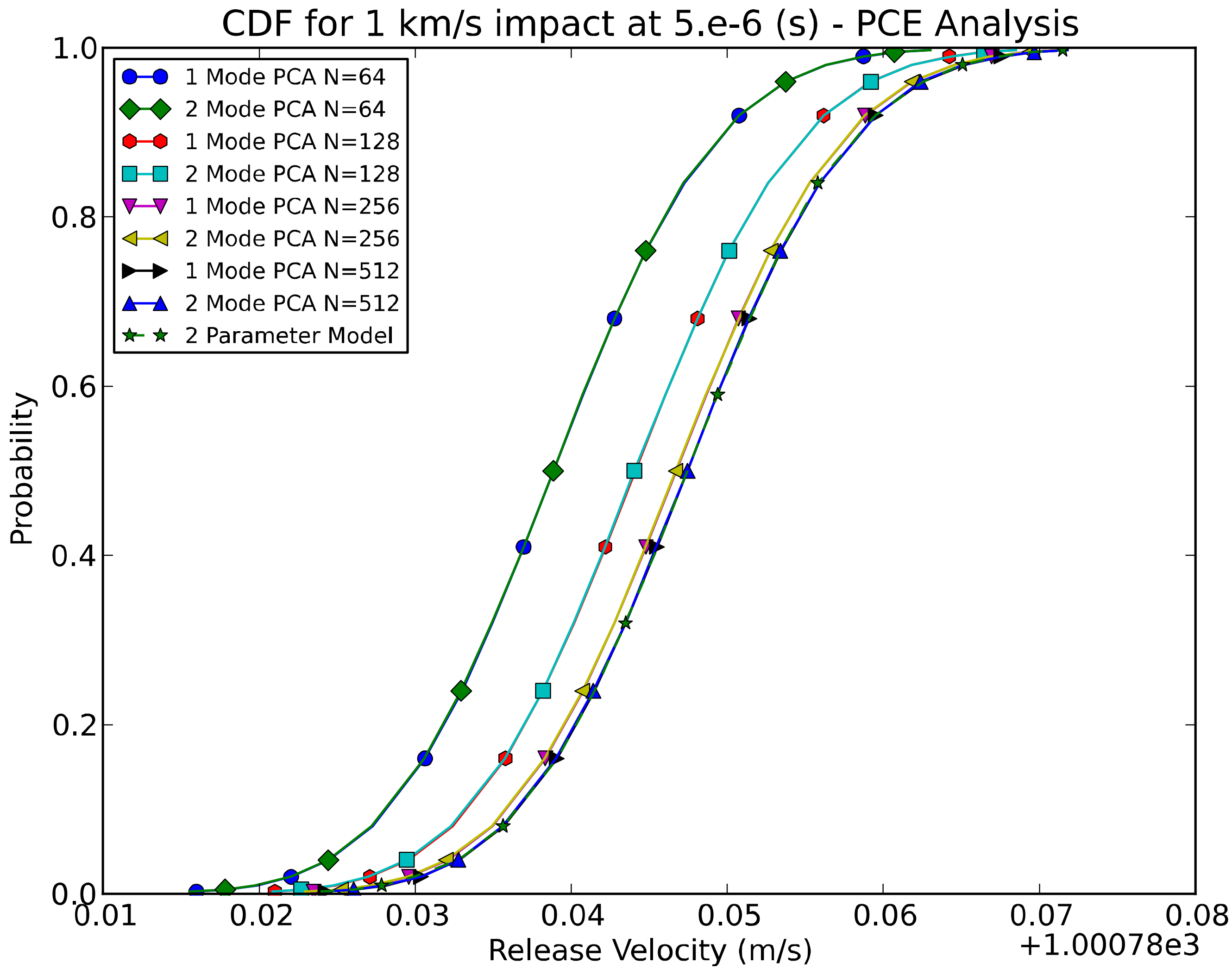

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Summary:

1) We assume noisy experimental data.
2) We determine the probability that sets of specific values for the parameters in the EOS model is representing the data.
3) This joint distribution of the EOS model parameters (a large number of points) is in turn represented by a statistical distribution with a (smaller) number of random variables.
4) Several options to obtain a distribution of outputs from the continuum code:
   a) Samples of the analytical EOS model parameters are generated and sent through the continuum code to generate a distribution of output.
   b) Samples of the EOS model parameters and corresponding tables are generated and sent through the continuum code to generate a distribution of output.
   c) Two steps:
      i. Samples of the EOS model parameters and corresponding tables are generated. Those tables are run through an analysis that amounts to a rotation to arrange combination of statistical variables in order of importance, resulting in a mean table and modes multiplied by random variables (similar to step 3).
      ii. (Fewer) sample tables are generated from these tables and run through the continuum code to generate a distribution of output.

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Data and EOS tables: Example of Xe

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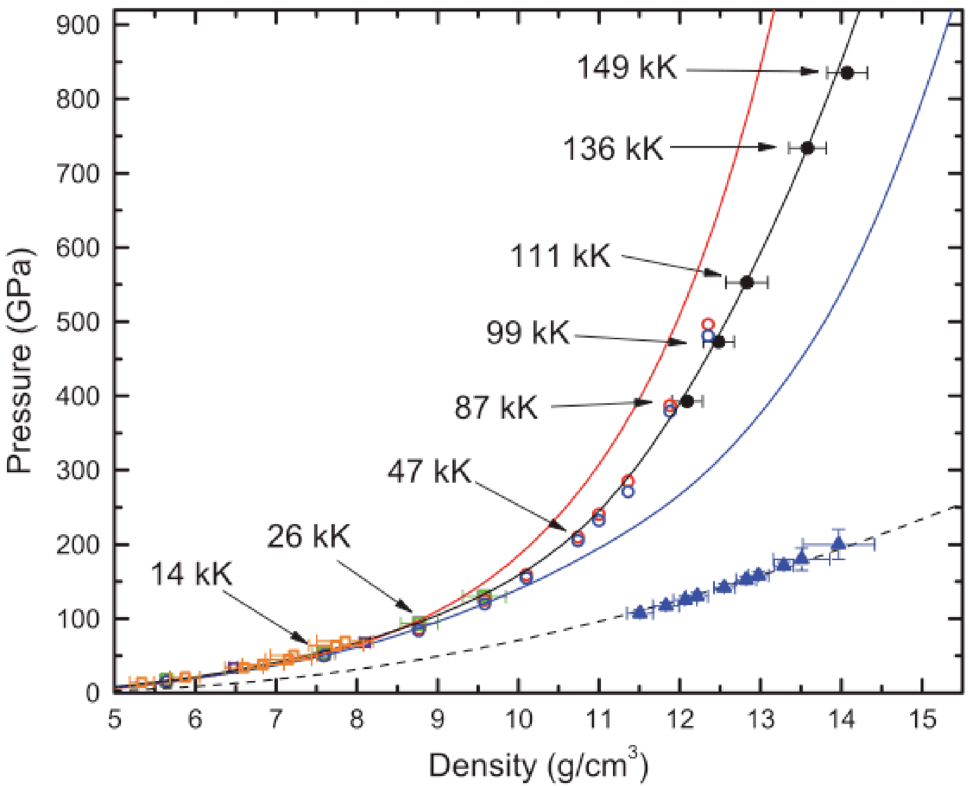


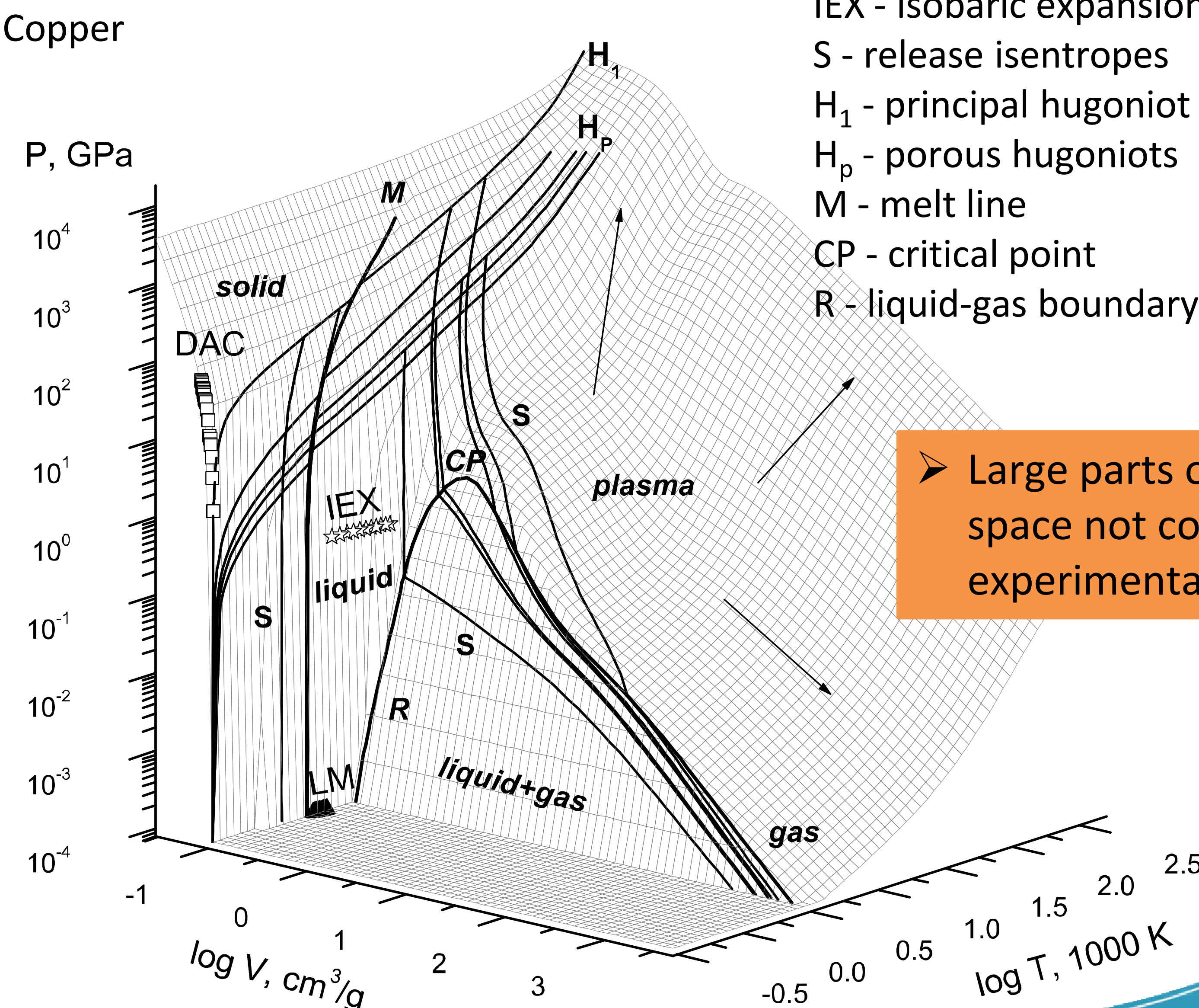
FIG. 3 (color). *P*-*ρ* Hugoniot plot. Lines and symbols as in Fig. 2. Black dashed line, 5191 298 K isotherm; blue triangles, solid xenon compression data [17]. Also indicated are Hugoniot temperatures calculated using 5191. Our DFT calculated isotherm [37] agrees with the experimental data [17].

Root et al. PRL 105, 085501 (2010)

Red circle: LDA
Blue circle: AM05
Black circles: Z data
Black line: New EOS 5191
Blue line: SESAME 5190
Red line: LEOS 540

Note: DFT calculations published *before* Z data was available. Shown is the Hugoniot. DFT data is added also in other parts of phase space (e.g., cold curve and melt line).

Data and EOS table: Copper



DAC - diamond anvil cell measurements
IEX - isobaric expansion experiments
S - release isentropes
H_1 - principal hugoniot
H_p - porous hugoniots
M - melt line
CP - critical point
R - liquid-gas boundary

- Large parts of parameter space not covered by any experimental technique.

Ann E. Mattsson