Radiative Shock Hydrodynamics: Experiments, Simulations and Uncertainty Quantification

CRASH PIs: Marv Adams, Paul Drake, James Holloway, Ken Powell and Quentin Stout

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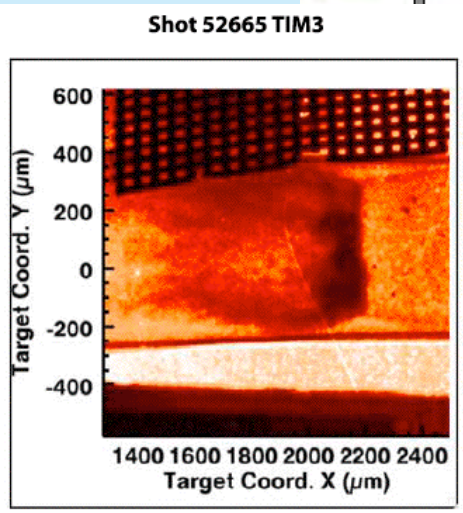
Summary of the CRASH Problem

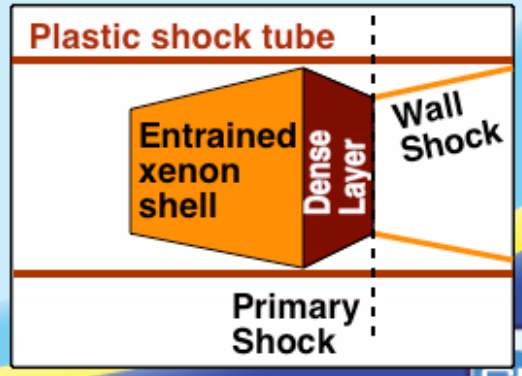
- Laser irradiates Be disk, driving shock into Xe-filled tube
- Radiative precursor heats wall of tube, leading to ablation
- Complex interaction among laser-driven shock, ablation-driven shock, and Xe-Be interface
- Relevant to astrophysics and fundamental high-energy-density physics

10^{15} W/cm^2
0.35 μm
1 ns pulse



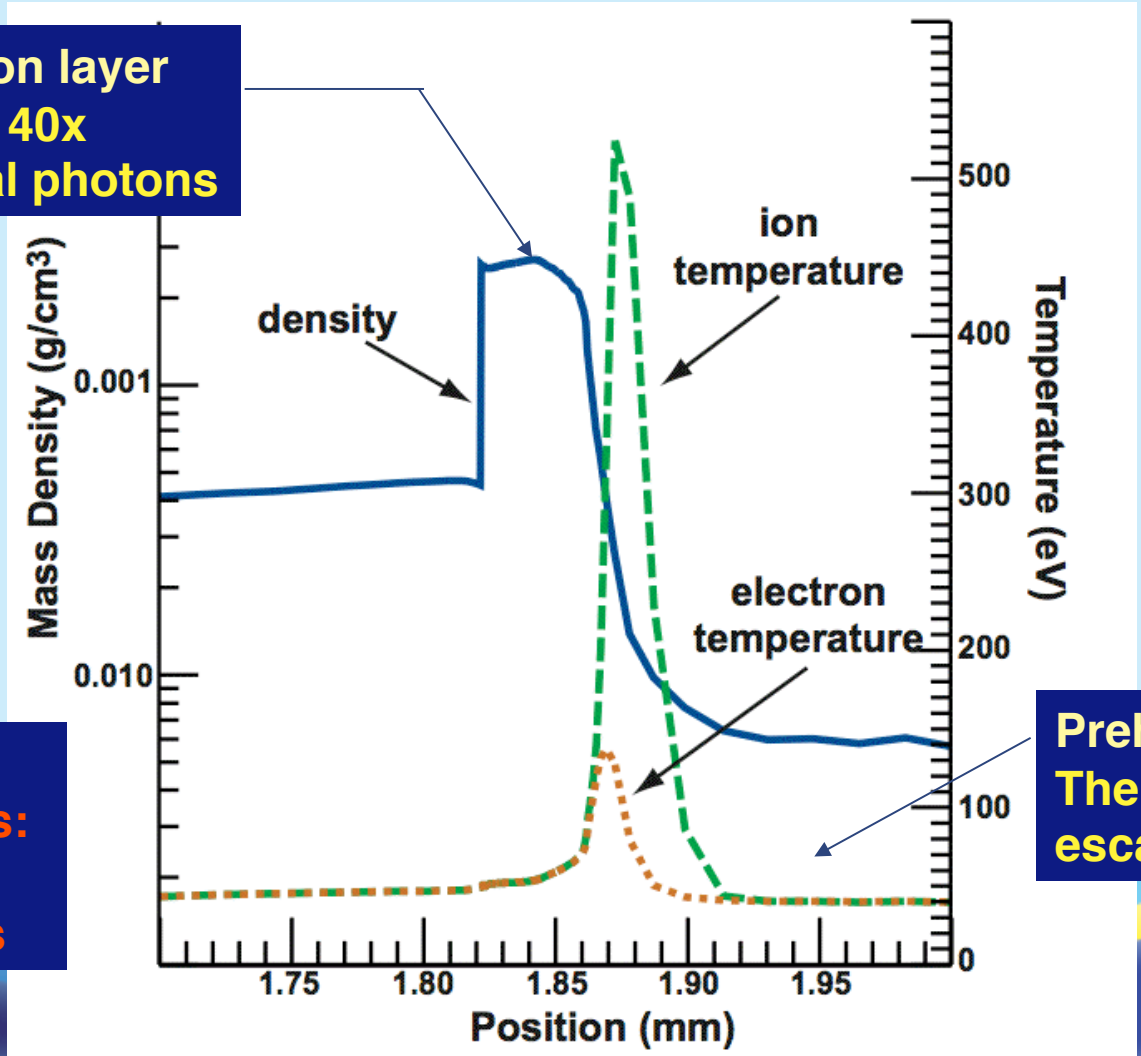
Radiograph

Schematic



Radiative shocks develop complex structure

Shocked xenon layer
Compressed 40x
Traps thermal photons



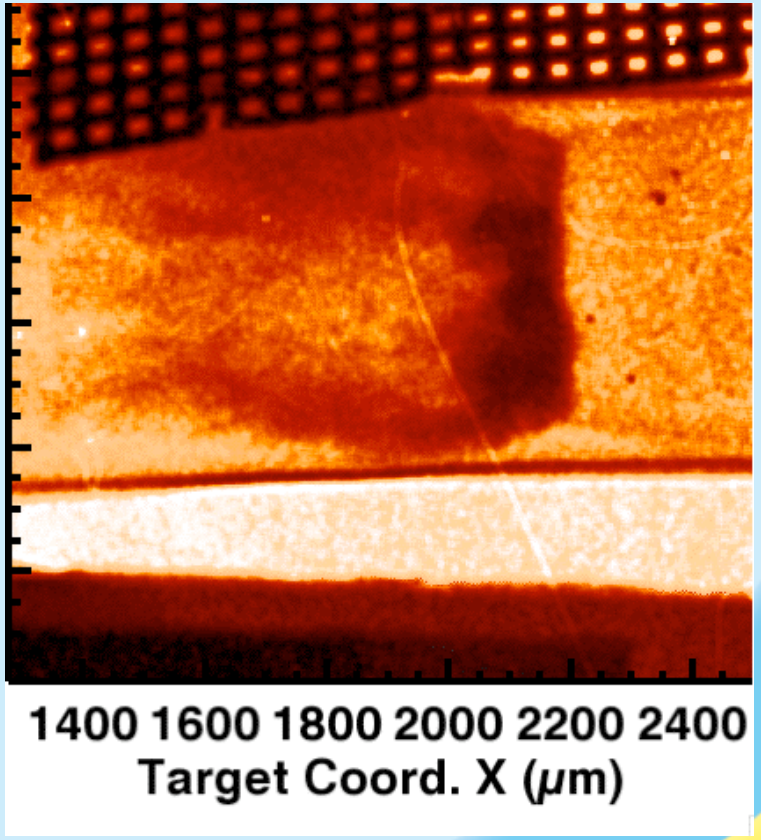
Other fun complications:
Instabilities
Wall shocks

Preheated region
Thermal photons escape upstream

Key outputs include:

- Shock position at observation time
- Distance of edge of shock from tube wall
- Angle of xenon edge just downstream of shock
- Measure of entrained Xe in radiograph

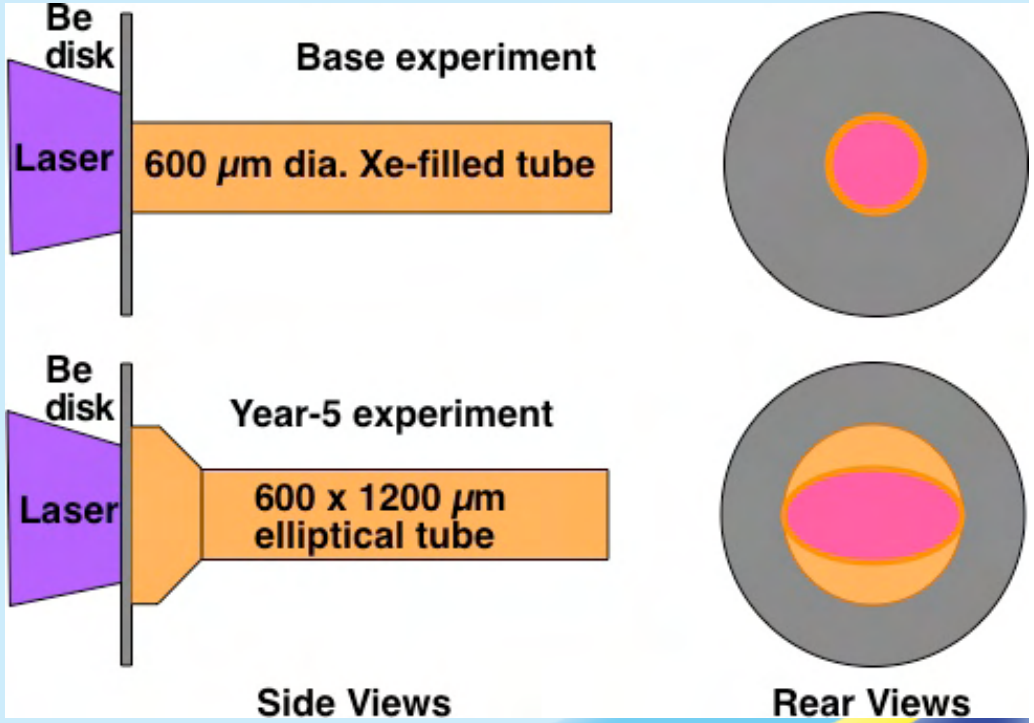
Determine sensitivities of Y and predict pdf of output $\pi(Y \mid X^*)$ for a new experiment X^*, accounting for uncertain inputs



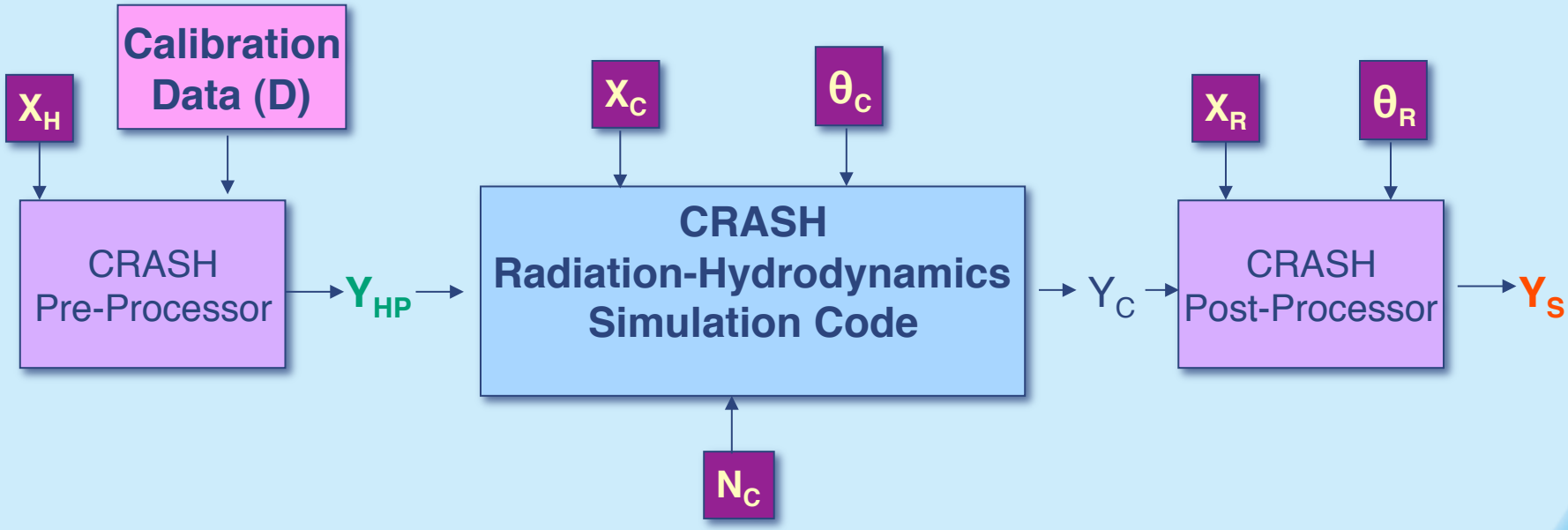
X-ray radiograph from experiment with average velocity 140 km/sec at 14 ns

Year 5 Experiment

- Go from 2D symmetry to 3D
- Predict outcome and uncertainty before doing year 5 experiment
- Demonstrate a predictive uncertainty comparable to the observed experimental variability



Summary of the CRASH Calculation

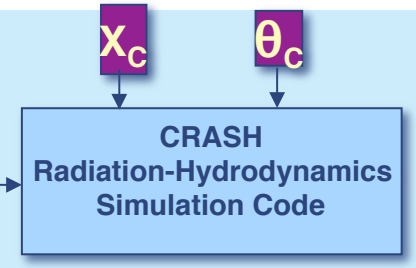


$$
\begin{aligned}
Y_{HP} &= C_{PRE}\left(X_H, D\right) = \text{Calibrated CRASH ICs} \\
Y_C &= C_{3D}\left(Y_{HP}, X_C, \theta_C, N_C\right) \\
Y_S &= C_{POST}\left(Y_C, X_R, \theta_R\right)
\end{aligned}
$$

X - Experiment parameters
θ - Physical Constants
N - Numerical Parameters

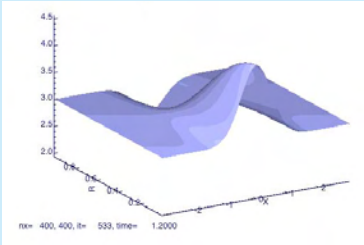
Y_S - Results to be analyzed with data by statistical methods

CRASH capabilities & tests

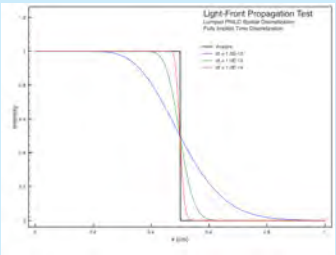


- TVD MUSCL Hydrodynamics
- Adaptive mesh refinement
- XYZ and RZ geometry
- Multimaterial w/ level sets
- Multigroup radiation diffusion (S_n pending)
- Electron physics
- Material properties (EOS and opacities)
- Simulated radiography
- All backed up by extensive testing

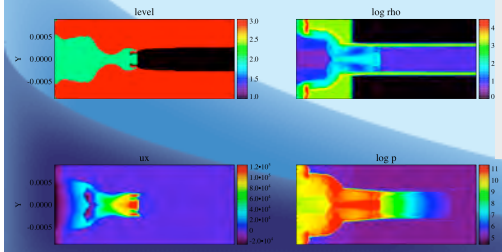
HEAT CONDUCTION



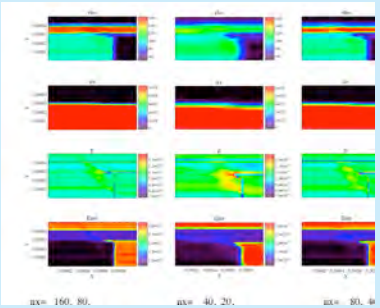
RADIATION TRANSPORT



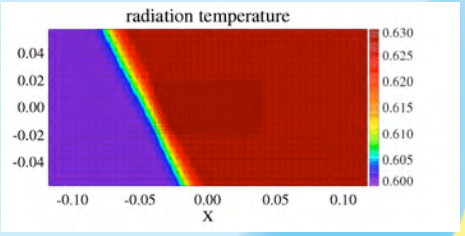
FULL SYSTEM



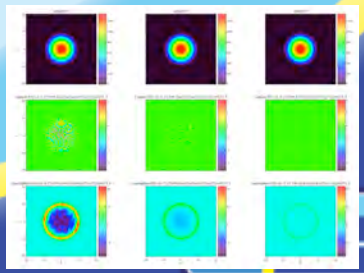
HYDRODYNAMICS



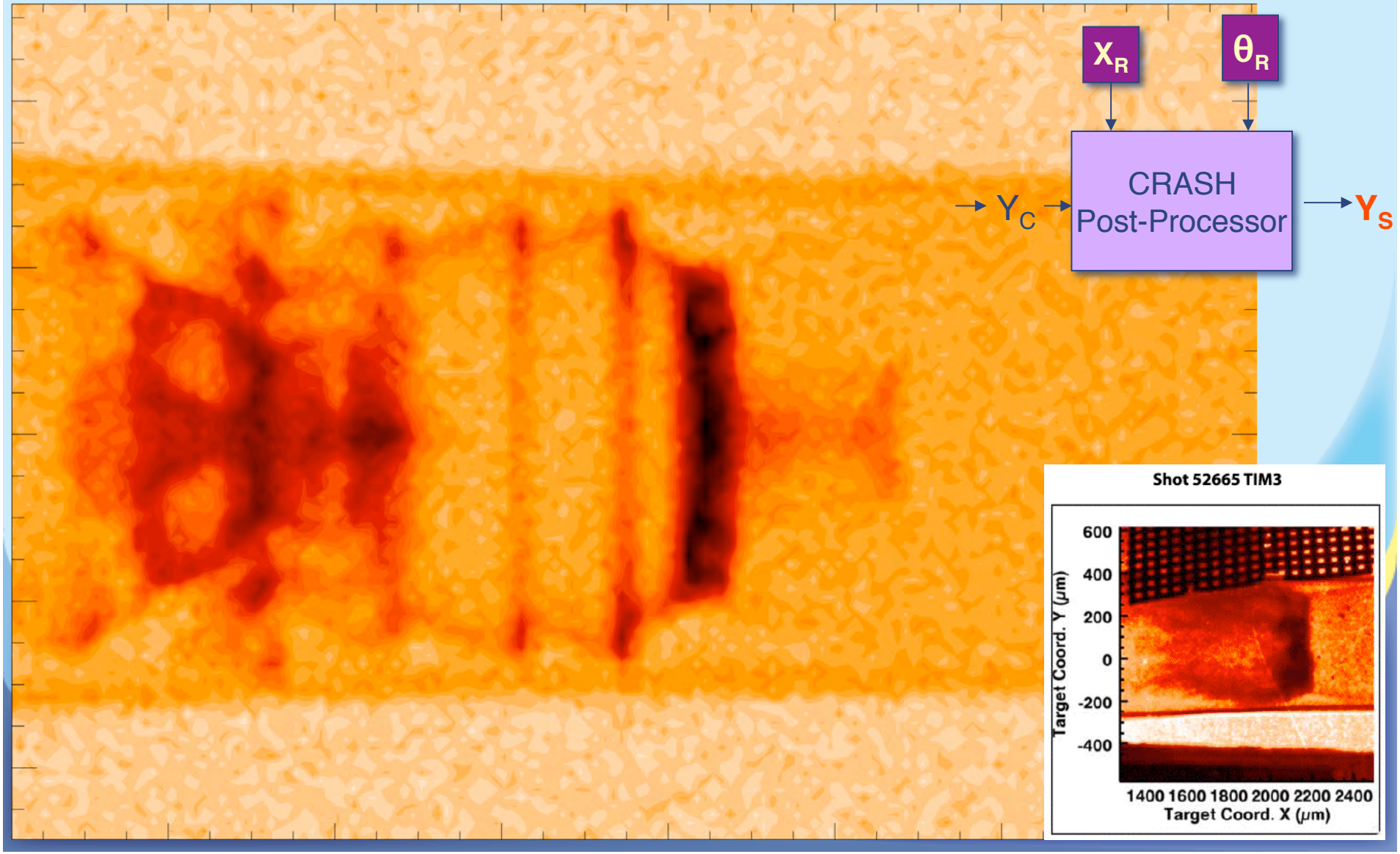
RADIATION HYDRODYNAMICS



SIMULATED RADIOGRAPHY



We simulate radiographs to compare with experiment



The CRASH test matrix

Verification test problems

Tested code components

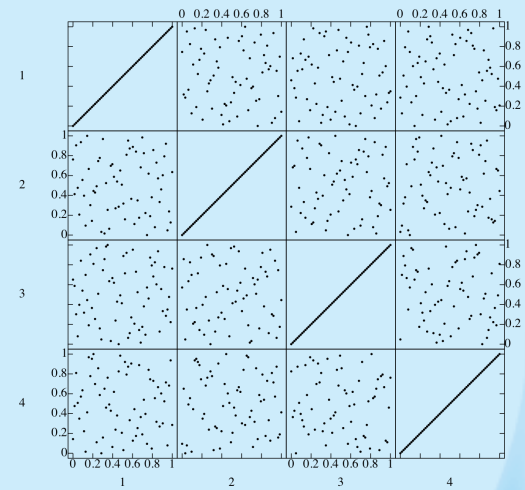
		Full System 1D	Full System 2D	Full System 3D	Full system (nozzle)	Full system (NIF)	Infinite medium	Light front	Light front (double)	Lowrie 1 (radiation)	Lowrie 2 (radiation)	Lowrie 3 (radiation)	Lowrie 3 (mod; electrons)	Multi-material advection	Multi-material wave	Radiography	Reinicke Meyer-ter-Vehn	Shu-Osher	Sound wave	Su-Olson	Uniform heat conduction
Active variables	rho	x	x	x	x	x				x	x	x	x	x	x	x	x	x	x		
	materials	x	x	x	x	x								x	x						
	u	x	x	x	x	x				x	x	x	x	x	x		x	x	x		
	E_int	x	x	x	x	x	x			x	x	x	x	x	x		x	x	x	x	x
	E_rad	x	x	x	x	x	x	x	x	x	x	x								x	
Radiation treatment	gray diffusion	x	x	x	x	x	x	x		x	x	x								x	
	multigroup diffusion	x	x	x	x	x	x		x											x	
	discrete ordinates	x	x	x	x	x	x	x	x											x	
Diffusion term	pure diffusion									x	x	x								x	
	flux-limited	x	x	x	x	x	x	x	x												
Equation of state	gamma law	x	x	x	x	x	x			x	x	x	x	x	x		x	x	x		
	self-consistent	x	x	x	x	x	x							x	x						
Heat Conductivity	uniform/analytic												x				x				x
	self-consistent	x	x	x	x	x															
Coupling	electron-ion	x	x	x	x	x							x								
Opacities	uniform/analytic						x	x	x	x	x	x								x	
	std tabular	x	x	x	x	x	x														
	self-consistent	x	x	x	x	x	x														
Multi-materials	level-set	x	x	x	x	x								x	x						
	mixed cell	x	x	x	x	x								x	x						
Dimensionality	1D x	x				x		x	x					x	x			x	x	x	x
	2D x-y							x	x	x	x	x	x	x				x	x		x
	2D r-z		x		x	x		x	x							x	x	x	x		x
	3D x-y-z			x	x	x		x	x	x	x	x	x			x	x	x	x		x
Grid resolution	uniform	x	x	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x	x	x
	fixed AMR	x	x	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x	x	x
	dynamic AMR	x	x	x	x	x		x	x	x	x	x	x	x	x		x	x	x	x	x
Time-evolution scheme	explicit													x	x			x	x		
	implicit	x	x	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x
	mixed explicit-implicit	x	x	x	x	x	x			x	x	x	x				x			x	x
Hydro scheme	HLLE	x	x	x	x	x				x	x	x	x	x	x		x	x	x		
	Godunov	x	x	x	x	x				x	x	x	x	x	x		x	x	x		
Implicit solvers	CG	x	x	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x
	GMRES	x	x	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x
Preconditioners	DILU/BILU	x	x	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x
Initial conditions	Hyades output	x	x	x	x																
	user specified					x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x

KEY

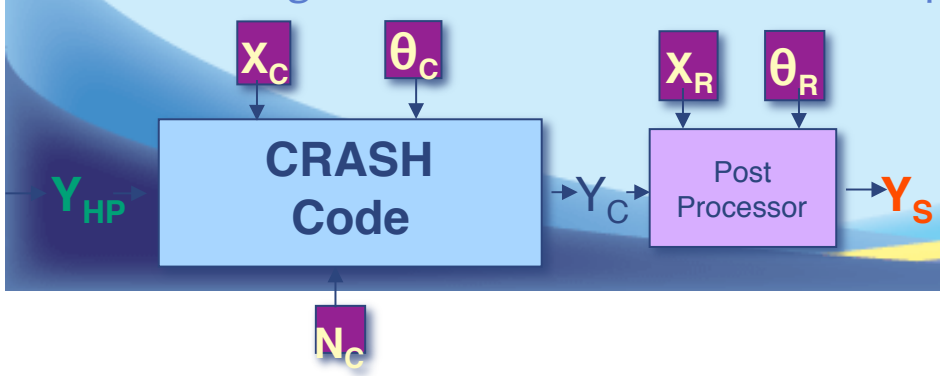
Implemented test covers this physics/numerics/code component	x
Not presently implemented	x
Test cannot cover this code component in a meaningful way	

Sensitivity analysis using statistical fitting

- Sample input space (Latin hypercube sampling)
- Compute outputs $y_i = \eta(x_i, \theta_i, y_{\mathrm{HP}i})$
- Fit a model $y = \hat{y}(x, \theta, y_{\mathrm{HP}})$
  - Gaussian Process model
  - Flexible regression models
- Estimate global sensitivity due to an input by:
  1. perturbing input variable randomly over samples
  2. refitting
  3. computing RMS difference
- Estimate parameter scale sensitivities using length parameters from GP model
- Marginalize over other variables to explore variation due to one or two variables



The LHD used for CRASH 3D sensitivity study

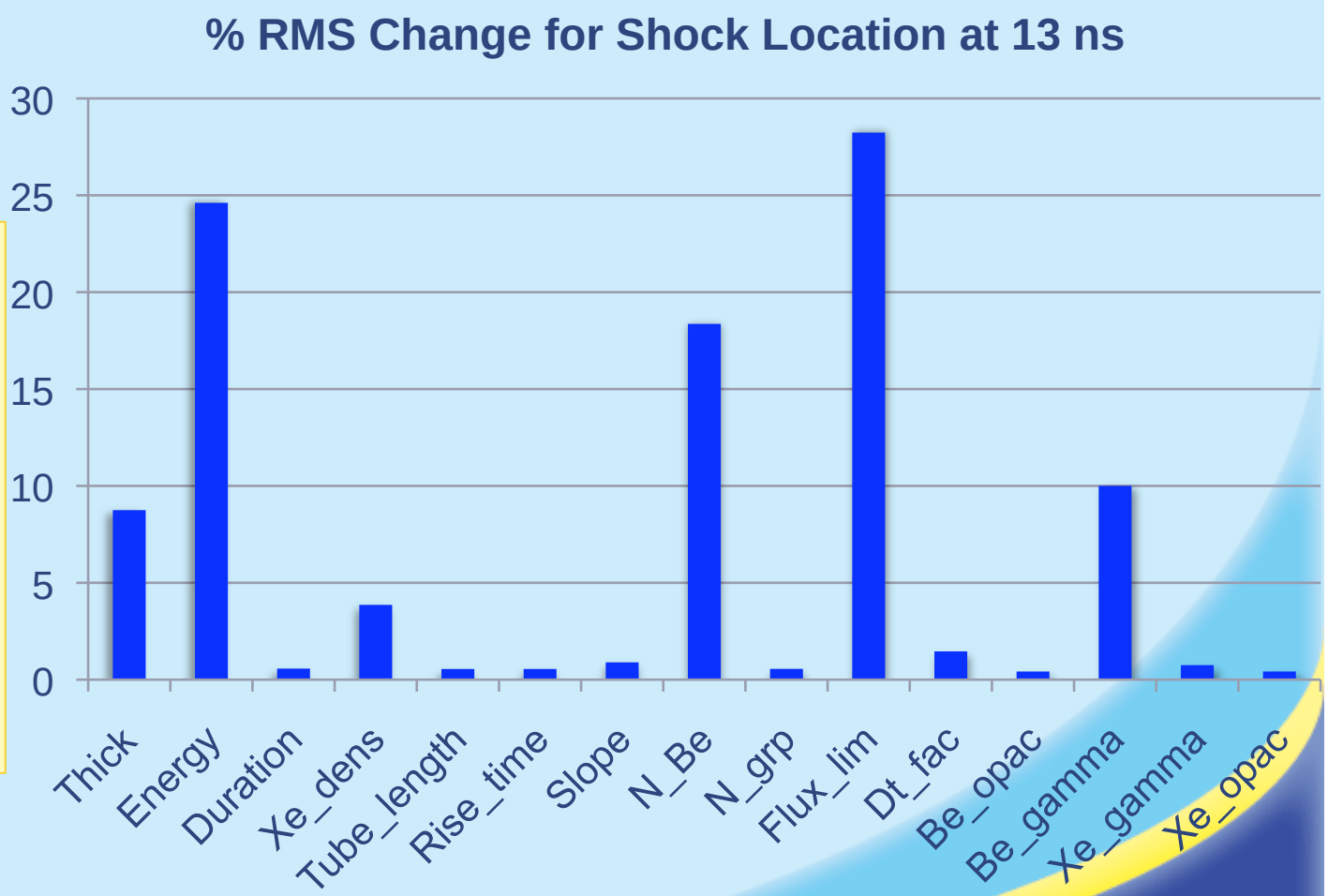


We can identify important influences on shock location

Based on 512 Hyades runs and MART fit

Informs selection of parameters for 3D study

- **Be Thickness**
- **Laser Energy**
- **Xe Density**
- **Be and Xe gammas**
- **Be and Xe opacity scale factors**



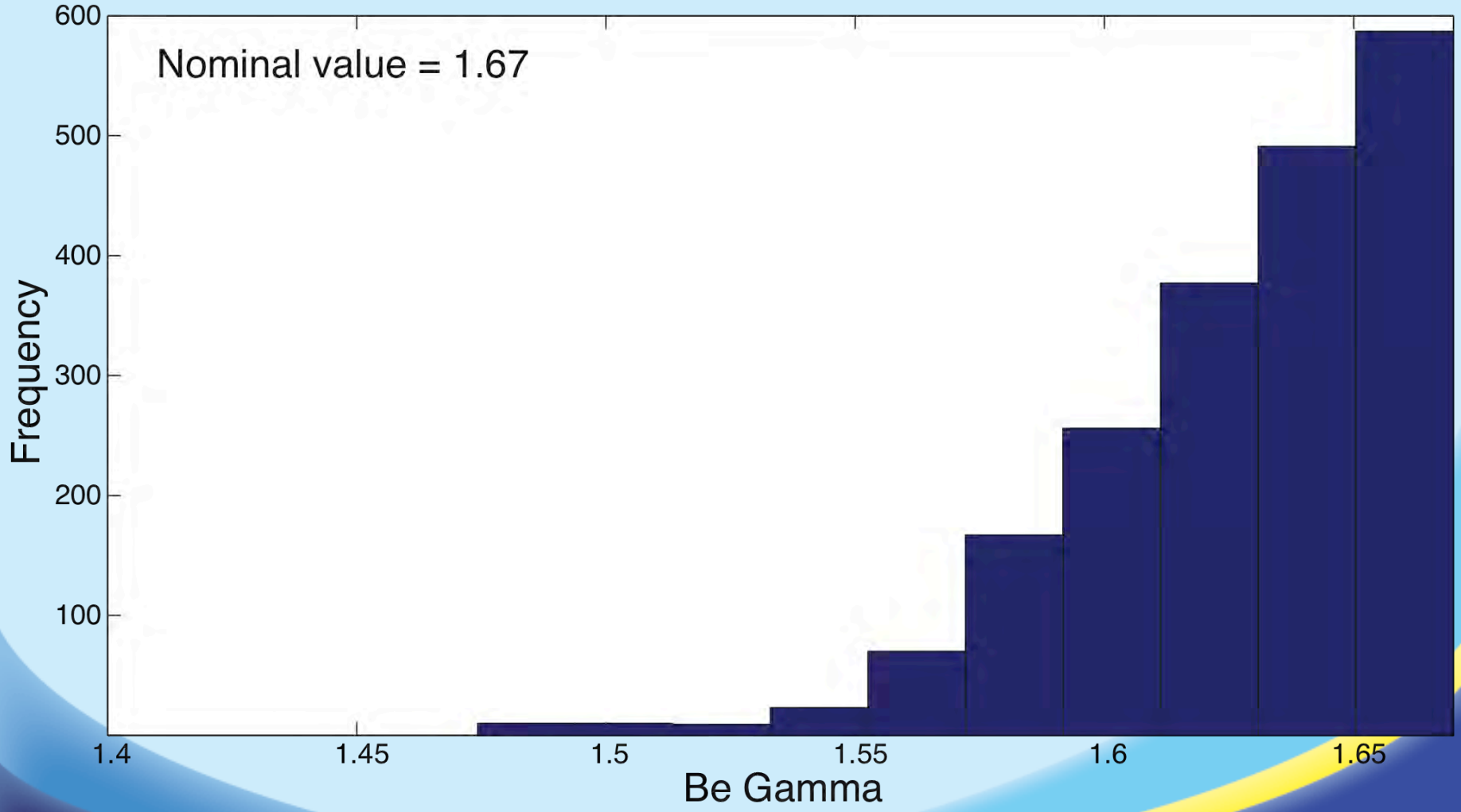
We build a predictive model to explore uncertainty

- Data for model are field experiments and set of code runs
- Model data as sum of 3 terms:

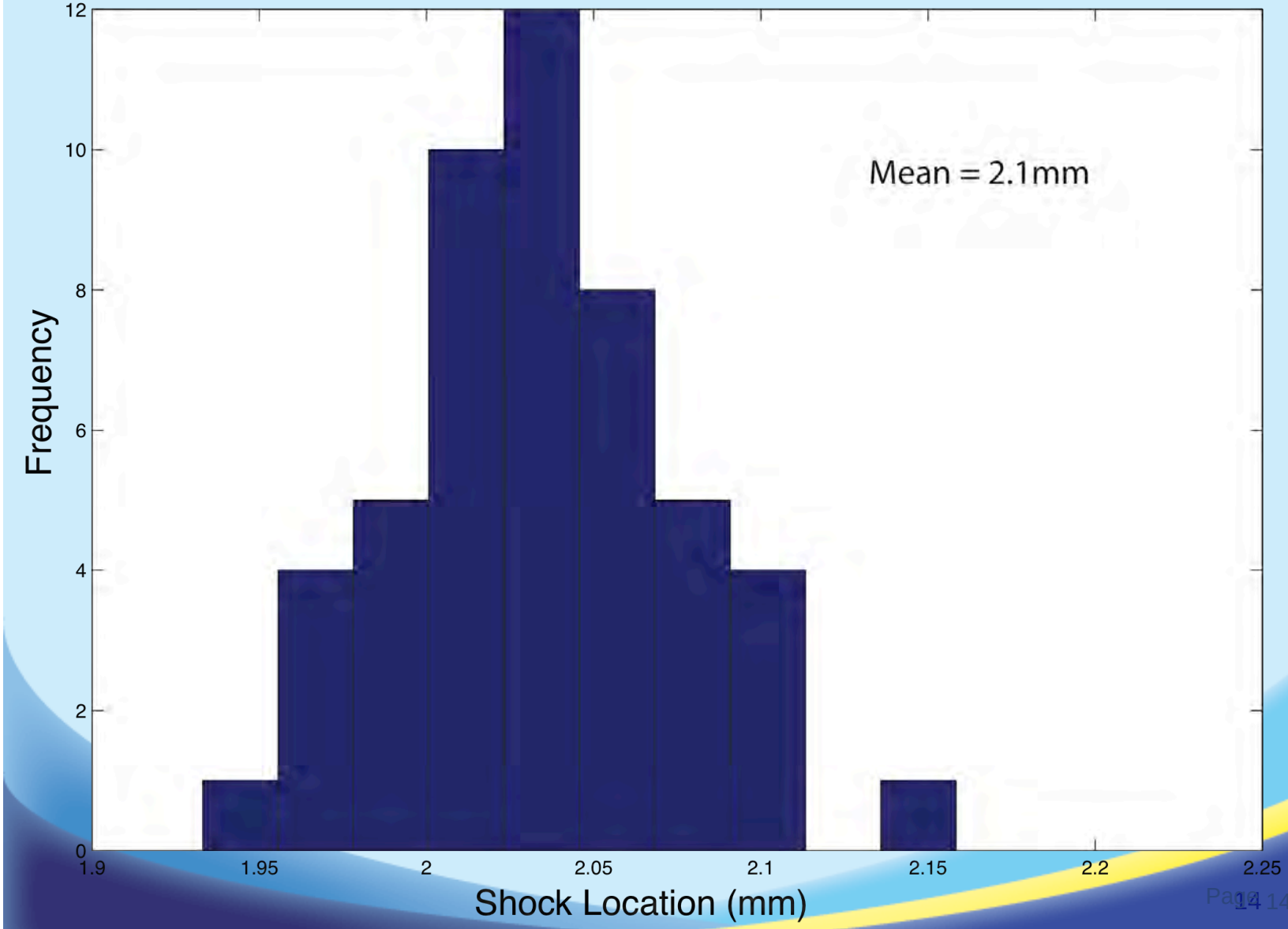
$$Y = \eta(X, \theta) + \delta(X) + \epsilon$$

- Such a model provides:
  - Mean and variance of output – predictive distribution
  - Tool to explore error in the model relative to experiment
  - Approach to determine a next experiment or simulation to reduce uncertainty

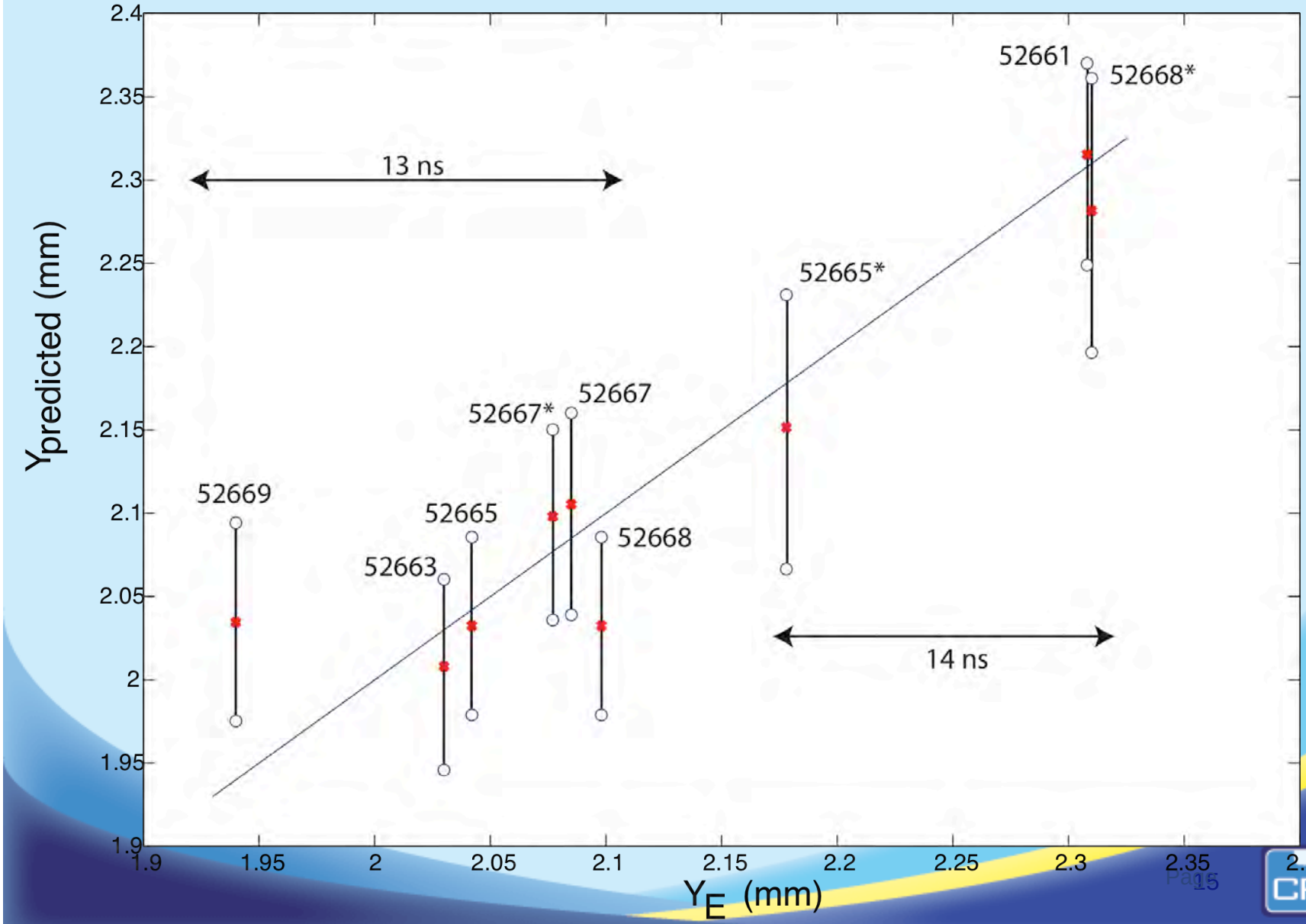
Posterior Distribution for Be Gamma



Posterior Prediction for Shock Location



Leave One Out Predictions for Shock Location



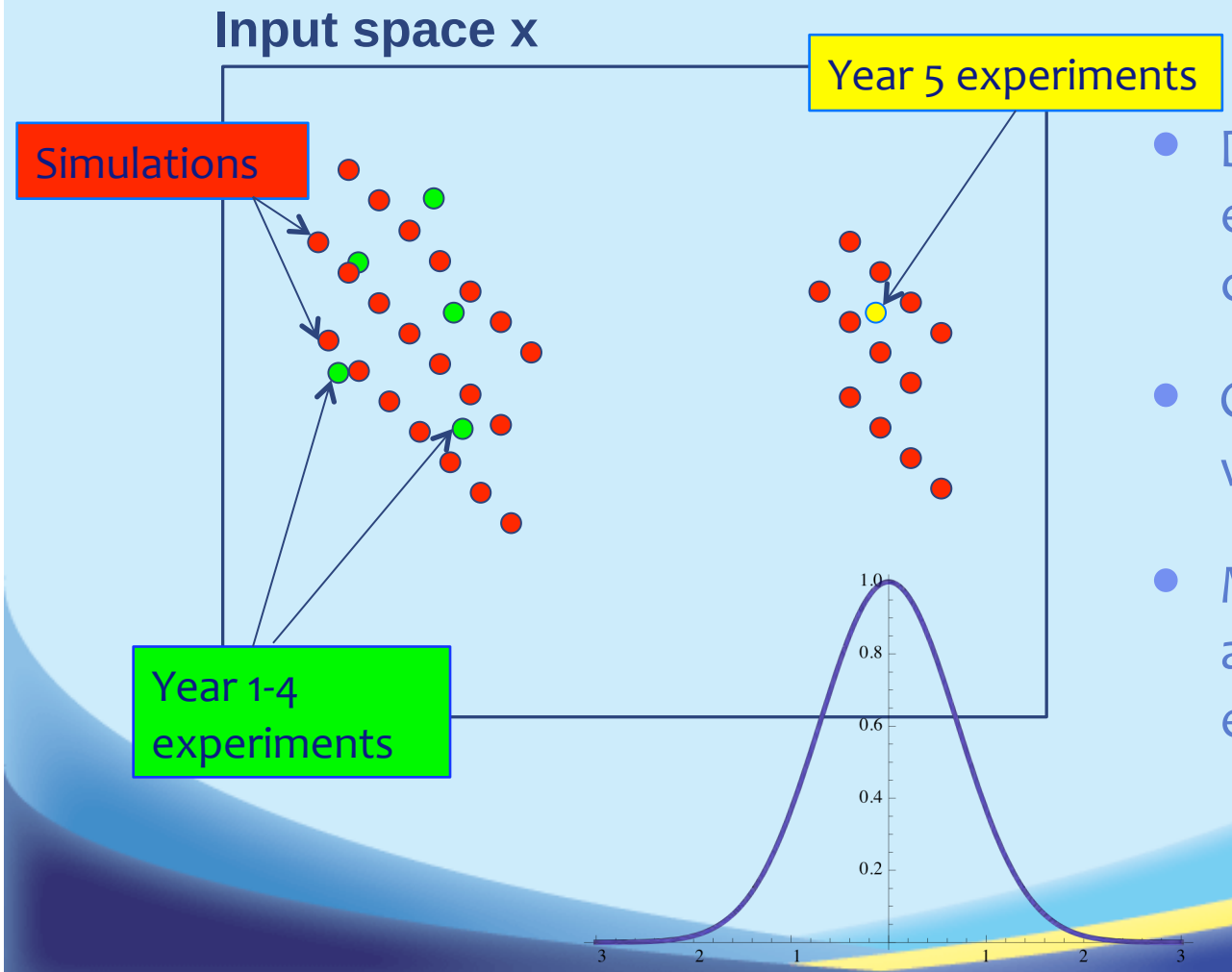
Next steps for the CRASH project

- Release CRASH 2.0
- Develop CRASH 2D/3D preprocessor
  - Analyze Hyades 2D runs
  - Quantify uncertainties in initial state
- Explore uncertainty due to all 3 stages:
  - Preprocessor, CRASH, Postprocessor
- Conduct a pure hydro sensitivity study in elliptical tubes
- Simulate year 5 experiment
- Design the year 3 experimental campaign based on these studies

CRASH's impact at Michigan & TAMU

- Culture change for students, faculty, and research scientists
  - Learning to think continuously about uncertainty
  - Over 20 graduate students are involved
- New graduate classes on uncertainty quantification
  - TAMU: Verification & UQ focus – McClarren
  - UM: UQ and SA focus – Holloway, Nair, Powell
  - Presence of many students from outside CRASH shows broad and growing interest

We are heading towards the year 5 elliptical tube

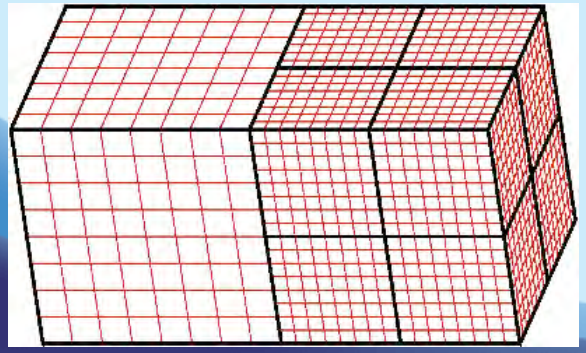


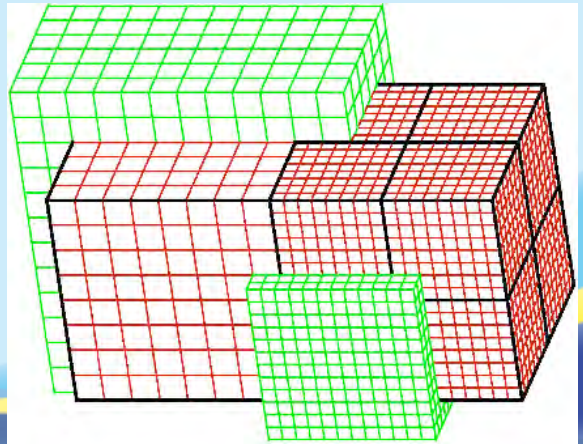
- Do computations and experiments with circular tubes
- Can do computations with elliptical tubes
- Must predict output y and its pdf for the elliptical tube

Questions?

CRASH Grid and Domain Decomposition

- Each block NxNxN (N typically 6, 8 or 10 – can be $N_1 x N_2 x N_3$)
- AMR divides one block into eight smaller blocks (in 3D)
- Blocks at different refinement levels logically similar - require the same amount of work
- Load balancing done by distributing blocks to processors
- Space-filling curve used to order blocks
- Blocks communicate via "ghost cells"





Elements of the Uncertainty Quantification Effort

- Experiment design
- Screening
- Emulator construction
- Prediction
- Calibration (solving inverse problems)
- Confidence/prediction interval estimation
- Analysis of multiple simulators
- Characterizing uncertainty propagation in this context

- This list is not exhaustive

Statistical Framework for Model Calibration

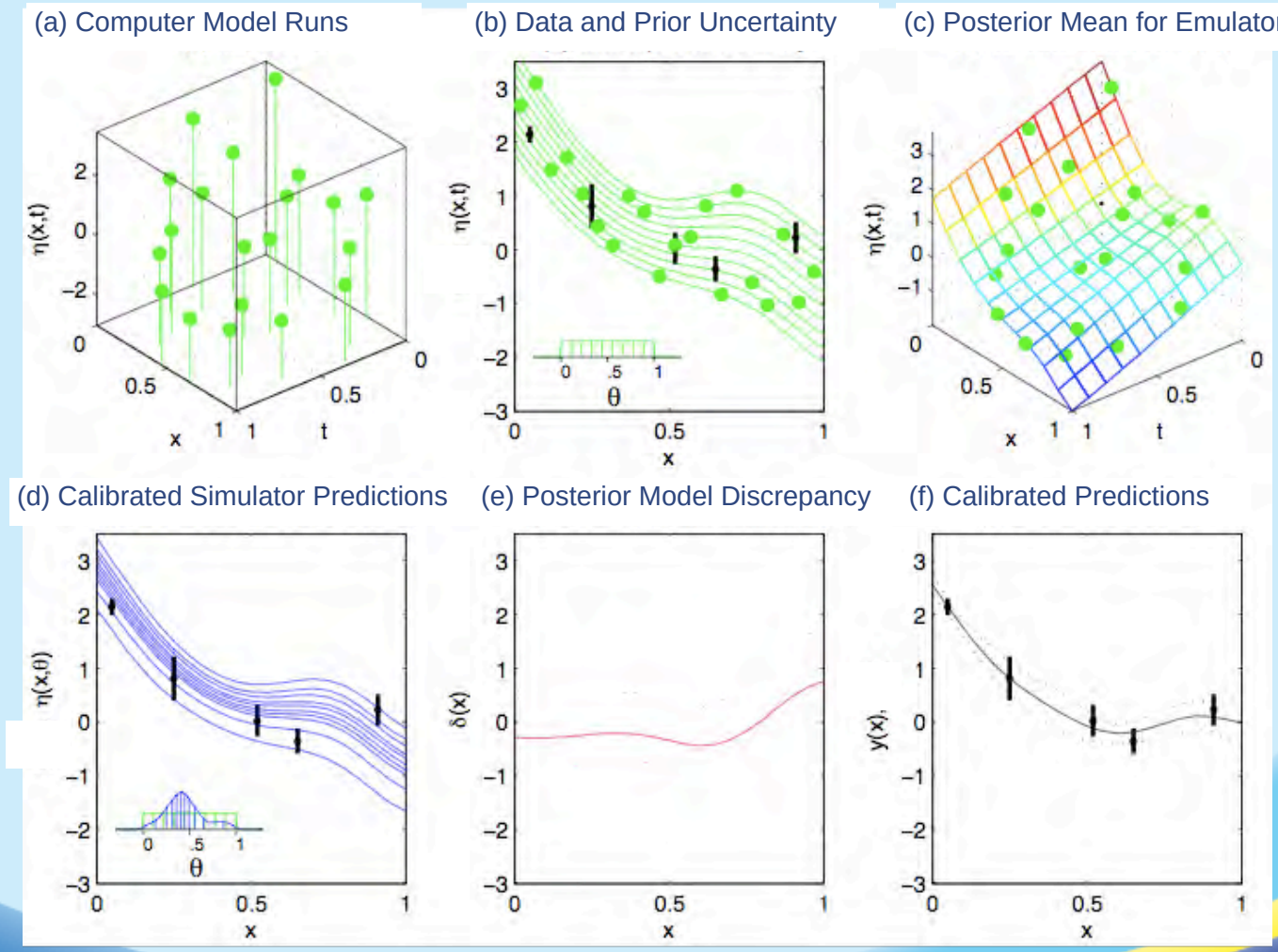
$$y_f(x_i) = \eta(x_i, \theta) + \delta(x_i) + \epsilon_i$$

$$y_s(x_j, t) = \eta(x_j, t)$$

where:

- x model or system inputs
- y_f system response
- y_s simulator response
- θ calibration parameters
- t value of calibration parameters used in code runs
- ϵ Gaussian observational error

Statistical Framework - Basic Idea



Solution of Rad-hydro equations: Gray Diffusion

- Radiation transport equation reduces to a conservation equation for the radiation energy

advection compression work diffusion energy exchange

$$\frac{\partial E_R}{\partial t} + \nabla \cdot (E_R \mathbf{u}) + p_R \nabla \cdot \mathbf{u} = \nabla \cdot \left[\frac{\lambda c}{\bar{\chi}} \nabla E_R \right] - \kappa_P c \left(E_R - \frac{4\sigma}{c} T^4 \right)$$

- Advection of radiation energy and the work due to the isotropic radiation pressure evaluated explicitly
- Diffusion of radiation energy and energy exchange between radiation and plasma evaluated implicitly

CRASH Coupled Approach – Hydro Governing Equations

$$\frac{\partial}{\partial t}\left\{\begin{array}{c}\rho\\ \rho\mathbf{u}\\ \mathcal{E}+\frac{1}{2}\rho\mathbf{u}\cdot\mathbf{u}\\ \mathcal{E}_e\end{array}\right\}+\nabla\cdot\left\{\begin{array}{c}\rho\mathbf{u}\\ \rho\mathbf{u}\mathbf{u}+p\mathbf{I}\\ \mathbf{u}\left(\frac{1}{2}\rho\mathbf{u}\cdot\mathbf{u}+\mathcal{E}+p\right)\\ \mathbf{u}\mathcal{E}_e\end{array}\right\}=\mathbf{S}$$

$$\mathbf{S}=\left\{\begin{array}{c}0\\ -\mathbf{S}_{rm}\\ \nabla\cdot C_e\nabla T_e-S_{re}\\ -p_e\nabla\cdot\mathbf{u}+\nabla\cdot C_e\nabla T_e+\frac{\rho k_B(T_i-T_e)}{M_pA\tau_{ei}}-(S_{re}-\mathbf{S}_{rm}\cdot\mathbf{u})\end{array}\right\}$$

radiation/electron momentum exchange

electron conduction

Compression work

collisional exchange

radiation/electron energy exchange

Predictive science is more than prediction

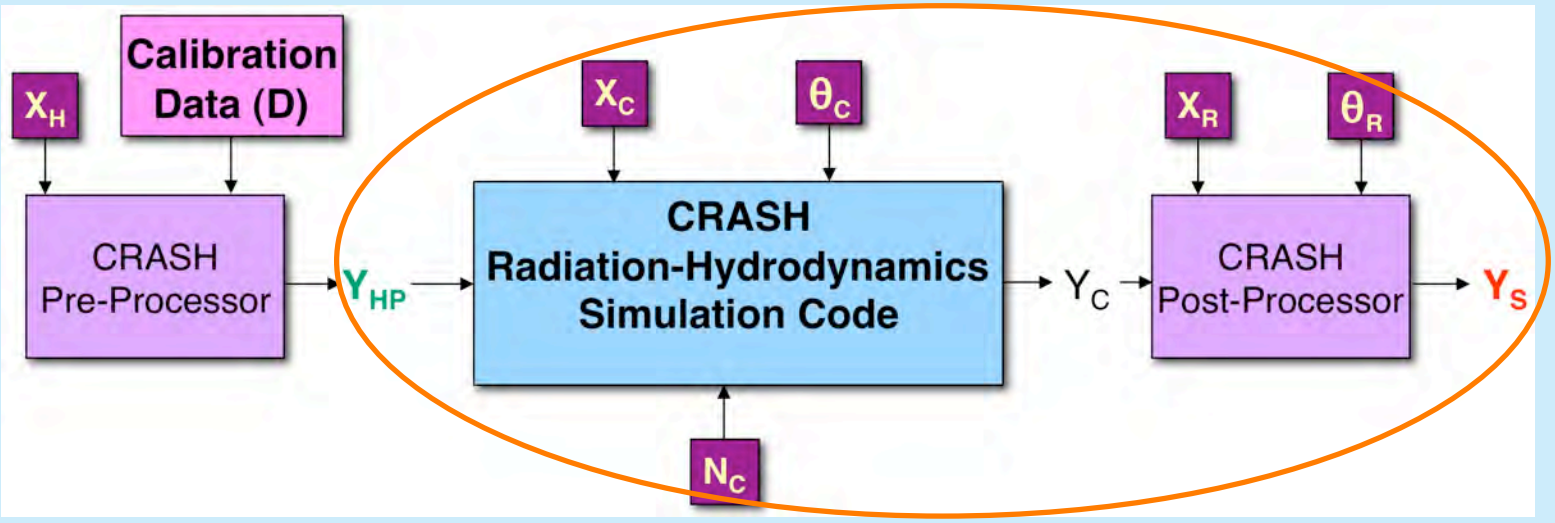
- Knowledge of the sensitivity of the output to variations in the input
  - Which input parameters, when varied over their probable ranges, generate the significant variations in output
- An understanding of the significant sources of uncertainty in output
- An estimate of the predictive *distribution* of outputs over
  - Uncertainty in physics parameters
  - Uncertainty in experimental parameters
  - Uncertainty in statistical fitting parameters
- Successful prediction means that the experimental result is, with reasonable probability, within the range predicted by the code

Verification and Testing

- New program units are implemented with unit tests
  - Unit tests must be complete and run in seconds.
- New features are implemented together with verification tests
  - Weekly verification tests are run on a 16 core Mac.
  - Tests should cover all aspects of the new feature.
  - Using grid convergence studies and model-model comparison.
- Compatibility and reproducibility of features are checked with the functionality test suite
  - Nightly runs ensure that bugs are discovered early
  - Running on 7 different platforms/compilers tests portability

We understand CRASH as a map from input to output

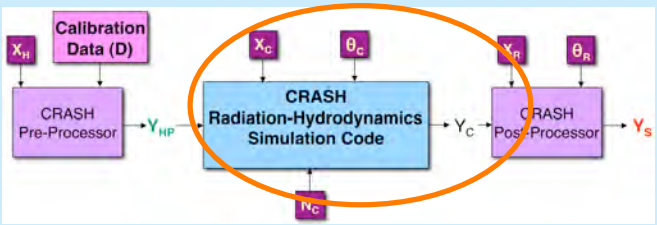
- CRASH maps inputs to output $$Y_s = \eta(X, \theta, Y_{\mathrm{HP}})$$



- We want to characterize the variations in η around interesting ranges of inputs $(X, \theta, Y_{\mathrm{HP}})$
  - Sensitivities
  - Predictive distributions
- Numerics converged sufficiently to be small contributor to overall uncertainty

Focus of current UQ efforts

A predictive model provides a pdf of outputs



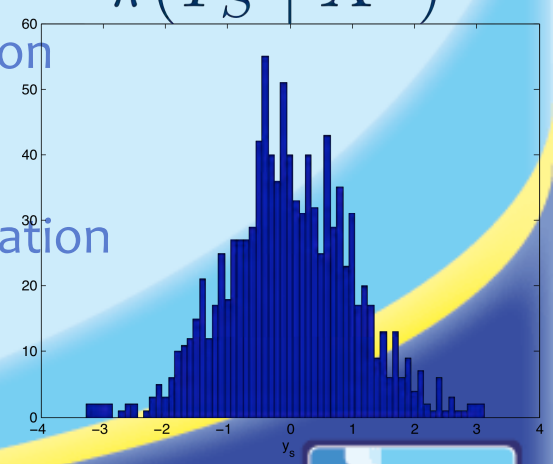
- Construct predictive model of output

$$Y_s = \hat{Y}(X, \theta, Y_{\mathrm{HP}}, \mathrm{Measurements})$$

along with posterior calibration pdf

$$\pi(\theta \mid \mathrm{Measurements})$$

- Combine with estimated $\pi(X)$ or input ranges to account for input uncertainty

- Such a model provides:
  - Mean and variance of output – predictive distribution
  - Tool to explore error in the model relative to experiment
  - Approach to determine a next experiment or simulation to reduce uncertainty

$$\pi(Y_S \mid X^*)$$