



Center for Radiative Shock Hydrodynamics

April 2013 TST meeting

Project Overview
R Paul Drake

Shock waves become radiative when ...

- radiative energy flux would exceed incoming material energy flux



where post-shock temperature is proportional to u_s^2 .

- Setting these fluxes equal gives a threshold velocity of 60 km/s for our system:

Material	xenon gas		
Density	6.5 mg/cc	Initial ion temperature	2 keV
Initial shock velocity	200 km/s	Typ. radiation temp.	50 eV

I will show you

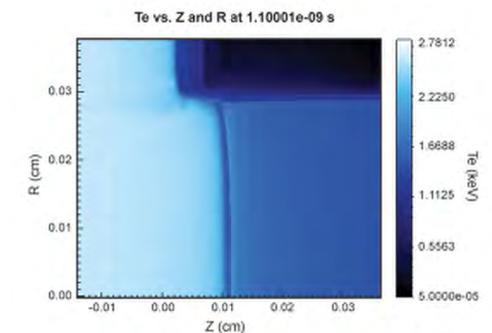
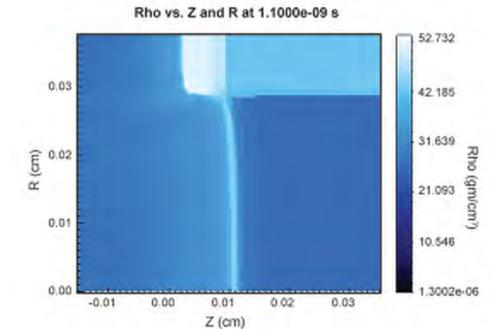
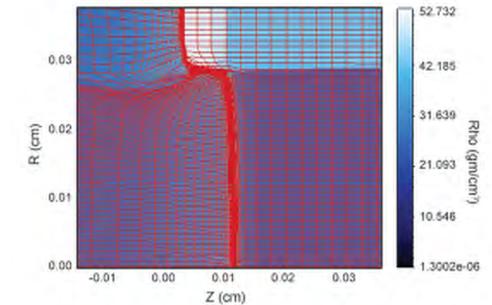
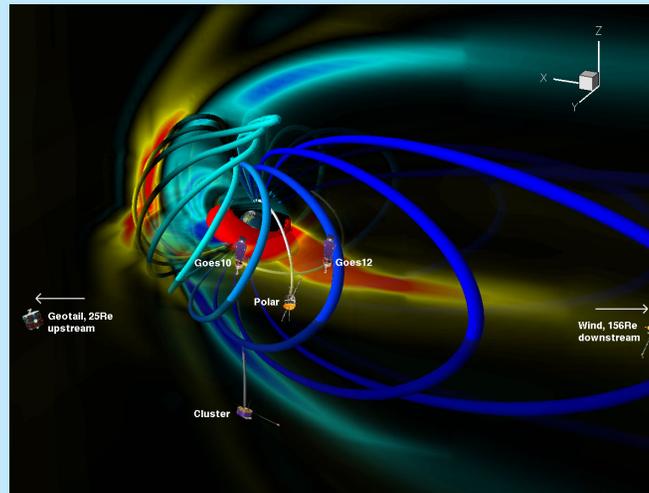
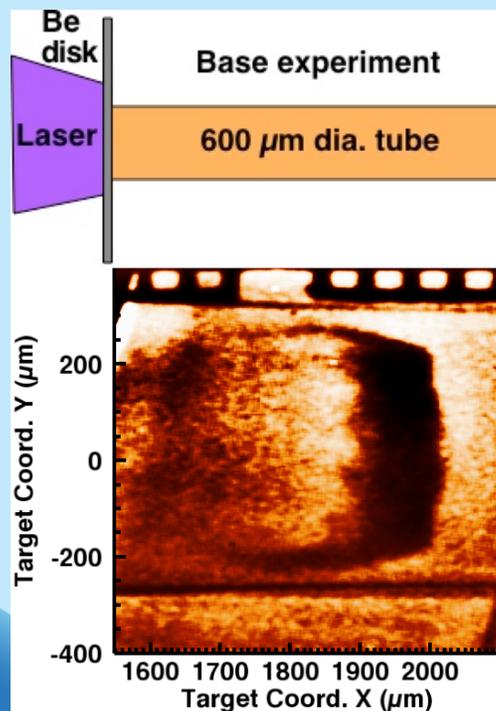
- Where we are, and
- How we got here, and
- Point toward ongoing work on a few issues discussed later today

CRASH is completing the primary project goals

- **CRASH has completed the year 5 (elliptical tube) experiment and analysis of the data**
- **The CRASH code has run effectively since late 2011 in support of run sets for assessment of predictive capability**
 - Also has proven effective in support of other experiments
- **CRASH has completed an initial assessment of predictive capability by comparing predictions based on run sets and circular-tube data to elliptical-tube data**
 - For shock location the predictions differ from observations by about 10%
 - This is of order the experimental variability and achieves our stated goal
 - Work with other metrics is ongoing
 - Difference perhaps attributable to combined effects of diffusion rad tran model and 3D geometry

We started with a few pieces

- A base experiment
- A space weather code
- A (black box) laser energy deposition code
- A primitive version of PDT for linear Boltzmann

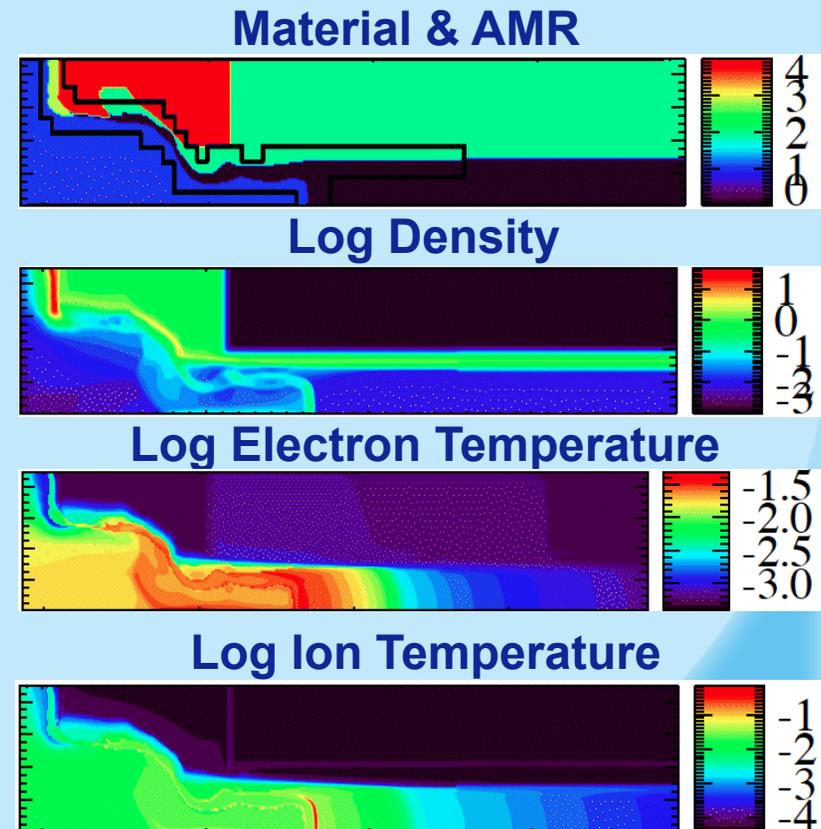


We extended the code to high energy density

- **CRASH 3.2**
 - Hydro equations with relevant source terms
 - Dynamic AMR
 - Level set interfaces
 - EOS
 - Self-consistent EOS and opacities for 5 materials
 - STA Xe opacities
 - Multigroup-diffusion radiation transport
 - Electron physics and flux-limited electron heat conduction

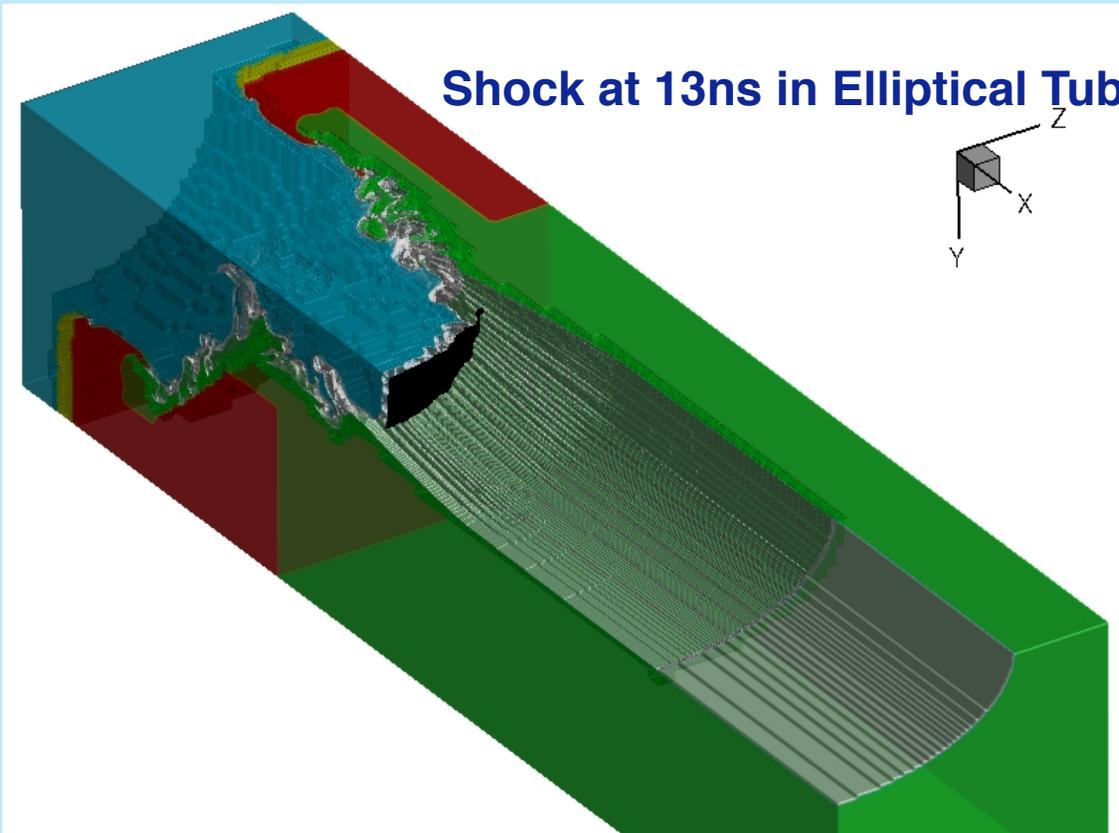
- This involved implementation of many verification tests

- Eventually we added a laser package



3D Nozzle to Ellipse @ 13 ns

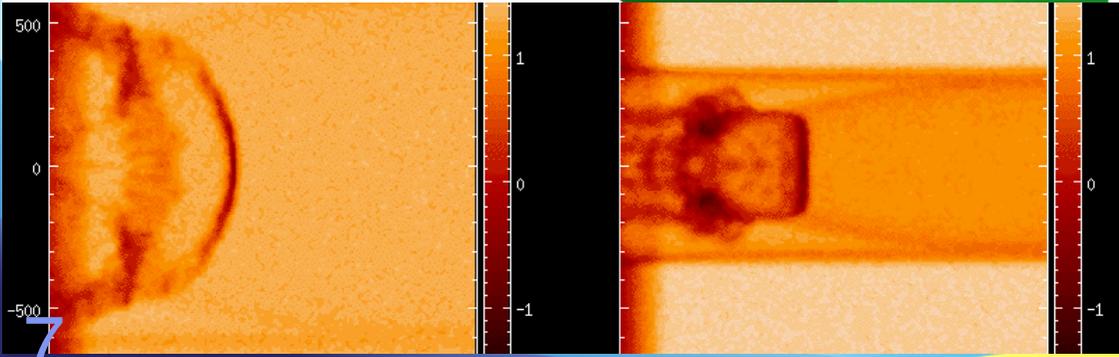
A key point in code development was simulations of the year-5 experiment



Elliptical simulations
(H2D initiated):

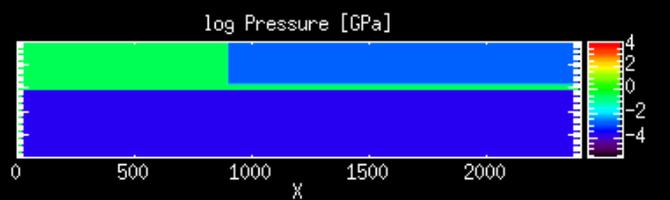
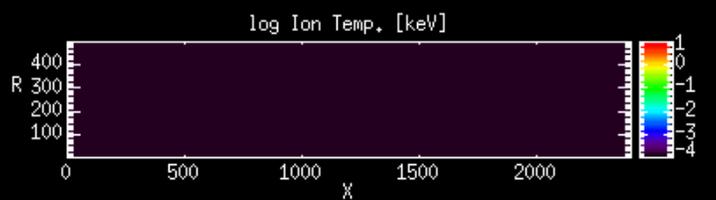
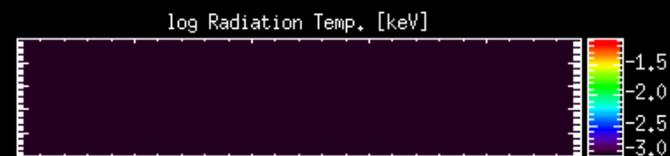
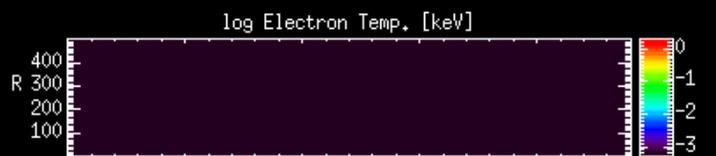
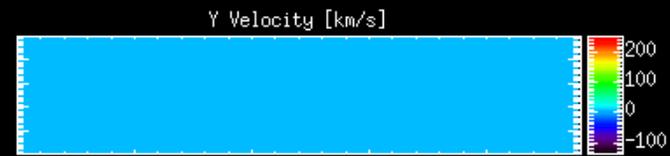
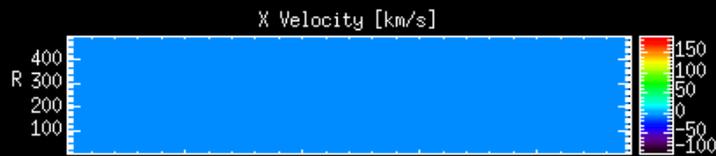
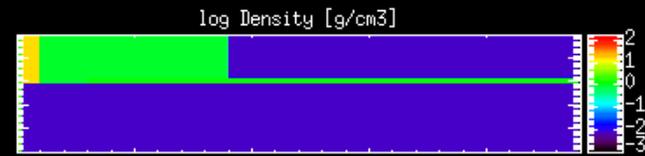
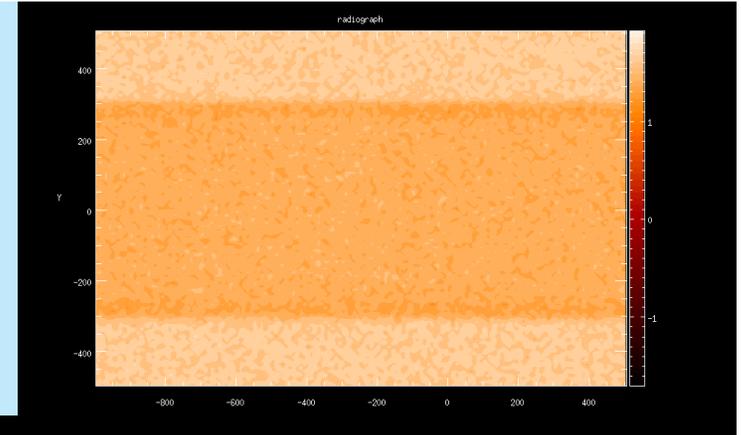
Van der Holst et al,
HEDP 2012

13 ns multigroup



Doing all this gave reasonable fidelity for the base experiment

- By the middle of year 4

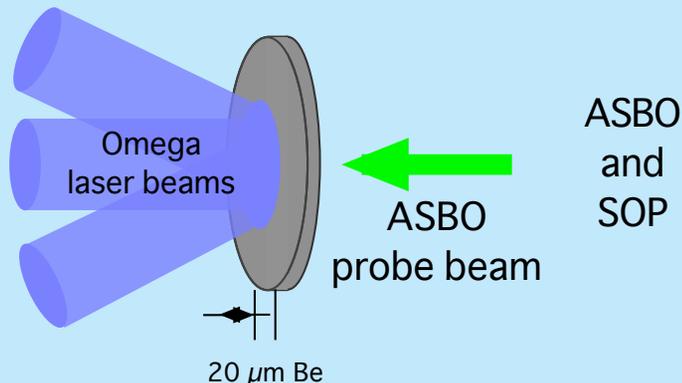
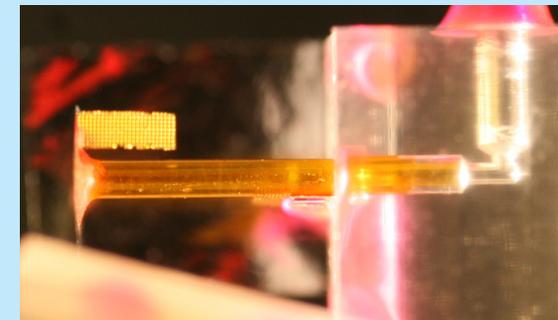


time = 0.0 ns

The experiments addressed the needs of UQ

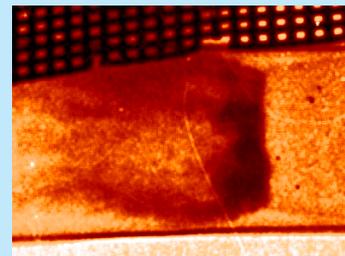
- The year 1 and 5 experiments assessed experimental variability for the circular and elliptical cases
- The year 2 through 4 experiments were mainly in service of code fidelity

Early time radiographs

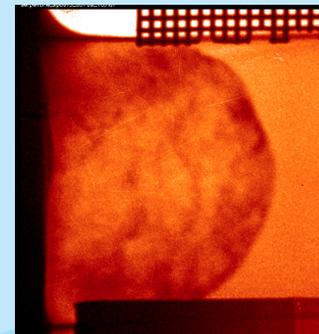


Shock breakout

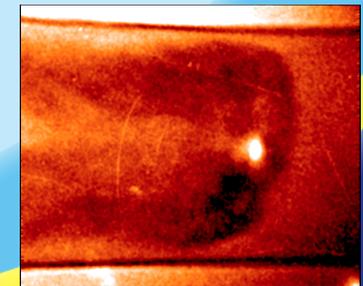
600 μm tube



1200 μm tube



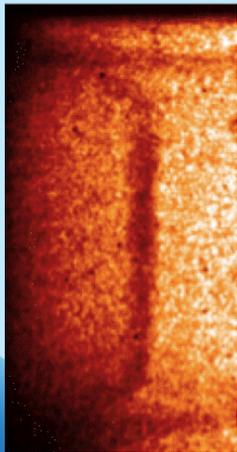
Circular nozzle



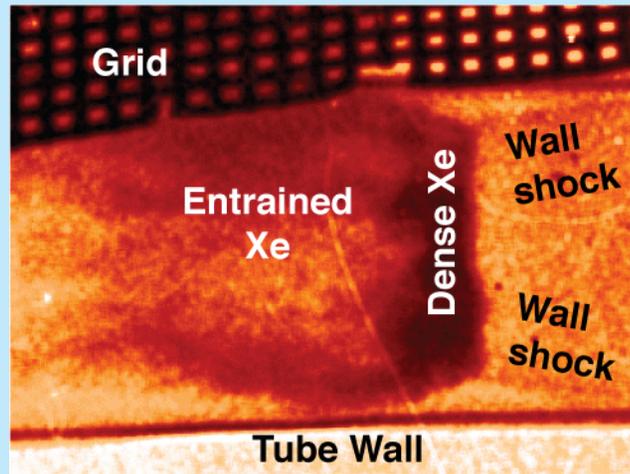
Our radiographic studies provided foundational data for code assessment

- Bayesian analysis of tilt gives compression ~ 22
 - Doss HEDP, A&SS 2010
- Shock-shock interactions give local Mach number
 - Doss PoP 2009
- Shape of entrained flow reveals wave-wave dynamics
 - Doss PoP 2011
- Thin layer instability; scaling to supernova remnants
 - Doss thesis & to be pub.

3.5 ns

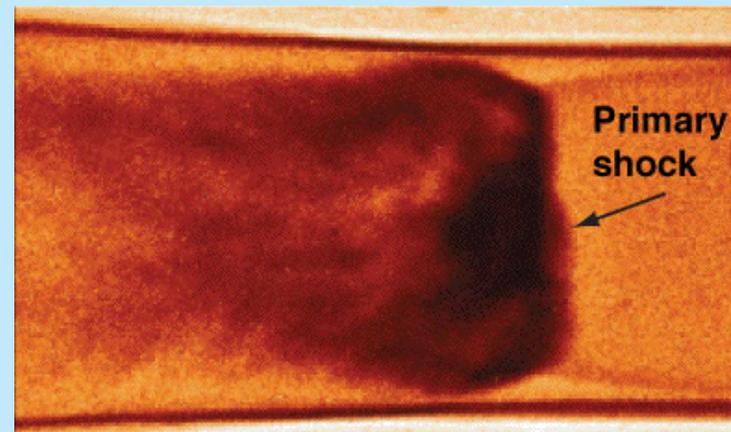


13 ns



Radiographs

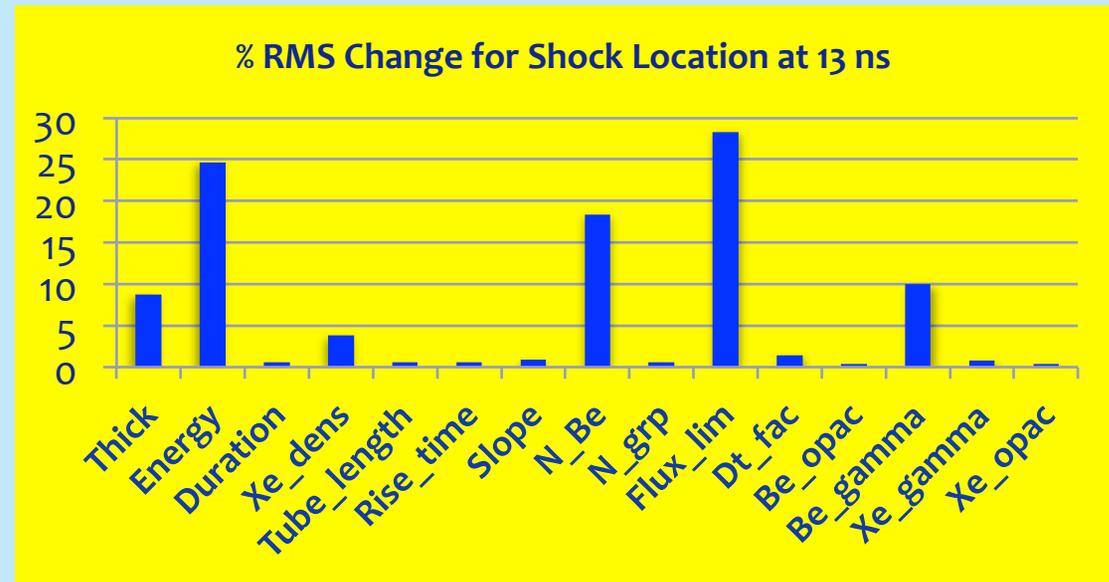
26 ns



Credit:
Carolyn Kuranz

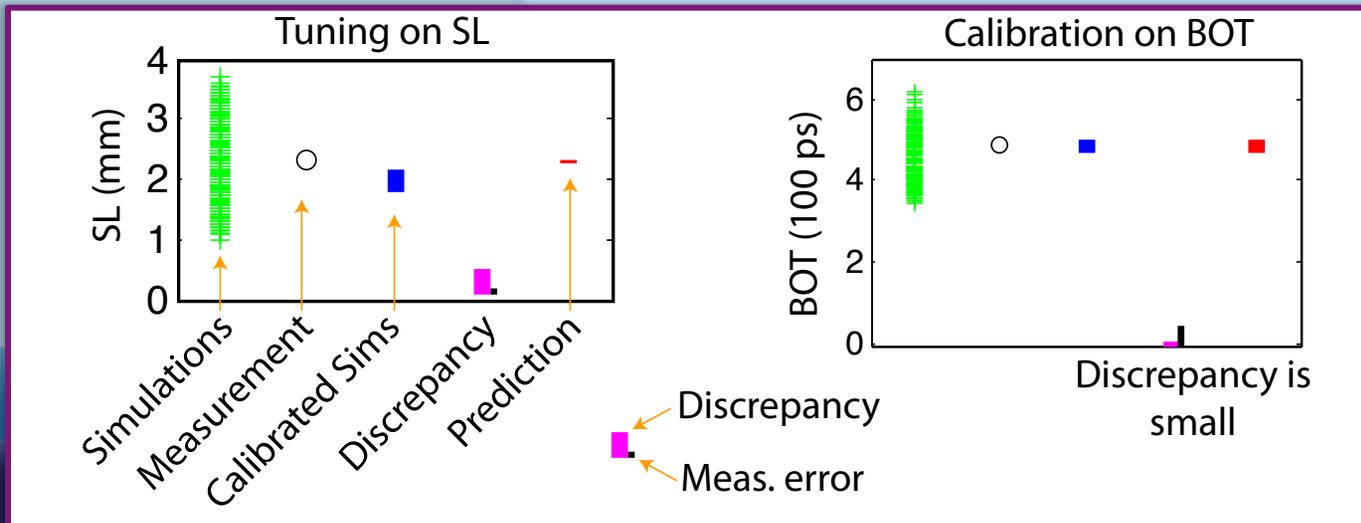
We used the work of our early years to develop and demonstrate techniques for prediction

- Sensitivity studies
- Approaches to metrics
- Predictive studies using 1D simulations



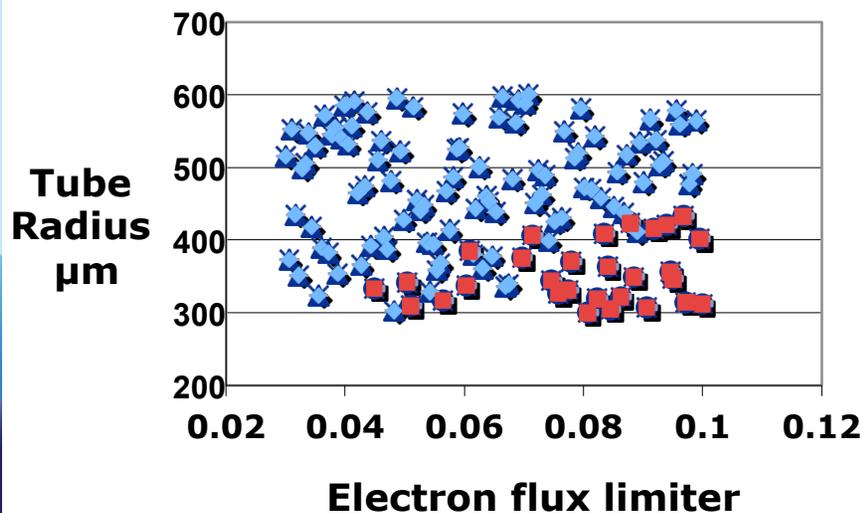
$$y_m = \eta(x, \theta) + \delta(x) + \epsilon$$

$$y_c = \eta(x, \theta_c)$$



As our codes evolved, we did many run sets to support UQ

- A substantial fraction of our activity
 - Defining
 - Initiating via a formal process
 - Running (as platforms change)
 - Processing
 - Analyzing
 - Reacting
- Many people & interactions
 - RS 4: 104 2D on base expt
 - RS 5: 512 1D on numerics
 - RS 6: 128 2D on numerics
 - RS 7: ~~128~~ 99 for nozzles
 - The final H2D runset (**ugh!**)
 - RS 8: 27 2D Nozzle properties
 - RS 9: 10 3D Ellipticity and shape
 - RS 10: 128 2D base CRASH
 - With laser package
 - RS 11: 128 2D base CRASH
 - Updated laser physics and parameter ranges from RS10
 - RS 12 -14 discussed later



H2D could not get the job done

From early work, we developed a new statistical model for combining outputs from multi-fidelity simulators

- Used simulations from 1-D and 2-D models
- 2-D models runs come at a higher computational cost
- Used all simulations, and experiments, to make predictions
- **1-D CRASH Simulations**
 - 1024 simulations
 - Experiment variables: Be thickness, Laser energy, Xe fill pressure, Observation time
 - Calibration parameters: Electron flux limiter, Laser energy scale factor
- **2-D CRASH Simulations**
 - 104 simulations
 - Experiment variables: Be thickness, Laser energy, Xe fill pressure, Observation time
 - Calibration parameters: Electron flux limiter, Wall opacity, Be gamma

Our joint model using two simulation codes

Common theta values put
in M1 & M2

M1-theta tuned
to model M2

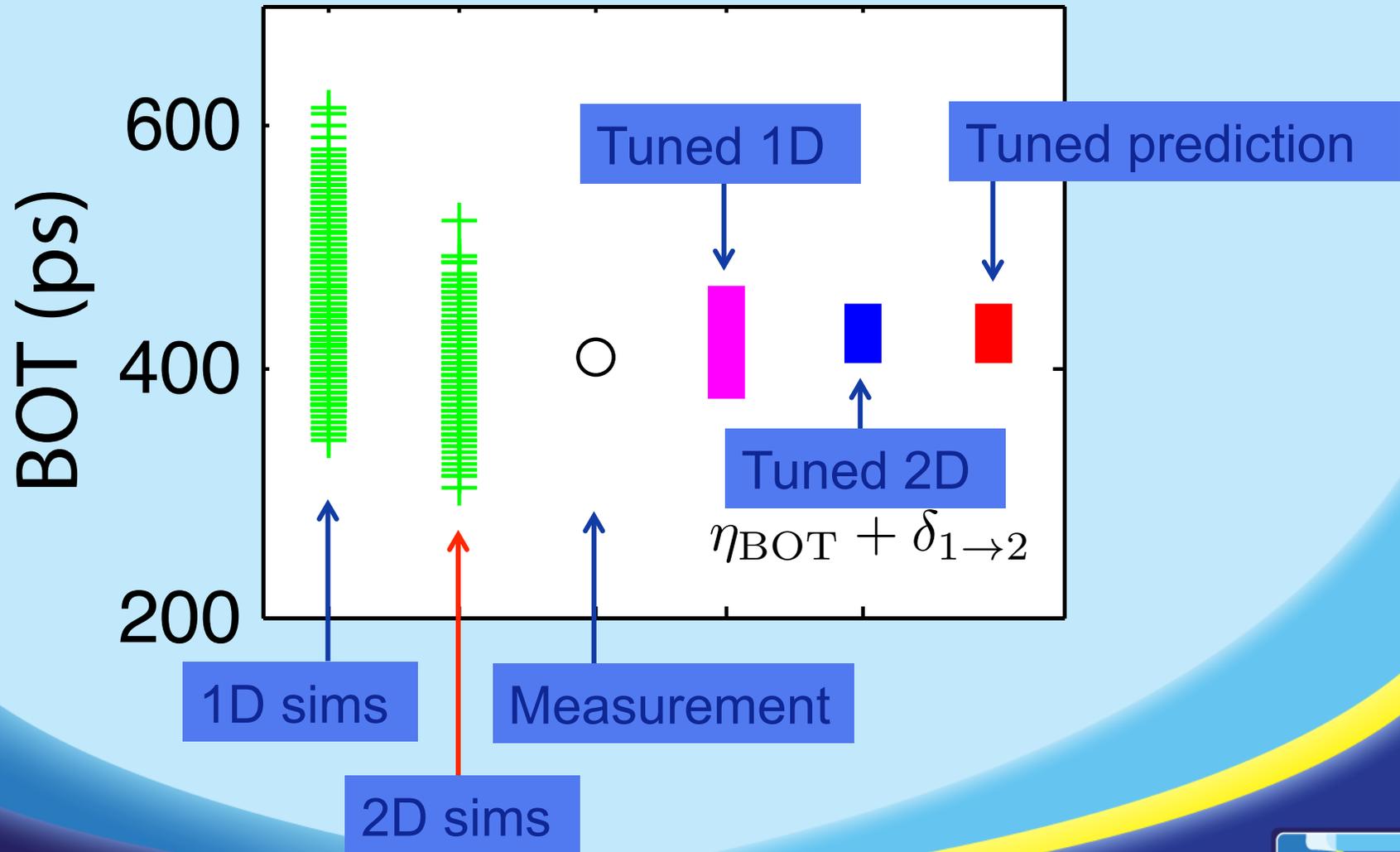
Theta values put in
model M1 only

Theta values in
M2 only

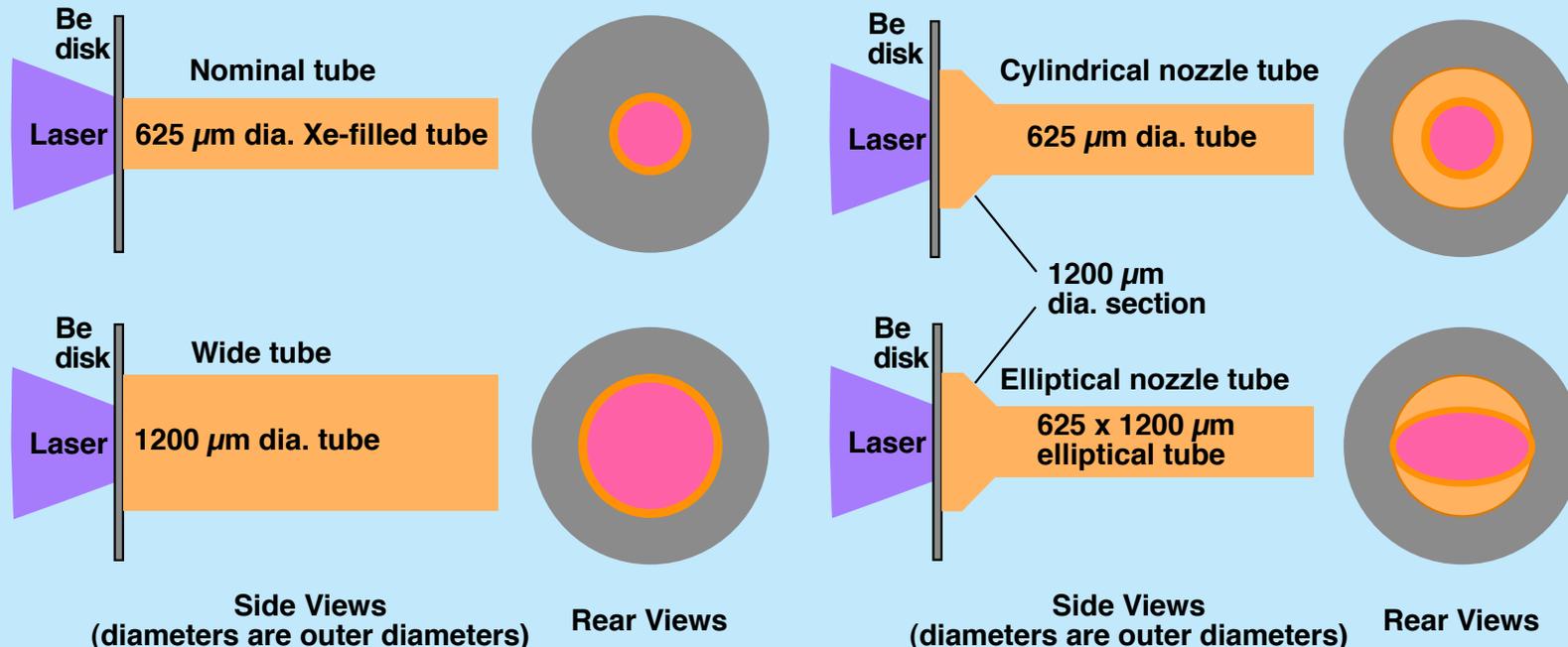
$$\begin{aligned} \text{BOT}_1 &= \eta_{\text{BOT}}(x, t_1, t_c) \\ \text{BOT}_2 &= \eta_{\text{BOT}}(x, \theta_1, t_c) + \delta_{1 \rightarrow 2}(x, t_2, t_c) \\ \text{BOT}_m &= \eta_{\text{BOT}}(x, \theta_1, \theta) + \delta_{1 \rightarrow 2}(x, \theta_2, \theta) \\ &\quad + \delta(x) + \epsilon \end{aligned}$$

Tuned values of theta

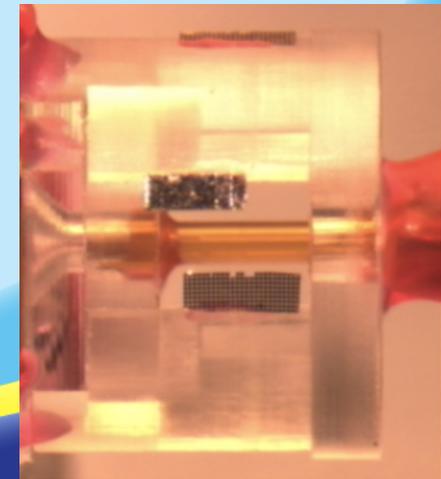
We used 1D & 2D run sets to predict shock breakout time



The year 4 and 5 experiments were new



- We met the necessary challenges in fabrication
 - The circular to elliptical transition was not trivial



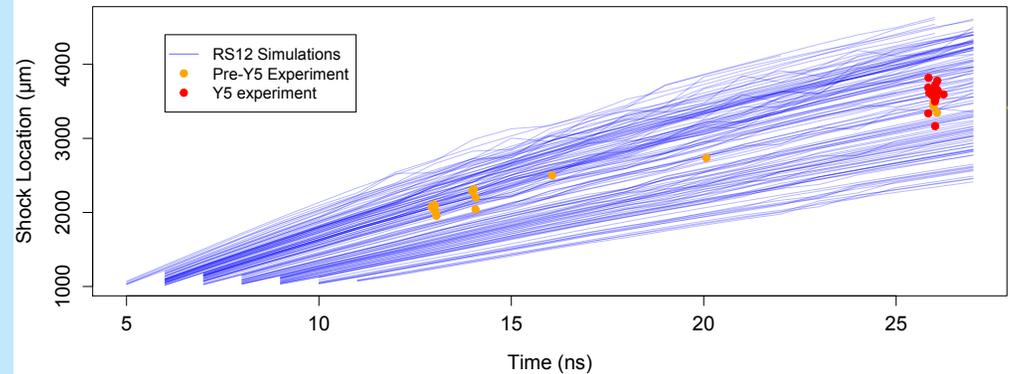
We used CRASH 3.2 to do run sets in support of predictions for the year 5 experiment

- **RS12:**
 - 128 2D base CRASH runs
 - Laser package with fully 3D ray tracing
 - Revised parameter ranges to adequately provide coverage of reasonable values
- **RS13:**
 - 80 3D base CRASH runs with gray radiation
 - Laser deposition phase carried out in 2D CRASH with conditions mapped to the 3D mesh after the laser pulse ends
 - Full year-5 experimental geometry
- **RS 14:**
 - Same as RS13 with multigroup radiation
 - Still running, slowly

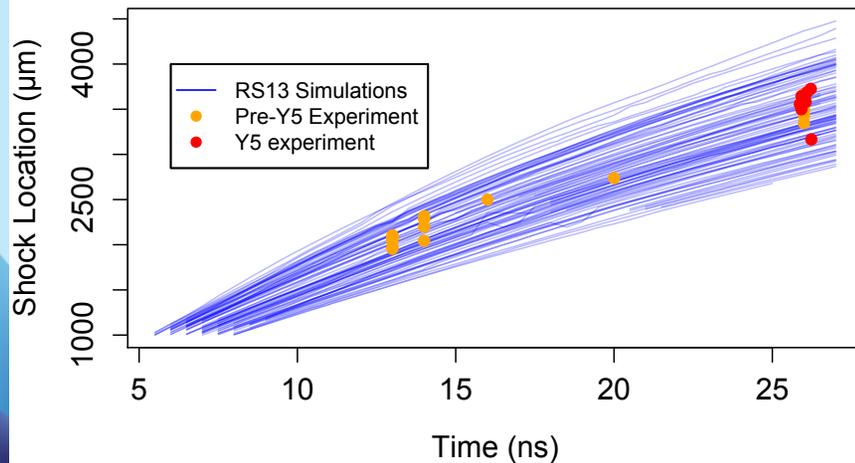
It is far from trivial to get adequate run sets

- **Challenges include**
 - Spanning what turns out to be the data
 - Identifying need for changes in the runs when the experiment evolves
 - One improves with practice

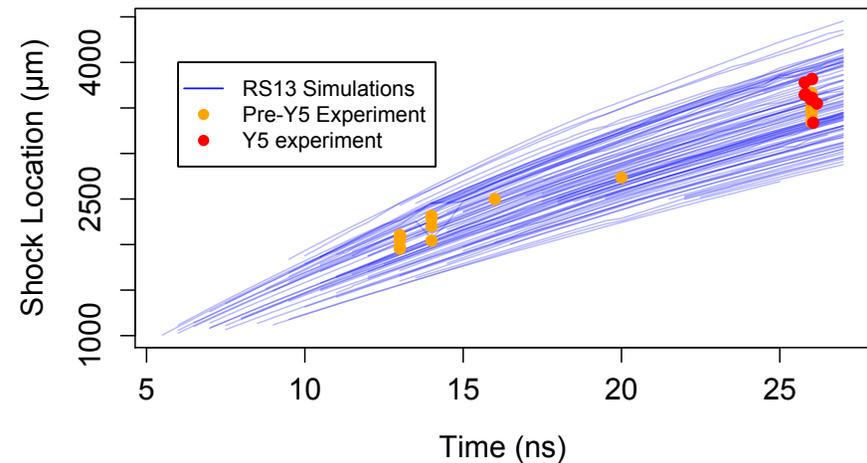
Shock location vs time from cylindrical runs



Shock Location vs Time on the Major Axis



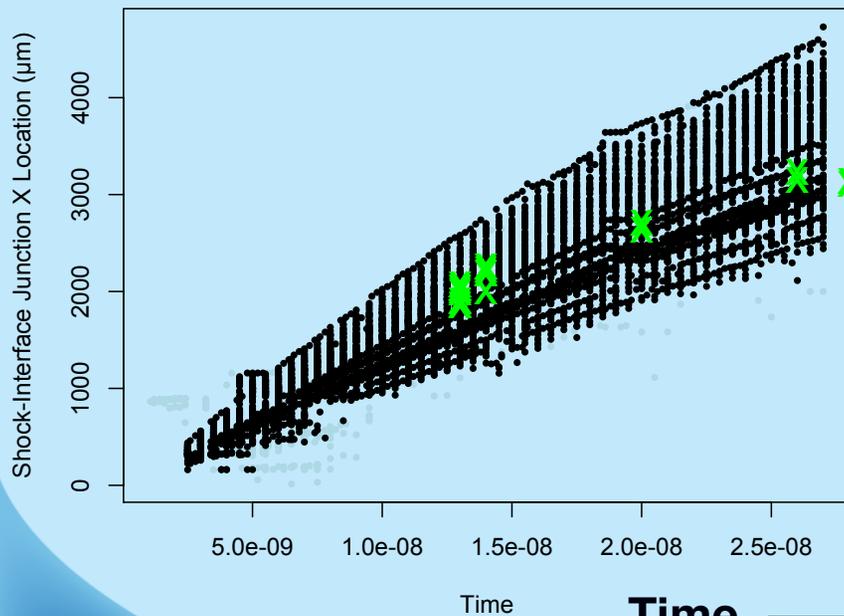
Shock Location vs Time on the Minor Axis



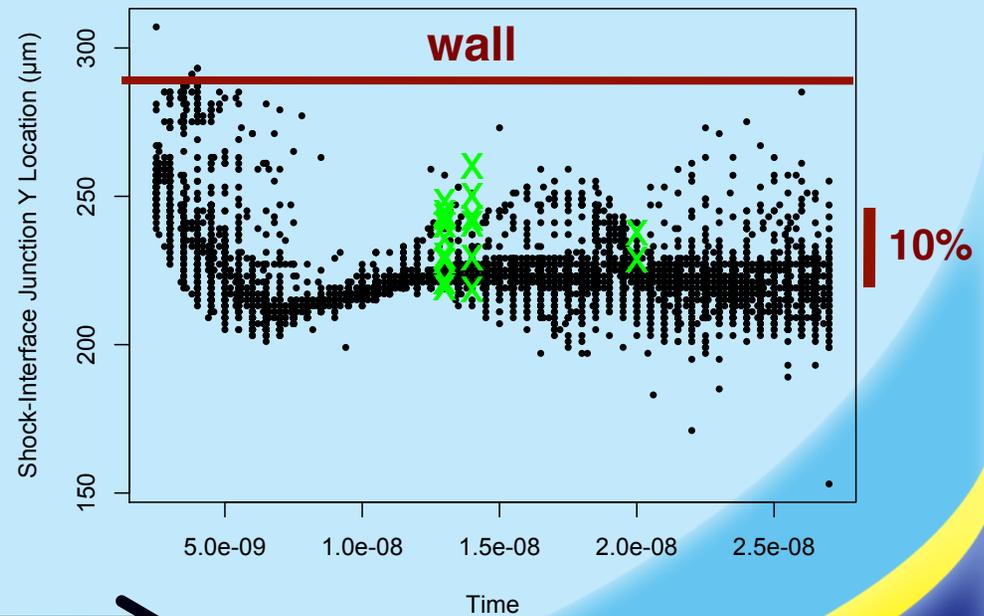
We are (just) now able to use the junction of the primary shock and wall-shock interface as metrics

- Results from RS12 and cylindrical tube data
 - Each black dot is from one run at one time
 - Green X's are experimental data

Location along axis



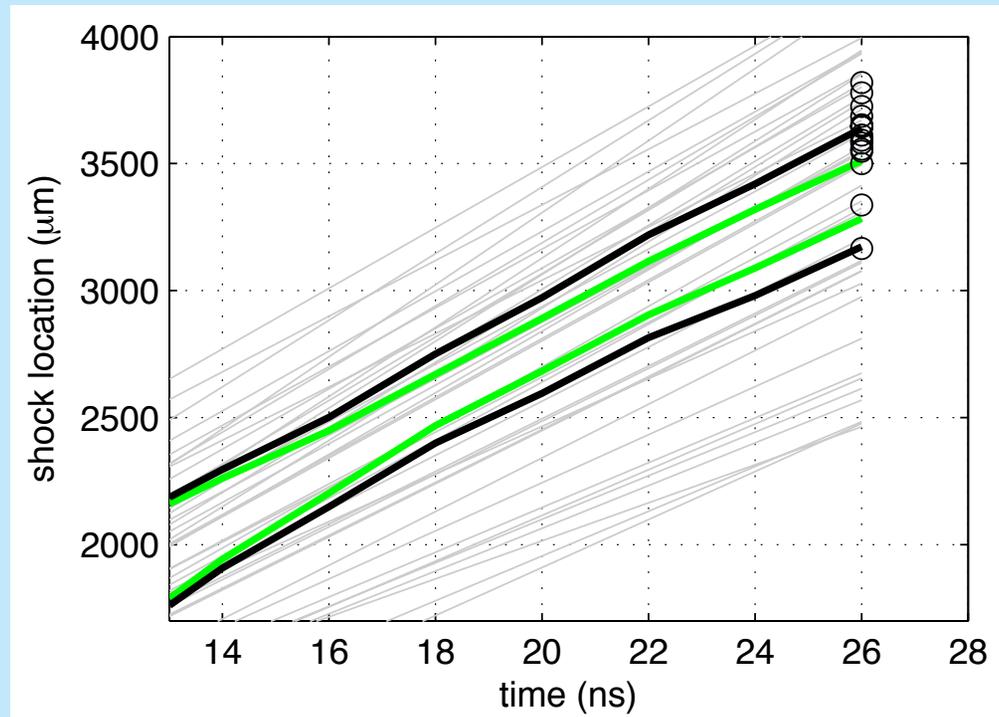
Location transverse to axis



- Mike Grosskopf will explain the details

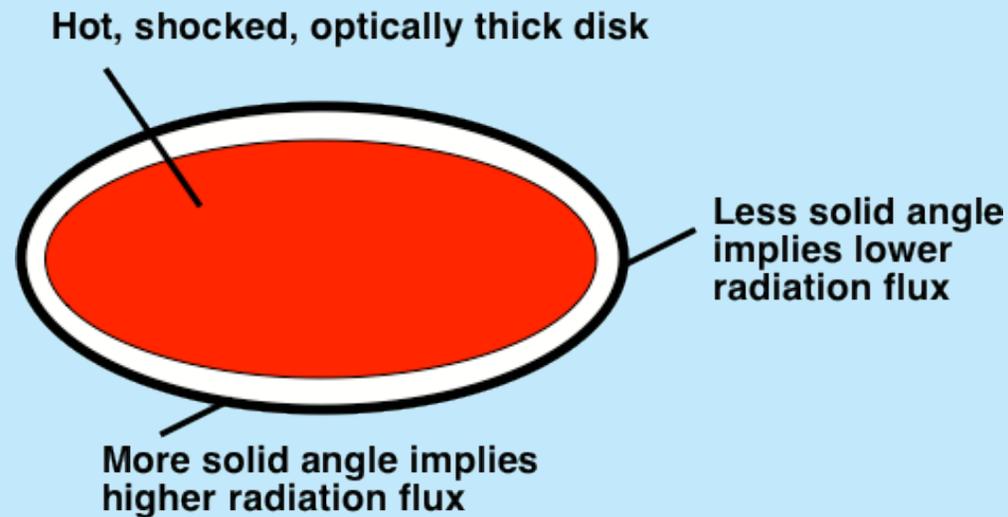
We applied our predictive methodology to the year 5 experiment

- You will hear much more about this next from Derek Bingham
- Median prediction = 3401.3
- All but one observation is within 10% of median prediction
- Largest value is differs from median by 10.92%



The difference between predictions and observations may reflect the detailed interplay of radtran and hydro

- The wall shock in the nozzle helps choke off some downstream flow
 - Our diffusive radtran model should get the wall heating wrong
 - < 20% difference in net forward momentum would match the data



- We are at the level of differences of order the experimental variability: this was our stated goal

Throughout we made progress in code development

- **CRASH 3.2**
 - Flux limited electron heat xport
 - EOS source adaptivity
 - Laser package
 - Improved multigroup preconditioner
 - Better use of level sets
 - Improved scaling with HYPRE
 - Non-LTE
- **PDT**
 - Implemented thermal radiation
 - Improved single-core performance
 - Optimal sweeps → parallel scaling
 - Developed STAPL; ported PDT
- **After CRASH 3.2**
- **Improved physics**
 - Non-LTE
 - Field-aligned heat conduction
 - Magnetic field effects in rz-geometry
- **Improved algorithms**
 - Support for higher-order schemes
 - Semi-implicit resistivity terms
- **Improved code**
 - Generalized initialization routines, including using 2D output to initialize 3D run
 - Finalized integration with the improved adaptive-mesh library, BATL

Years 1 through 4 involved many elements of progress in UQ

- **Predictive studies**
 - Predictive study involving calibration
 - Predictive study with calibration from H2D run set
 - Predictive method involving joint models
 - Predictive study with joint models and calibration/tuning

- **UQ**
 - Deep analysis of experimental sources of uncertainty
 - Radiograph interpreters for integrated metrics
 - Hydro validation studies
 - Extensive studies of output sensitivities
 - Experimental parameters
 - H2D parameters and use
 - Physical parameters
 - Fidelity with AMR
 - Solver details

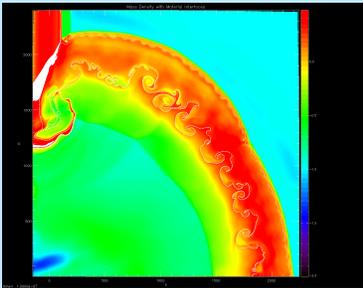
- **Continued solid code engineering practices**
 - Many code verification tests
 - Our code comparison project proved useful to LANL

We did a fair bit of physics along the way too

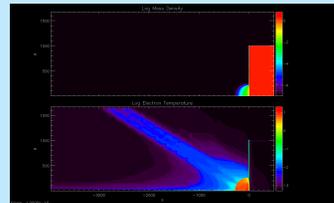
- **We published or are preparing papers on**
 - Wall shock and related flows
 - Relevant radtran & radhydro theory
 - The specific physics of our shocks
 - X-ray driven walls theory
 - SN/FLD comparison
- **We also did substantial work on**
 - Obtaining STA opacities
 - Non-LTE effects
 - SN/FLD comparison

We now use CRASH in support of all our HED experiments

Diverging Rayleigh-Taylor



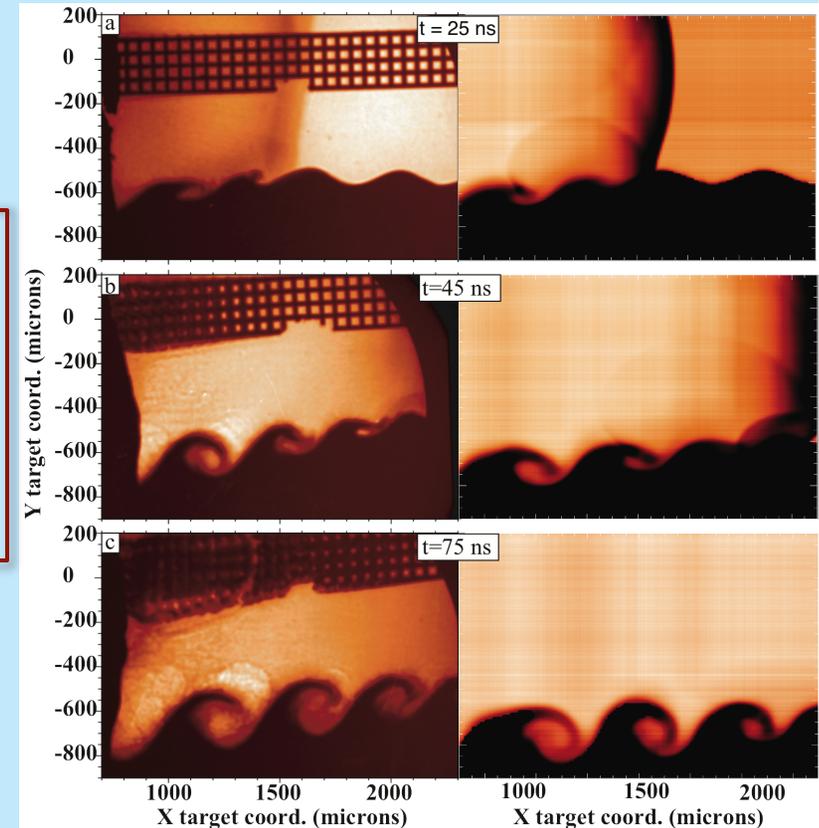
Ablative flows



Kelvin Helmholtz experiments

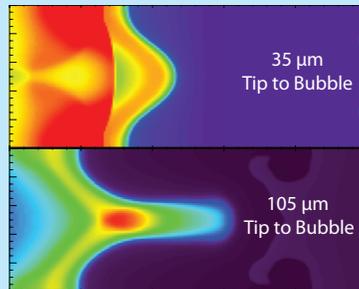
Data

CRASH



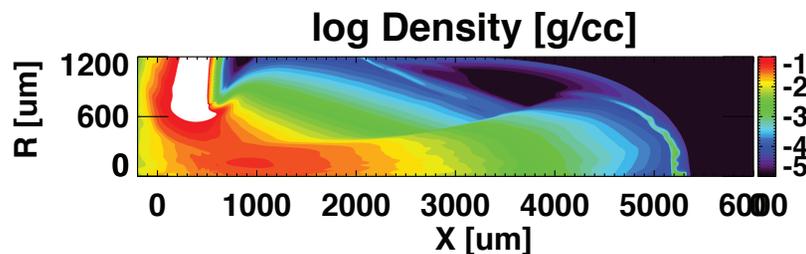
High Drive:
310 eV Tr source

Low Drive
207 eV Tr source



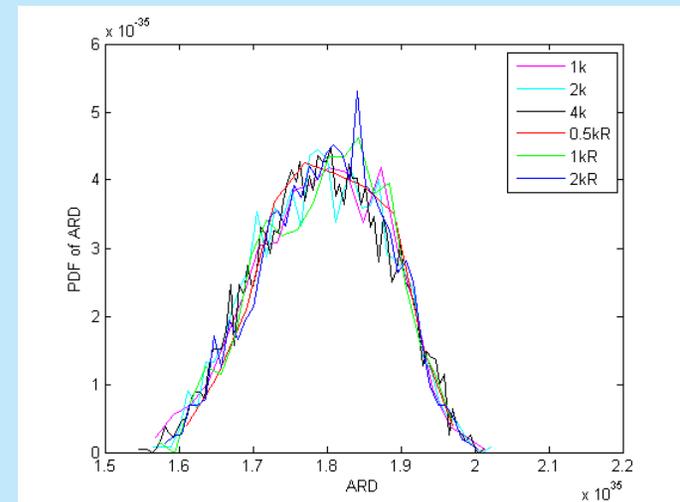
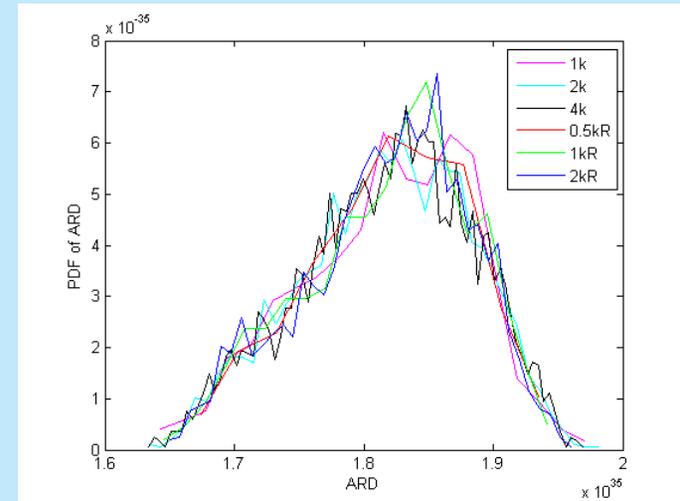
Rayleigh-Taylor growth in the presence of a radiative shock

Plasma jets



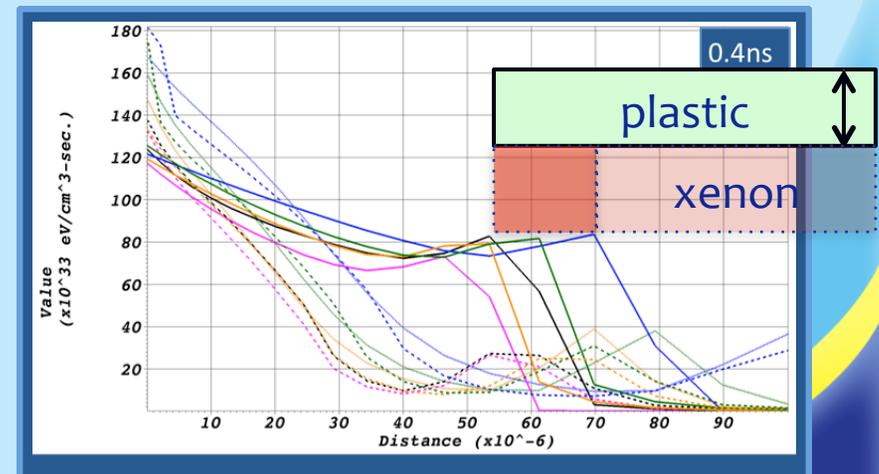
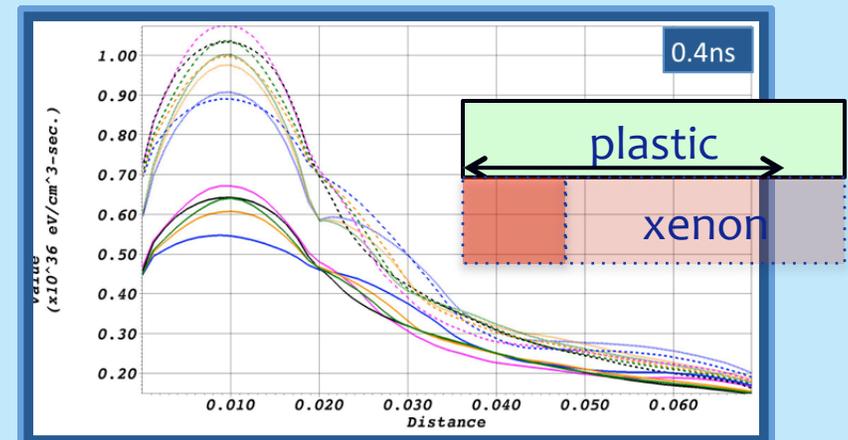
With PDT and CRASH-opacity we studied opacity UQ

- Treated inputs to CRASH-opacity code (not opacities themselves) as the uncertain inputs.
- Used 1D axial and radial problems to screen parameters
 - Involved 32k runsets – sets of 32k opacity tables with 32k PDT runs
- Used thousands of 2D runs (each with unique opacity table) to explore variations in Absorption Rate Densities in plastic wall.



With PDT we studied energy deposition in the wall

- We varied spatial, energy, and directional resolution
- We examined Abs.Rate.Density (ARD) as a function of time and position in the plastic
- Gray is terrible. 10-group not grossly different from 50-group, which is close to 99-group.
- S6 (24 directions in 2D) and S8 (40) show differences relative to S16 (144).



We have also addressed several issues of past concern

- **Diffusion vs transport (Myra and TAMU Talk)**
- **Non-LTE effects (Sokolov talk)**
 - Evidence indicates no important effects for metrics
- **Solution verification (Fryxell talk)**
 - We have convergence on simple tests that extrapolates to small errors
 - Other tests and the full problem do not match well the assumptions underlying standard simple solution verification models
- **Also figured out how to extract better metrics for the wall shock, finally (Grosskopf talk)**

Grad student summary

- **5 continuing students whose graduate student support has been > 40% from CRASH Sponsor funds.**
 - All have made lab visits
- **9 continuing students doing CRASH-related research having had < 40% CRASH sponsor fund support.**
 - 3 have made lab visits
- **19 graduated Ph.D.s (projected through summer 2018) who received direct or indirect CRASH support.**
 - 12 of them made 18 lab visits.
 - 4 of them are now working at NNSA labs and several others are working at other DOE labs
- **5 students who have left CRASH orbit or dropped.**
- **38 students total whose research has been directly or indirectly supported by CRASH**

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 - This is of order the experimental variability and achieves our stated goal
 - Work with other metrics is ongoing
 - Difference perhaps attributable to combined effects of diffusion rad tran model and 3D geometry

Supplemental material follows

CRASH Faculty	Where & what	UQ/APC	Scient. Comp.	Modeling & Theory	Experiments
Paul Drake, Director	UM Prof. AOSS				
Predictive Capability beyond traditional V&V					
James Holloway, Co-PI, lead	UM Prof. Nuclear	X		X	
Bruce Fryxell, chief scientist	UM AOSS Res. Sci.	X	X	X	
Natasha Andronova	UM AOSS Res. Sci.	X			
Krzysztof Fidkowski	UM Prof. Aero	X		X	
Bani Mallick	TAMU Prof. Stats	X			
Vijayan Nair	UM Prof. Stats & IOE	X			
Derek Bingham	SFU Prof. Stats	X			
Scientific Computing					
Quentin Stout, Co-PI, lead	UM Prof. CSE	X	X		
Nancy Amato	TAMU Prof. CompSci		X		
Lawrence Rauchwerger	TAMU Prof. CompSci		X		
Code Development and Traditional V&V					
Ken Powell, Co-PI, lead	UM Prof. Aero		X	X	
Gabor Toth, Software Archit.	UM AOSS Res. Sci.		X	X	
Igor Sokolov	UM AOSS Res. Sci.			X	
Bart van der Holst	UM AOSS Res. Sci.			X	
Eric Myra	UM AOSS Res. Sci.	X	X	X	
Ben Torralva	UM MSE Res. Sci.		X	X	
Modeling and Theory					
Marv Adams, Co-PI	TAMU Prof. Nuclear	X	X	X	
Tamas Gombosi	UM Prof. AOSS			X	
Ed Larsen	UM Prof. Nuclear	X		X	
Eric Johnsen	UM Prof. Mechanical			X	
Smadar Karni	UM Prof. Math			X	
Bill Martin	UM Prof. Nuclear	X	X	X	
Ryan McClarren	TAMU Prof. Nuclear	X	X	X	
Jim Morel	TAMU Prof. Nuclear			X	
Phil Roe	UM Prof. Aero			X	
Katsuyo Thornton	UM Prof. MSE			X	
Bram van Leer	UM Prof. Aero			X	
Marcel Klapisch	ARTEP			X	
Michel Busquet	ARTEP			X	
Experiments					
Paul Keiter	UM AOSS Res. Sci.				X
Carolyn Kuranz	UM AOSS Res. Sci.				X

Grad Students	Advisor	UQ/APC	Scient. Comp.	Modeling & Theory	Experiments
Baker, Eric	Larsen			X	
Barbu, Anthony	Adams and Morel			X	
Cheatham, Jesse (graduated)	Holloway and Martin			X	
Chou, Jason	Fryxell and Drake	X			
Dahm, Johann	Fidkowsky	X			
Davidson, Greg (graduated)	Larsen			X	
Di Stefano, Carlos	Kuranz and Drake				X
Doss, Forrest (graduated)	Drake			X	X
Edwards, Jarrod	Morel and Adams			X	
Fein, Jeff	Holloway and Drake	X		XX	X
de Frahan, Marc	Johnsen			X	
Gamboa, Eliseo	Drake				X
Goh, Joslin	Bingham	X			
Hetzler, Adam	Adams	X			
Huntington, Channing	Drake				X
Krauland, Christine	Drake and Kuranz				X
Magino, Peter	Morel			X	
MacDonald, Michael	Drake				X
Moran, Tiberus	Holloway			X	
Movahed, Pooyah	Johnsen			X	
Pandya, Tara	Adams			X	
Patterson, Nick	Thornton and Drake			X	
Poon, Patrick	Stout	X	X		
Smith, Tim	Rauchwerger		X		
Starinshak, Dave	Karni and Powell			X	
Stripling, Hayes	Adams	X		X	
Till, Andrew	Adams			X	
Visco, Tony	Drake				X
Wan, Wesley	Drake			X	
Young, Rachel	Kuranz and Drake		X	X	X
Zaide, Daniel	Powell and Roe			X	
Zhang, Zhanyang	Nair	X			
Technical Staff					
Mike Grosskopf	UM Sr. Res. Eng.	X	X		X
Donna Marion	UM Technician/Target Fab				X
Erica Rutter	UM Technician/ Codes	X	X		
Mauro Bianco	TAMU Post doc	X	X		
Guy Malamud	UM Post doc	X			
Avishek Chakraborty	TAMU Post doc				
W. Daryl Hawkins	TAMU Softwr Architect	X	X		
Sergey Manolov	TAMU Staff programmer	X	X		
Michael Adams	TAMU Staff programmer	X	X		
Administrative					
Kathy Norris	UM CRASH Admin				
Jan Beltran	UM Sr. Admin. Asst.				

We've invested real effort in scaling

- CRASH hydro on BG/L
- PDT transport on Sequoia (60% efficiency on 393k cores with STAPL-beta version)

