Various Challenges in Simulations Of Laboratory Astrophysics Experiments

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The team we work with at Michigan and on CRASH

- **Center for Radiative Shock Hydrodynamics (CRASH)**
  - **Staff:** Fryxell, Myra, Toth, Sokolov, van der Holst, Andronova, Torralva, Rutter, Trantham
  - **Grad students:** Patterson, Chou, and many others
  - **UM Professors:** Powell, Holloway, Stout, Martin, Larsen, Roe, van Leer, Fidkowsky, Thornton, Nair, Karni, Gombosi, Johnsen
  - TAMU: Adams, Morel, McClarren, Mallick, Amato, Raushberger, Hawkins
  - **Simon Frazer:** Bingham
  - ARTEP: Klapisch, Busquet

- **CLEAR Experimental Program**
  - **Grad students:** Visco, Huntington, Krauland, Di Stefano, Gamboa, Young, Wan, MacDonald
  - Many undergrads
  - **Staff:** Grosskopf, Klein, Lowenstern, Gillespie, Susalla
  - (Many scientific collaborators beyond UM not listed here)

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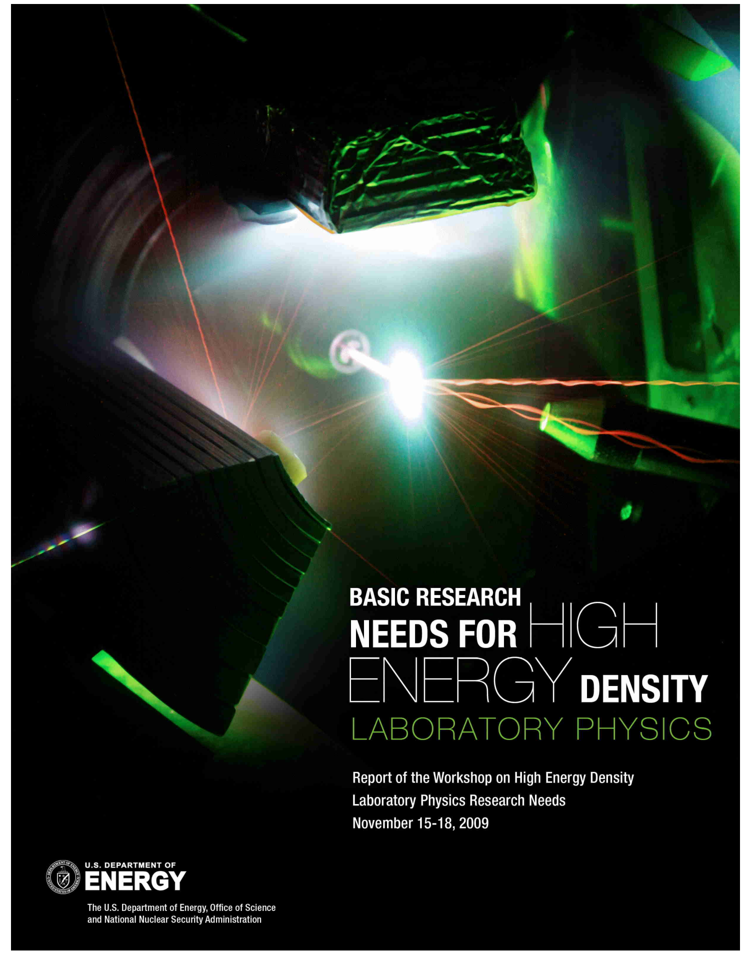
CRASH

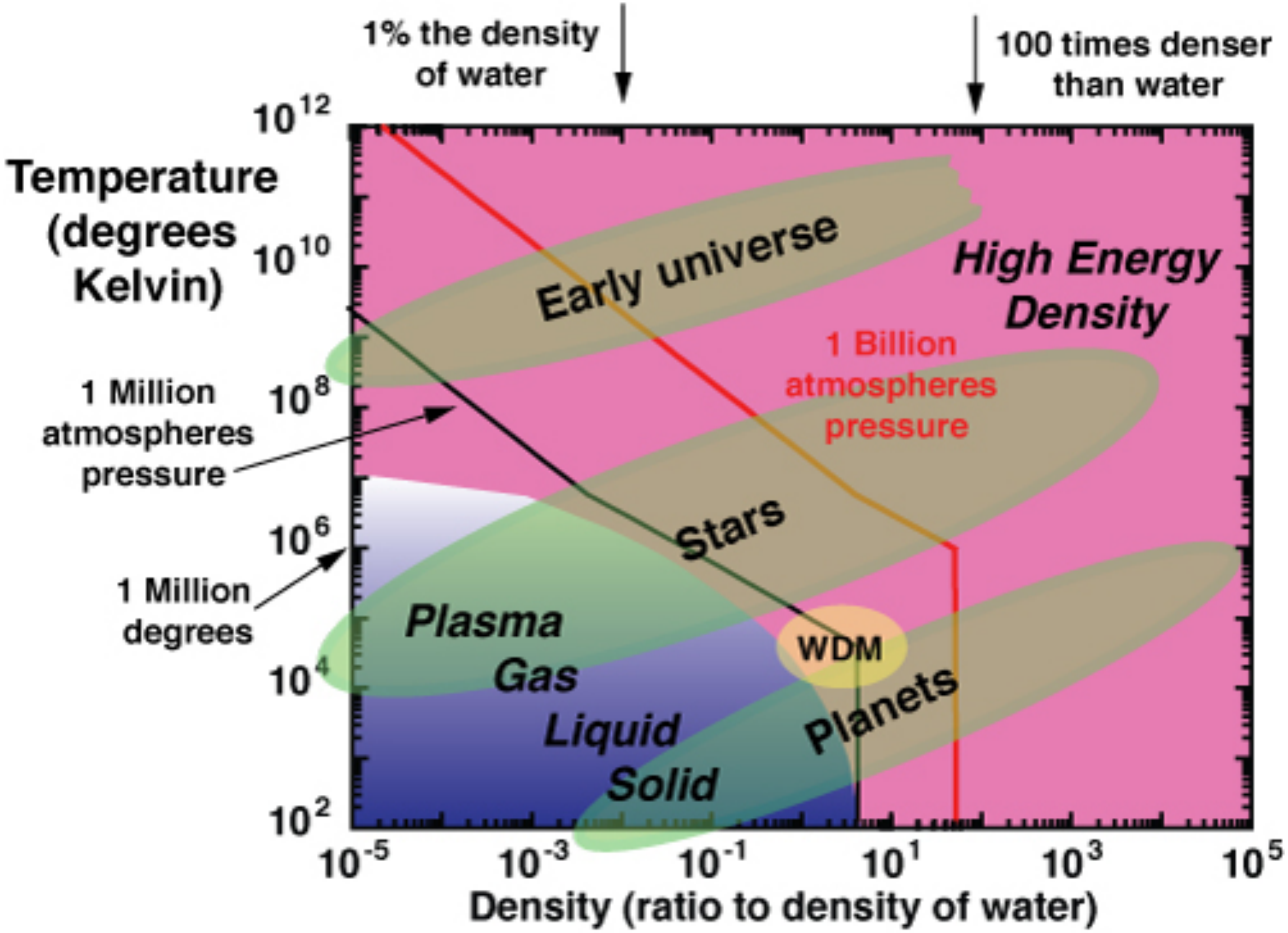
This talk will cover

- An introduction to laboratory astrophysics at High Energy Density (HED)
  - Material properties
  - Hydrodynamics
  - Radiation hydrodynamics

- Throughout
  - Examples from the CRASH project
  - Some observations on codes and UQ



The properties of high energy density matter connect with astrophysical systems

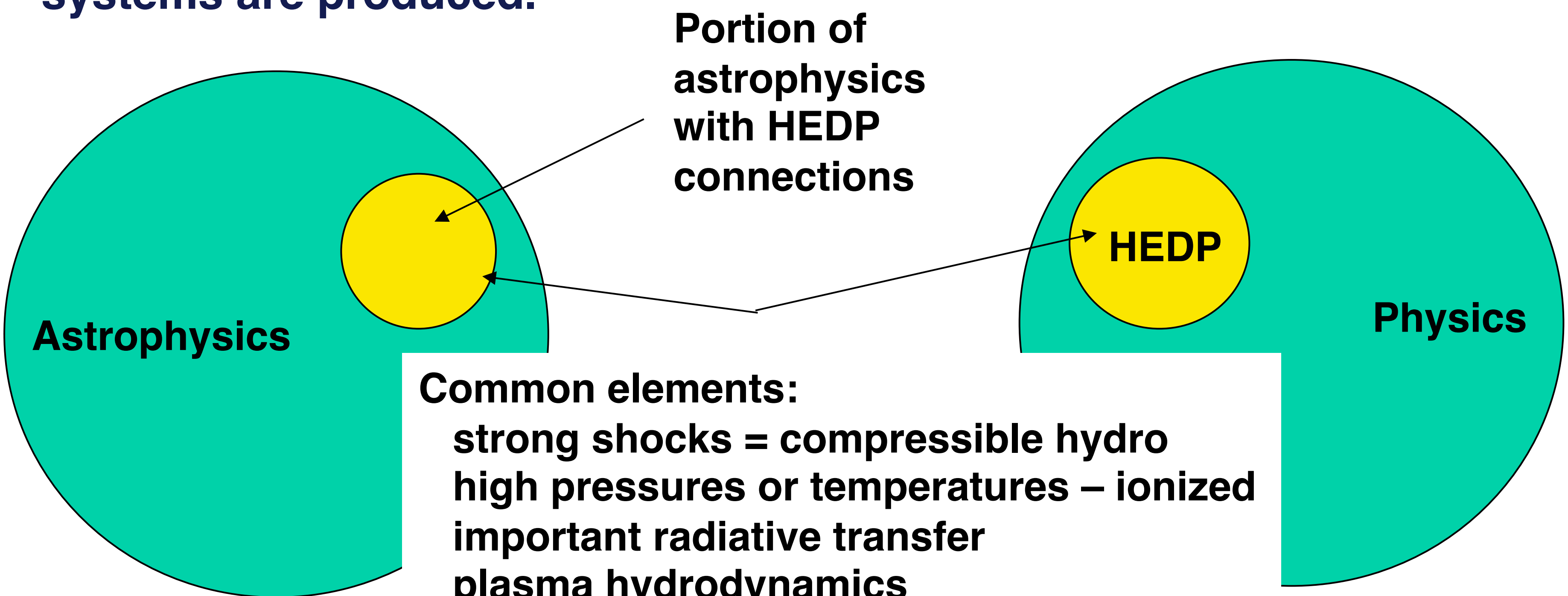


Quark-gluon plasmas

Drake,
Physics Today
June 2010

High-Energy-Density Physics has elements common to some astrophysical systems

HEDP involves the study of systems having a pressure > 1 Mbar (= 0.1 Tpascal = 10^{12} dynes/cm^2), and of the methods by which such systems are produced.

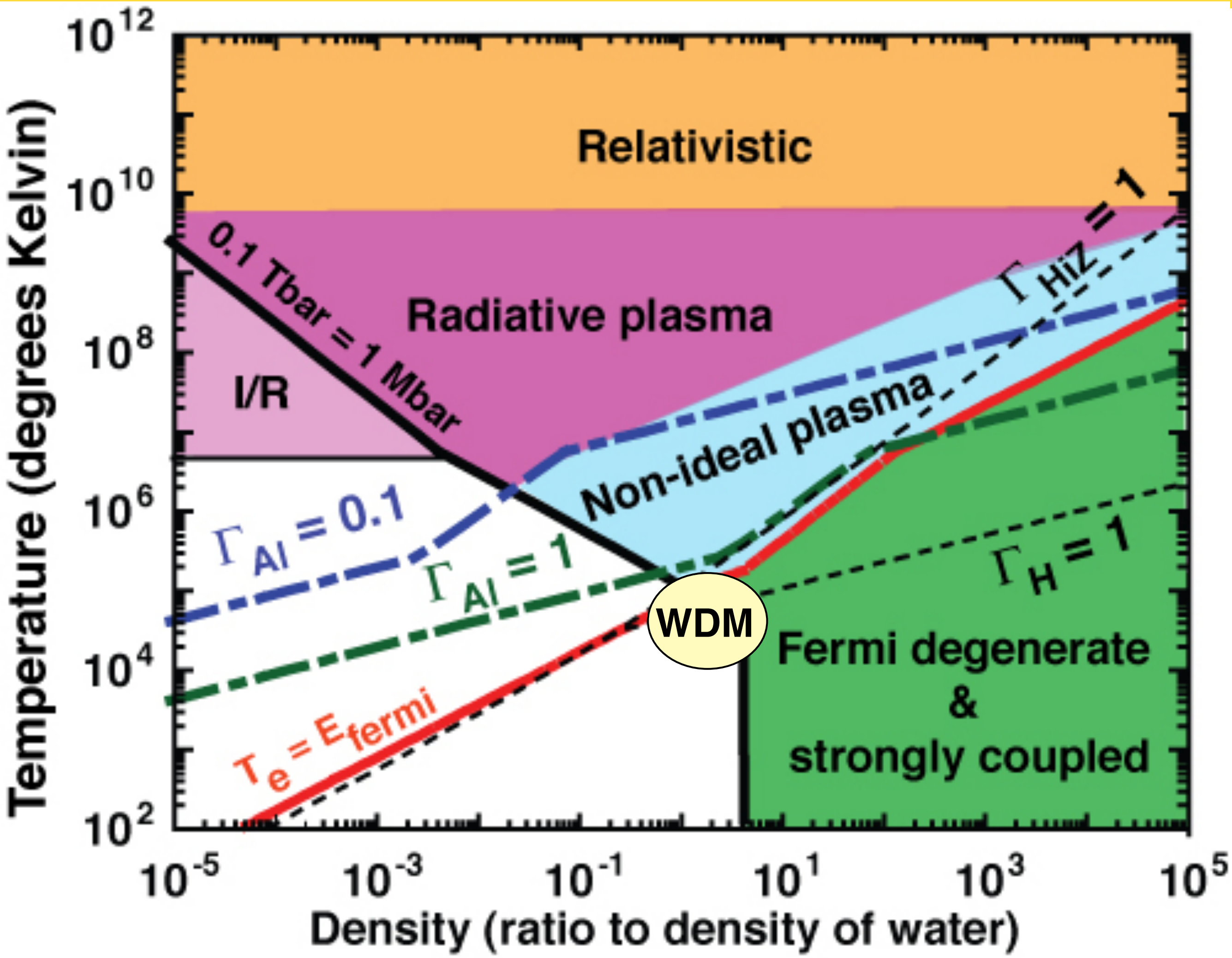


Common elements:

- strong shocks = compressible hydro
- high pressures or temperatures – ionized
- important radiative transfer
- plasma hydrodynamics

The "sexy" questions tend to arise from the connections
Nearly every problem in HEDP has astrophysical connections

HEDP behavior depends on a lot of physics, often hard to model numerically



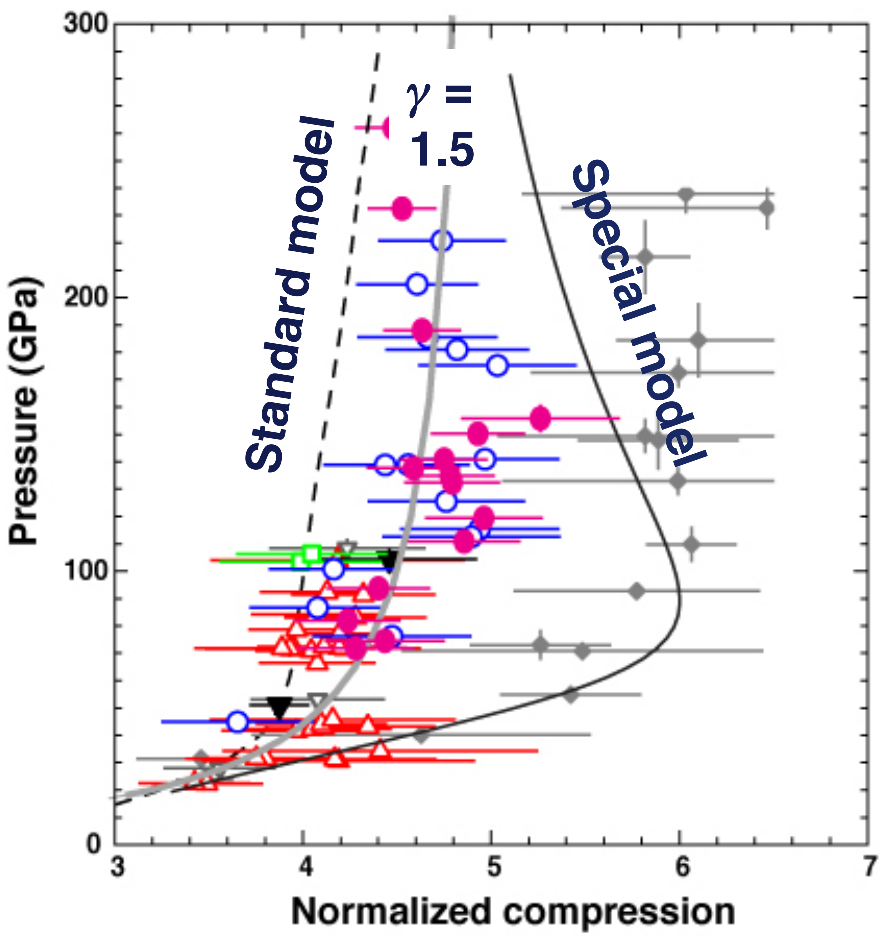
Drake,
Physics Today
June 2010

Material properties matter for astrophysics

- **Examples follow**
  - **Hydrogen and other equations of state**
  - **Iron opacities**
  - **Foam materials in experiments**

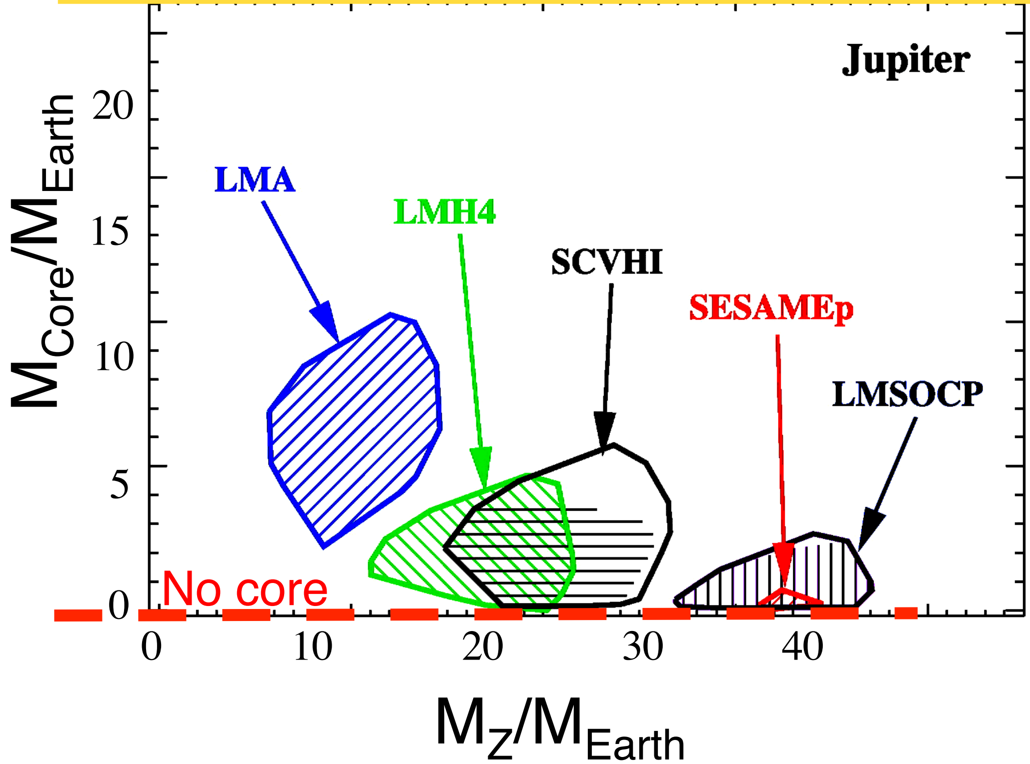
Warm dense matter is a big challenge

States produced by shock waves in D_2



- At pressure near 100 Gpa (1 Mbar)
  - Molecules dissociate
  - Ionization begins
  - Measurements are hard
- One cannot do the exact theory
  - Even molecular dynamics depends on approximate potentials

The different EOS models for hydrogen directly impact whether Jupiter is predicted to have a central dense core or not



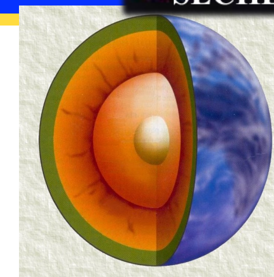
- Outlines show range of models matching Jupiter's properties within 2σ of observed
- Cannot yet tell whether Jupiter has a core
- The predicted age of Jupiter is is also sensitive to the H EOS, which affects luminosity

[D. Saumon and T. Guillot, Ap. J. 609, 1170 (2004)]

Adapted from slide by Bruce Remington

An EU consortium (SECHEL) has been funded to study iron properties using lasers

SECHEL

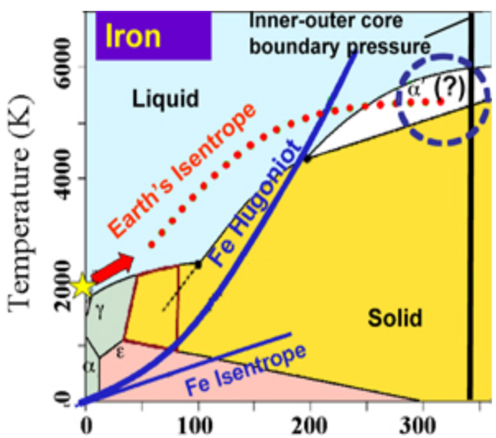


- A 3 years program has been funded by our national research agency (530,000 €) to determine iron properties at the Inner-Outer core Boundary

4 laboratories involved : LULI, CEA, LCD (Poitiers), IMPMC (Jussieu)

3 main objectives

Isentropic Compression



X-ray source > 40 keV

Find the good material (*Energy, spatial resolution, signal-to-noise*) for radiography & diffraction

Simulations & modelling

Multi-scale approach

Hydro+MD
Classic MD
QMD

Slide credit: Michel Koenig

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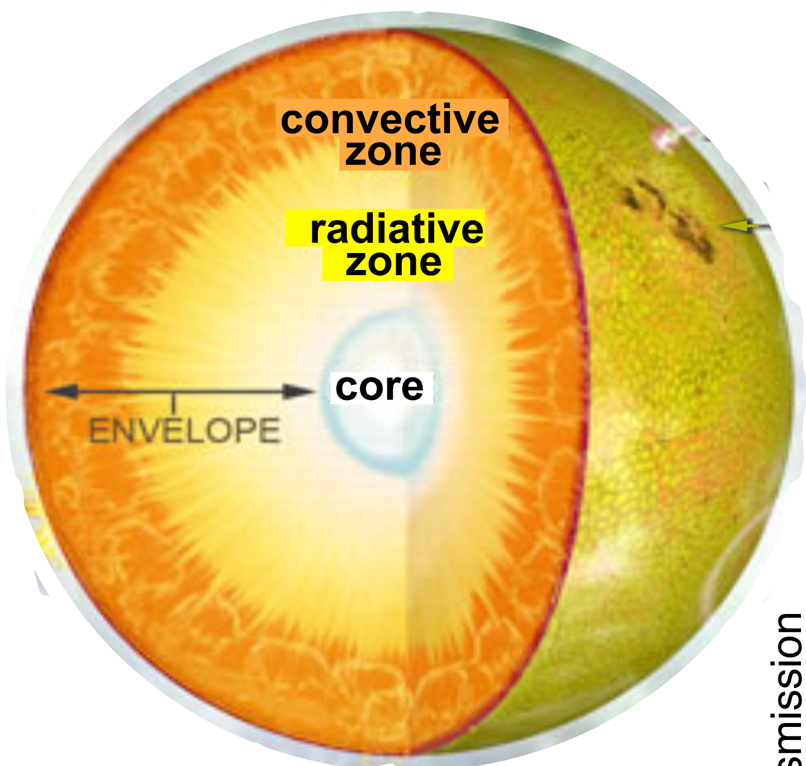
Laboratory experiments test opacity models that are crucial for stellar interior physics



2007 Don Dixon / cosmographica.com

Slide credit: James Bailey

Predictions of solar structure do not agree with observations (13 [illegible] CZ problem)

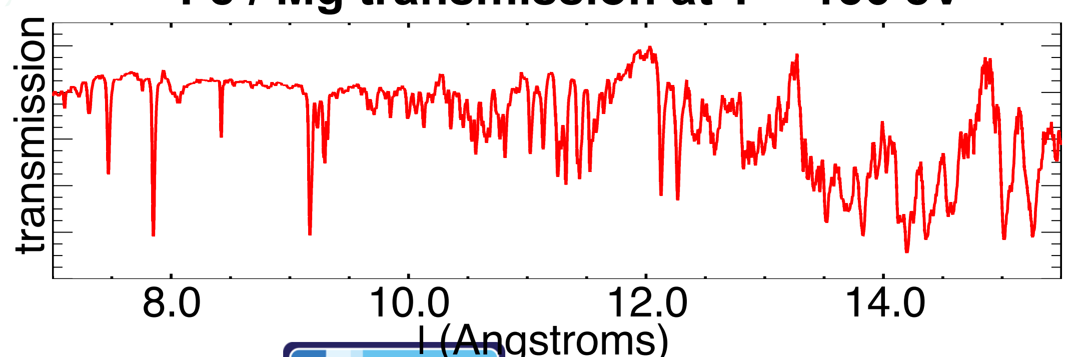
Solar structure depends on opacities that have never been measured

<u>Challenge: create and diagnose stellar interior conditions on earth</u>

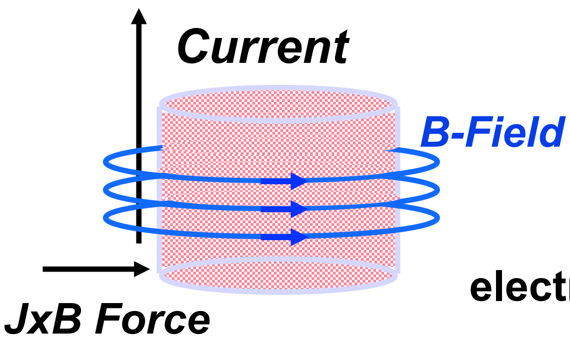
Z opacity experiments reach T ~ 156 eV

High T enables first studies of transitions important in stellar interiors

Fe / Mg transmission at T ~ 156 eV



Magnetically-driven z-pinch implosions provide one means to do studies like this, requiring bright x-ray sources



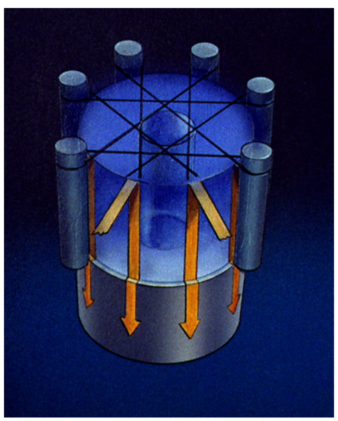
electrical energy

kinetic energy

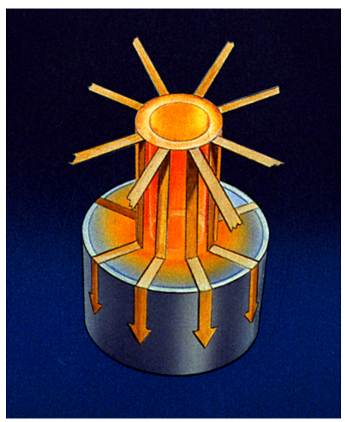
kinetic and electrical energy

internal (shock heating)

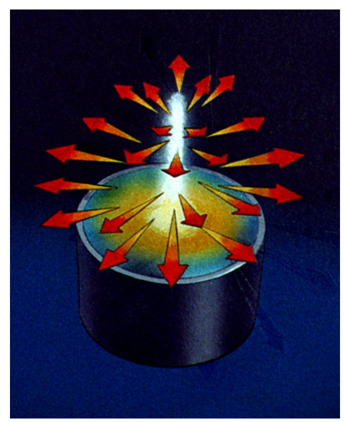
x rays



Initiation



Implosion

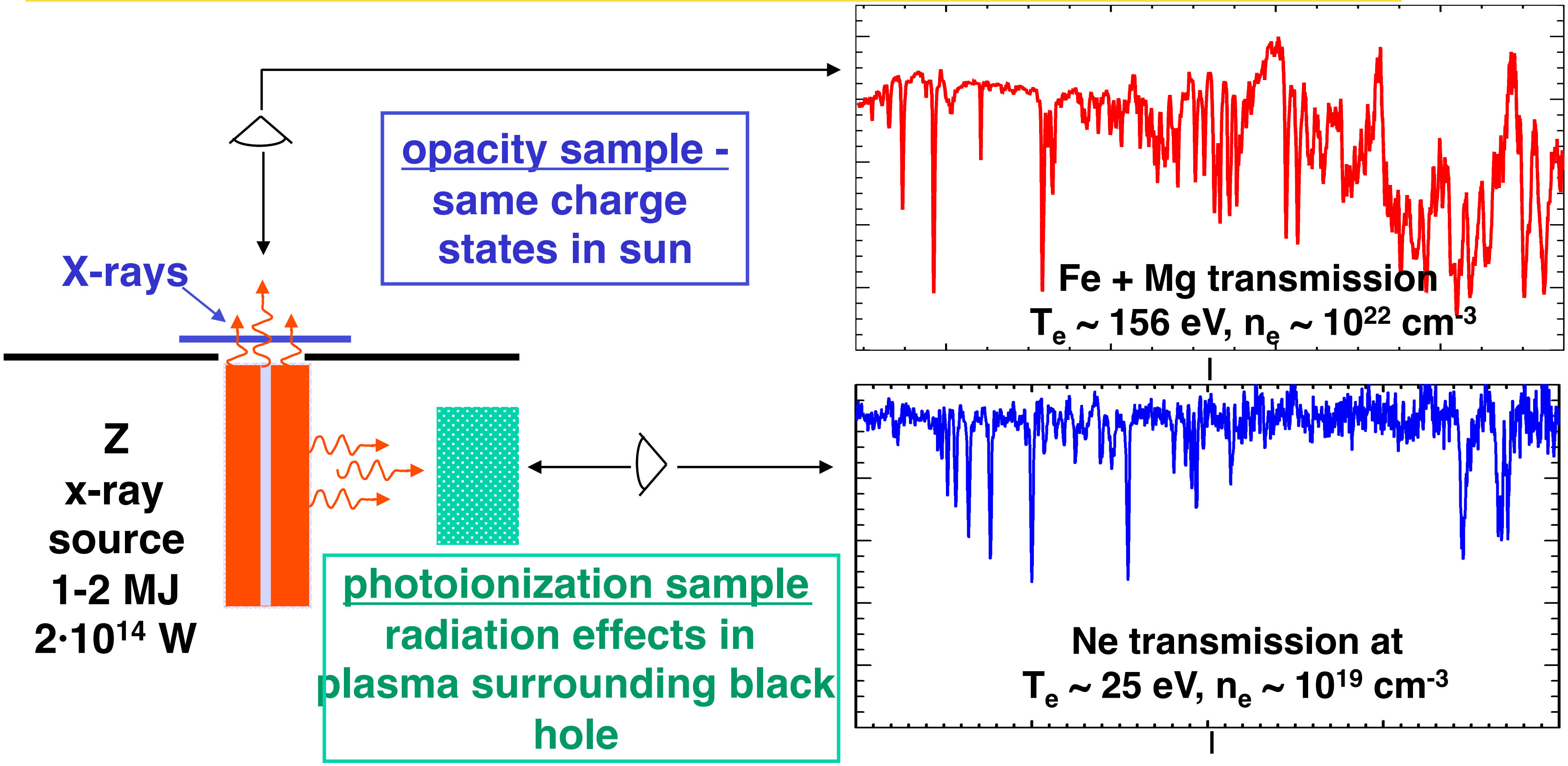


Stagnation

- **Energy: 1.5 MJ x-ray ≈ 15% of stored electrical**
- **Power: 200 TW x-ray**

Slide credit: James Bailey

Z pinches can do opacity and photoionization experiments, relevant to stellar interiors and accretion powered objects



Slide credit: James Bailey

[Jim Bailey, PRL (2007); and PoP 13, 056301 (2006)]

Experiments have to use foams

- Need to drive strong shocks across density differences of several (5 to 10)
  - The various layers all have to be diagnosable
  - Implies using plastic or other low-density solids
  - But these are > 100x times gas densities
  - The intervening density range becomes essential but is occupied by foam

- Alas, fluid-type EOS models are invalid for foams
  - Do not model destruction of foam cells during plasma formation
  - Do not model formation and decay of turbulence
  - Do not model hysteresis upon later cooling

Material properties matter for astrophysics

- **Modeling them is a big challenge**
- **EOS models**
  - If they apply
- **Opacity models**
  - Should self-consistency matter?
- **Uncertainty in such models**
- **Uncertainty in wrong models**

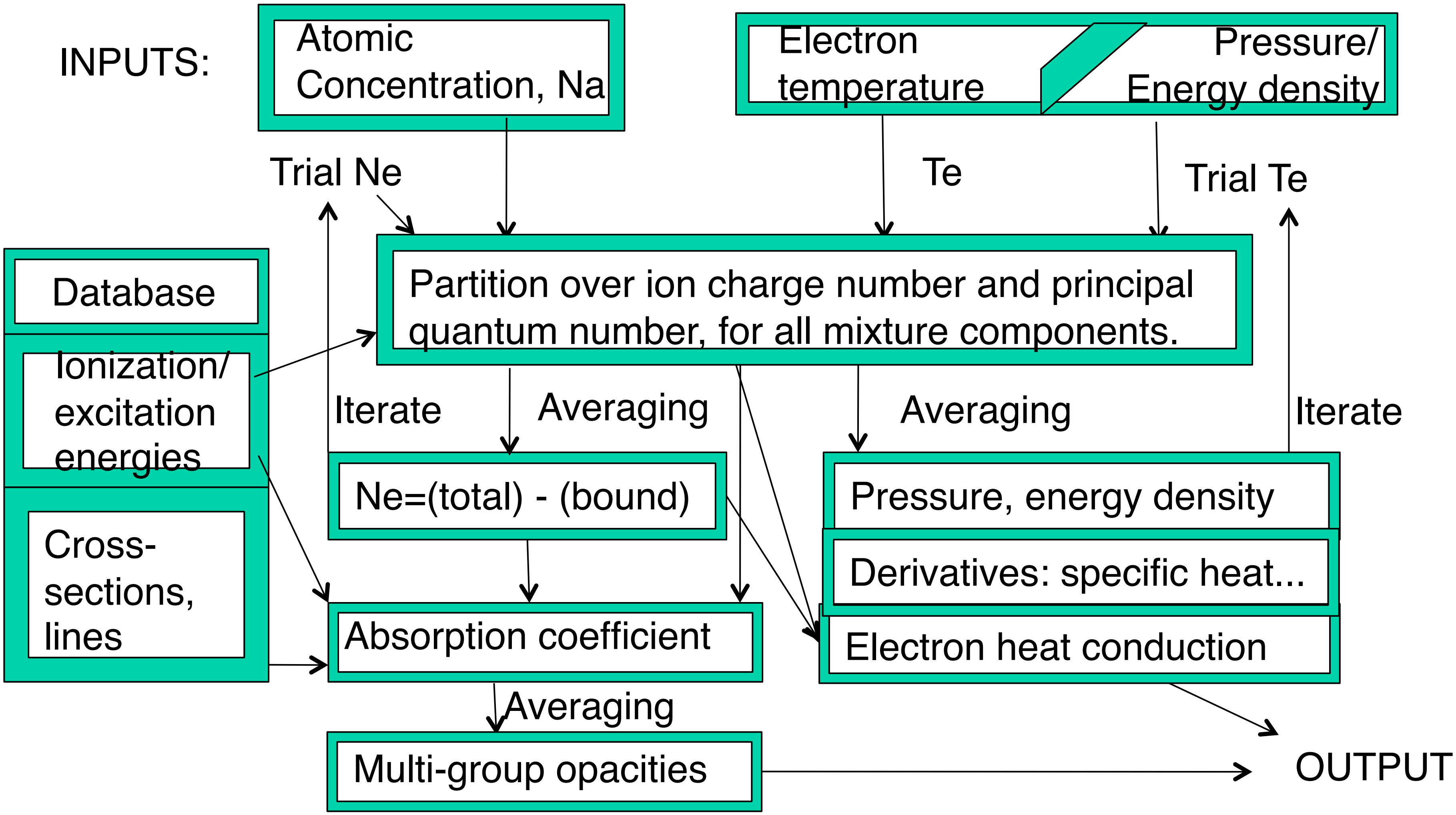
Our approach in CRASH

- **We were charged with quantifying uncertainty in simulated results**
  – **Uncertainty in EOS and opacity is part of this**

- **It's nearly impossible to deal *post facto* with uncertainty in a table of 10^N numbers**
  – **One can do fitting to reduce the number of dimensions and can address the uncertainty associated with the fit,**
  – **But this does not account for the numbers in the table being uncertain and for the uncertainties being correlated**

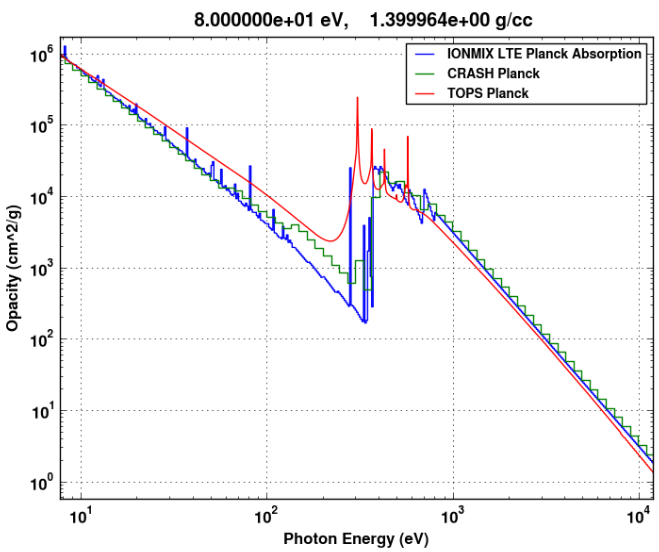
- **We took the approach of self-consistently evaluating EOS and opacity from atomic data**
  – **Allows propagation of uncertainties (in principle)**

EOS and opacity model: general scheme

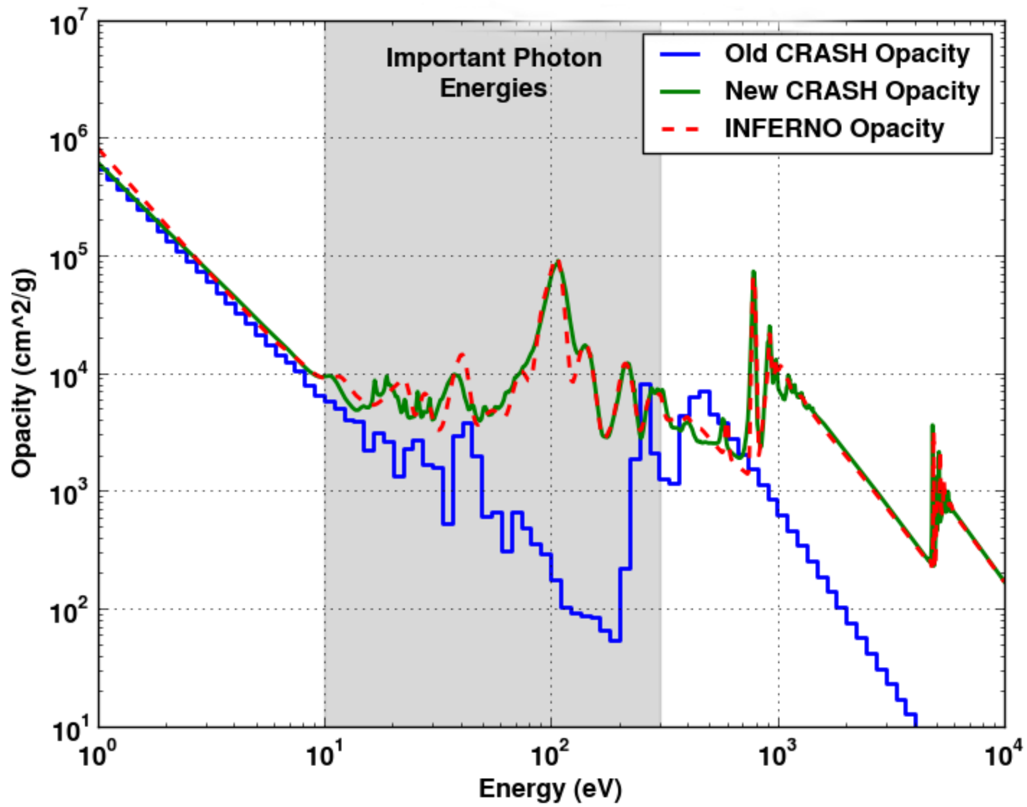


This worked well for low-Z but failed for Xe

Polyimide



Xe



Of course, agreement among models does not imply accuracy

Some observations about material properties

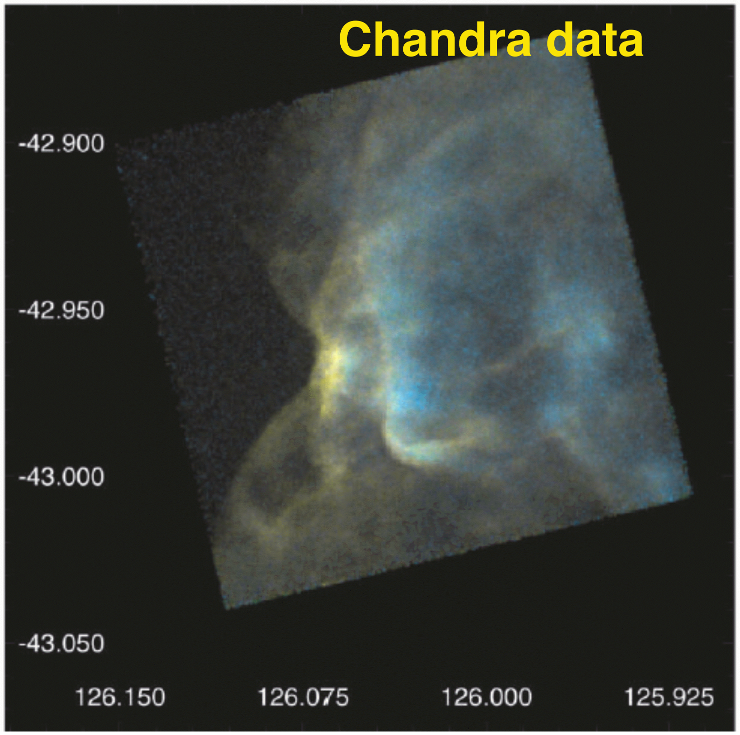
- Understanding uncertainty in EOS and opacity models is at best difficult
  - The atomic data approach is feasible at least at times
  - Purely theoretic approaches can generate usable results
    - But knowing their accuracy is problematic
  - Doing this well would require a major, extended effort

- The situation is even worse when EOS models are not valid
  - To handle such materials, more complex computational models are needed

Other issues in HED laboratory astrophysics

- Hydrodynamics
  - And physics that affects it
- Radiation hydrodynamics
  - We will discuss CRASH to develop this topic
- We will not address a couple other areas
  - Magnetic fields and MHD systems
  - Relativistic dynamics
- Why not just trust the codes?

Destruction of clumps in post-shock flow has been a research area with impact



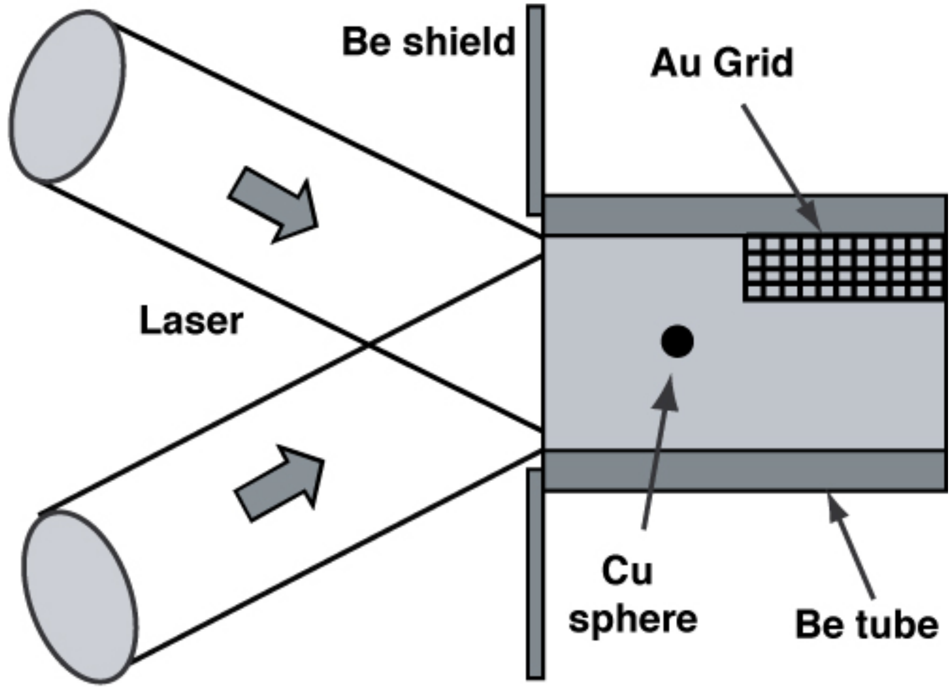
Well scaled experiment

Klein et al., ApJ 2003
Robey et al., PRL 2002

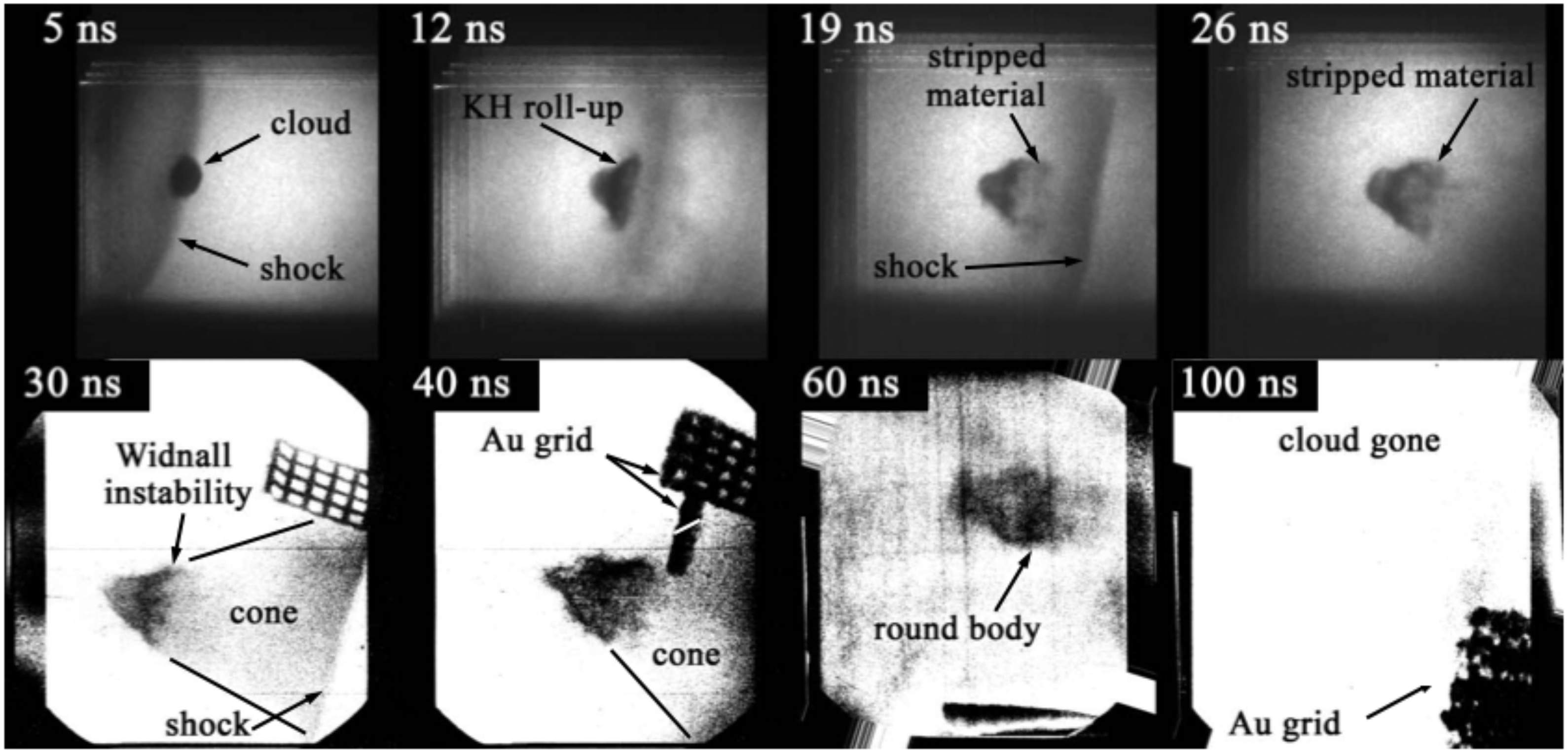
- **Experimental results used to help interpret Chandra data from the Puppis A supernova remnant**
- **Well-scaled experiments have deep credibility**
- **Una Hwang et al., Astrophys. J. (2005)**

How shock-clump experiments are done

- The experiment involves blast-wave-driven mass stripping from a sphere
- Early experiments used Cu in plastic; recent experiments use Al in foam



Observations of the Al/foam case continued until mass stripping had destroyed the cloud



- Hansen et al., ApJ 2007, PoP 2007

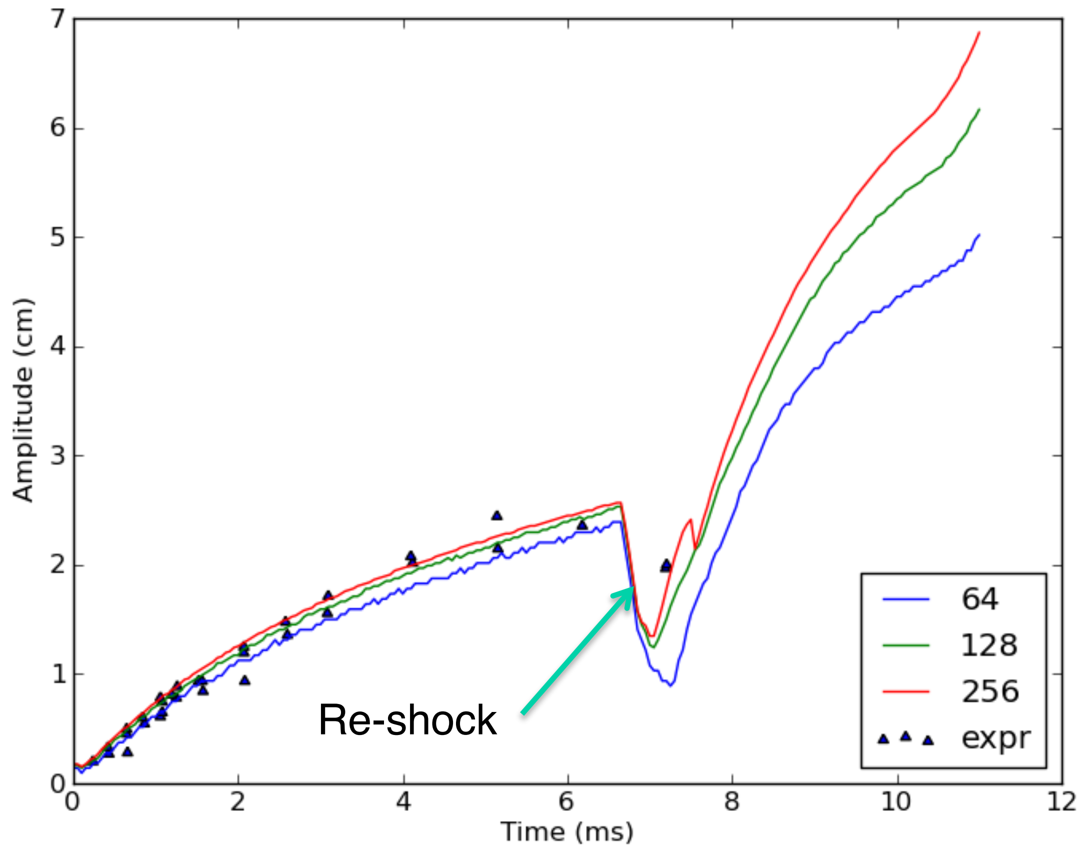
Simulating such experiments is not trivial

- Even leaving aside the EOS issues discussed above
- Many people act like their favorite hydro method is perfect
  - I'm not taken in by this any more
  - Astro types love their PPM
    - But PPM creates structure on unresolvable scales
  - Space weather modelers like more diffusive solvers
    - Probably mock up reconnection effects OK, but need a lot of zones to accurately capture instabilities
  - ALE codes seem popular in the labs
    - But these involve unquantified dissipation of vorticity
  - All the methods have seldom-mentioned parameters in the hydro scheme that affect the results
    - "limiters", "beta",

I've noticed that code developers seem to like best the methods that match their personalities

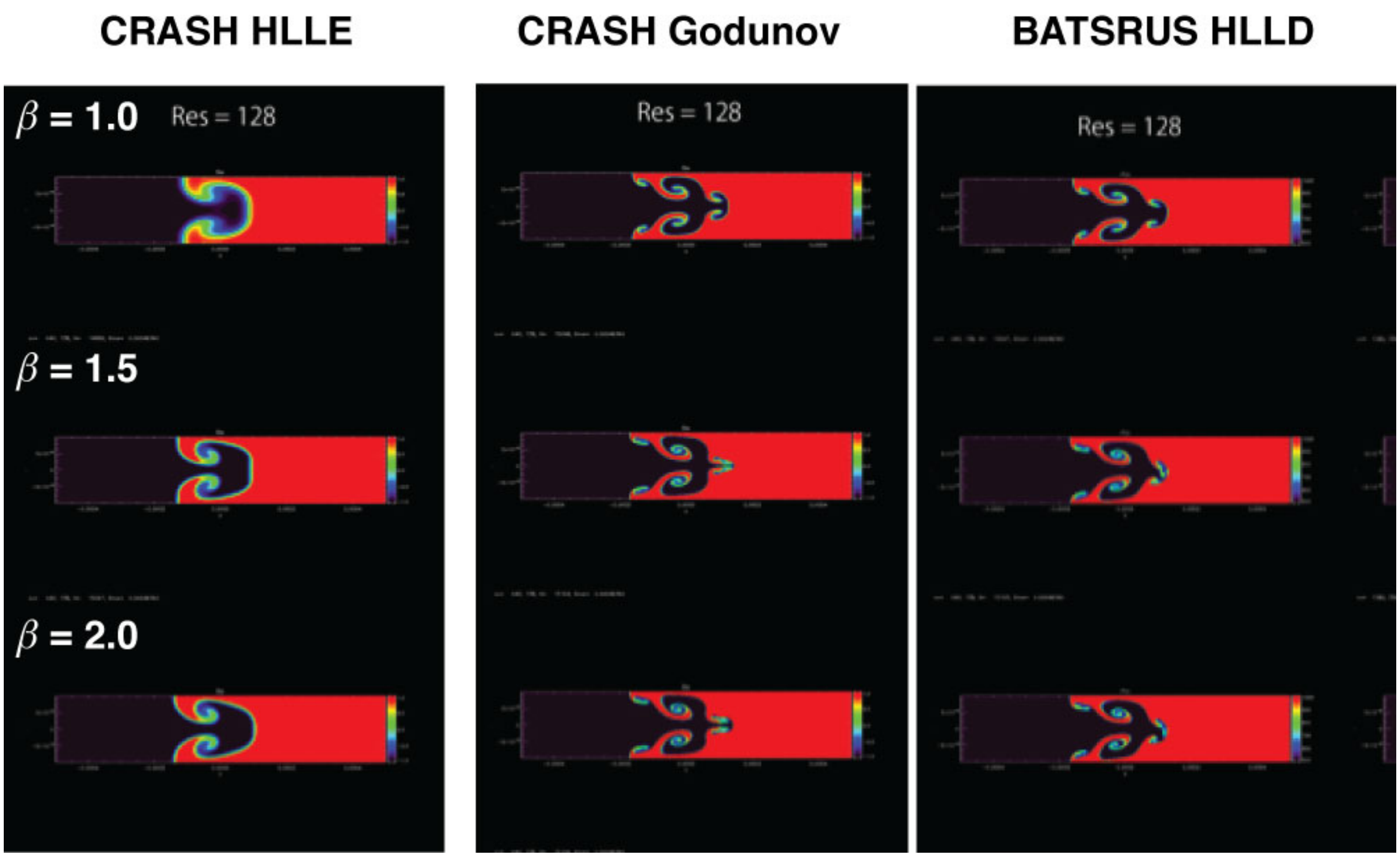
Any decent hydro code will prove able to reproduce some standard results

Modeling of Jacobs' Richtmyer Meshkov experiment using CRASH



But I have learned that there are some magical hydrodynamic adjustable parameters

Rayleigh Taylor at Embedded Interface, 128 zones resolution

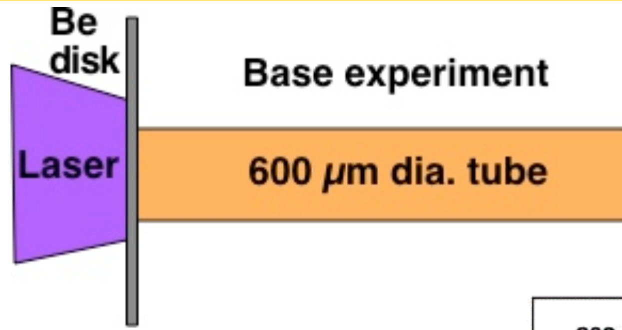


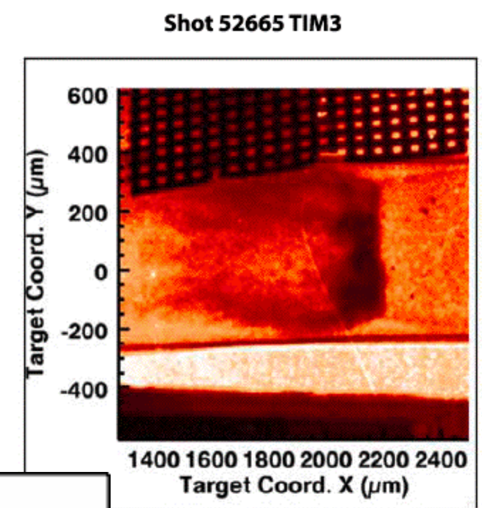
Now we turn to the CRASH project, and specifically its radiation hydrodynamics

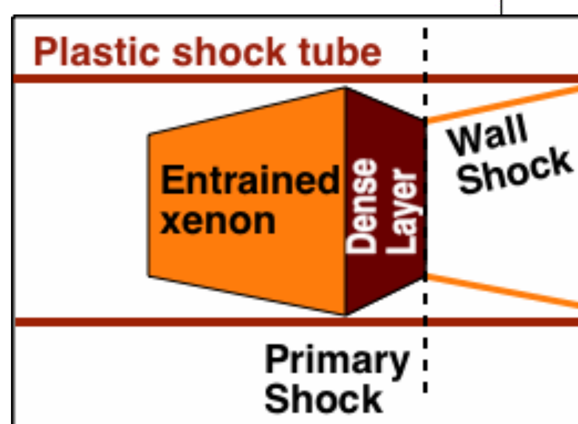
- In CRASH we are funded
  - To simulate a complex physical experiments
    - Radiative shock experiments
    - A radiation hydrodynamic code
  - To assess the predictive capability of the simulation
    - Using uncertainty quantification and related analysis
- Key papers
  - CRASH code: Van der Holst et al, Ap.J.S. 2011
  - CRASH Physics: Drake et al. HEDP 2011
  - 3D simulations: Van der Holst et al, HEDP 2012

The physical system of interest to CRASH is a radiative shock wave

- 1 ns, 4 kJ laser irradiates Be disk
- Drives 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

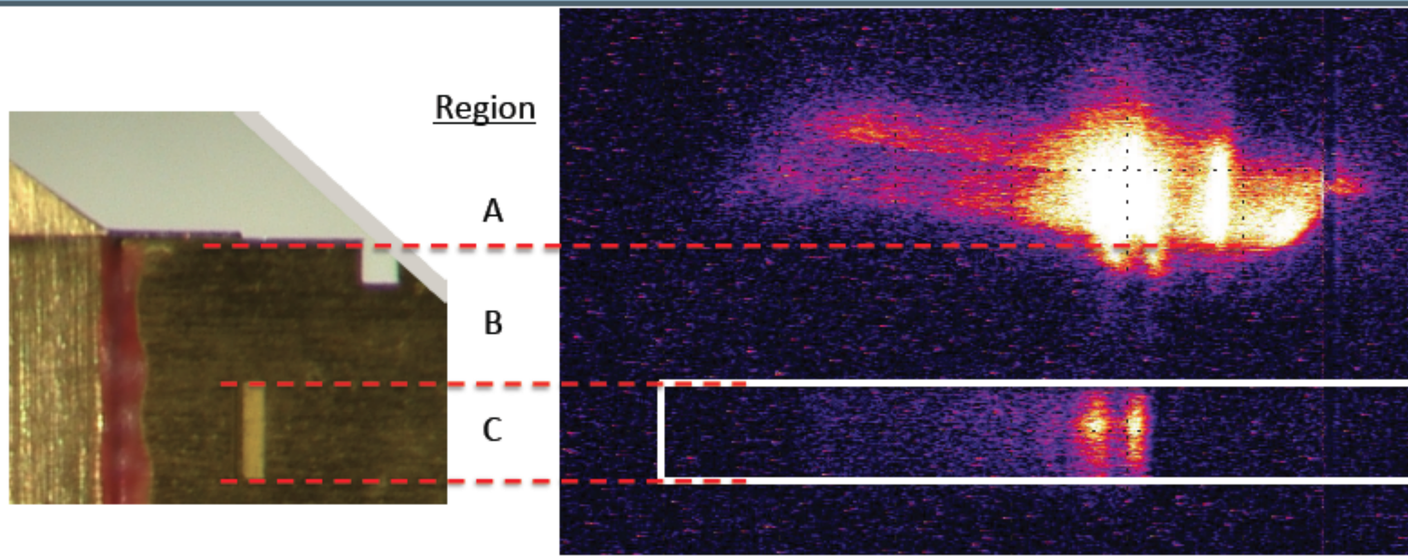




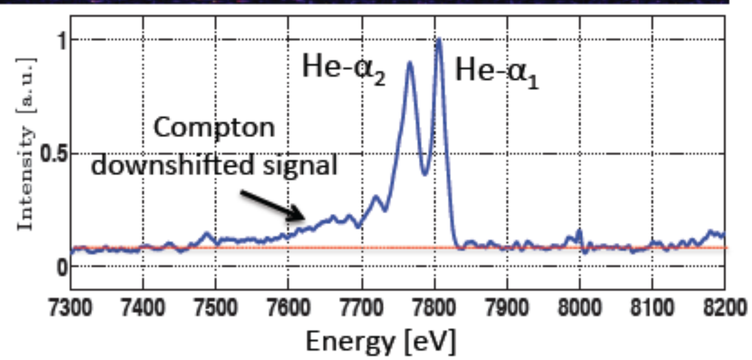


Just last week we got measurements from which we will get temperature profiles

- **Imaging spectrometer**
  - **Designed by UM student Eliseo Gamboa (J. Inst. 2011)**
  - **Built by LANL; experiment by UM student Chan Huntington**

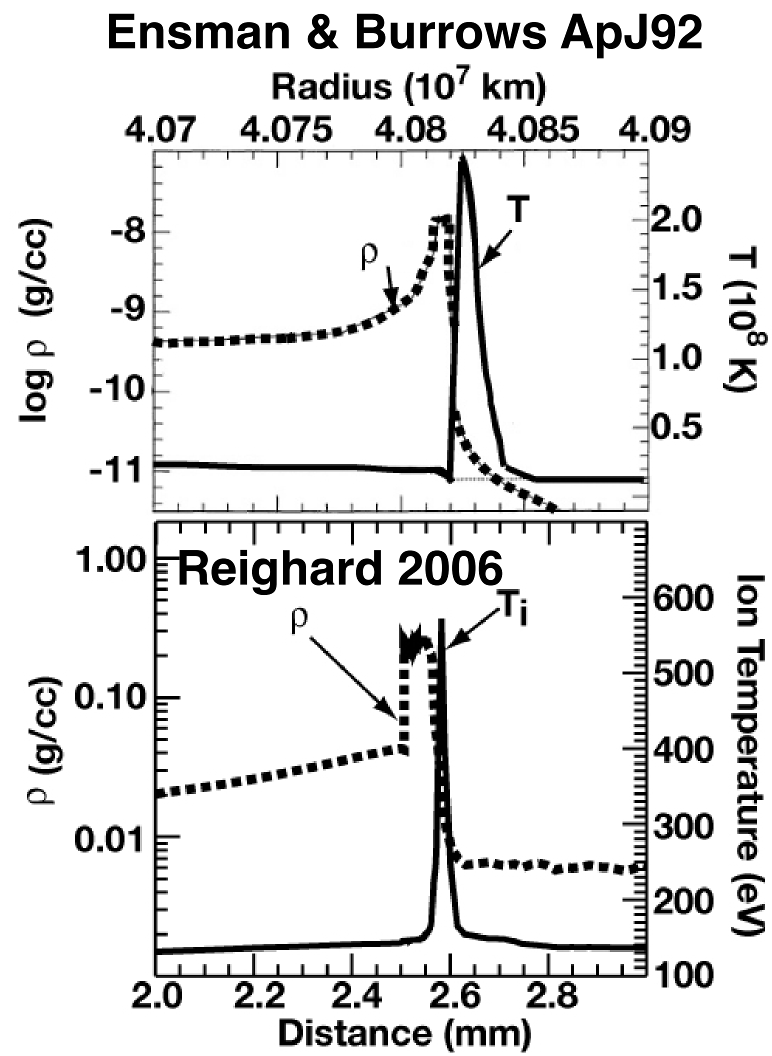


Region	Nominal dimension	Measured Dimension
A (Be plume)	~	>2 mm
B (gold shield)	1.5 mm	1.4 mm
C (scattering slit)	1040 μm	1000 μm



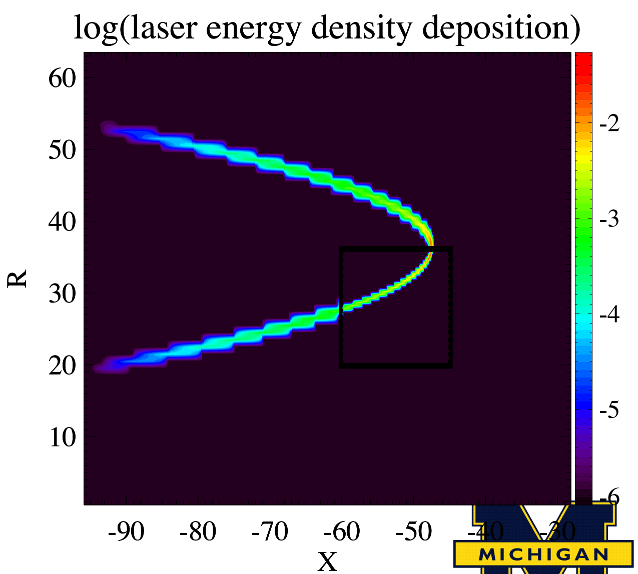
We find our motivation in astrophysical connections

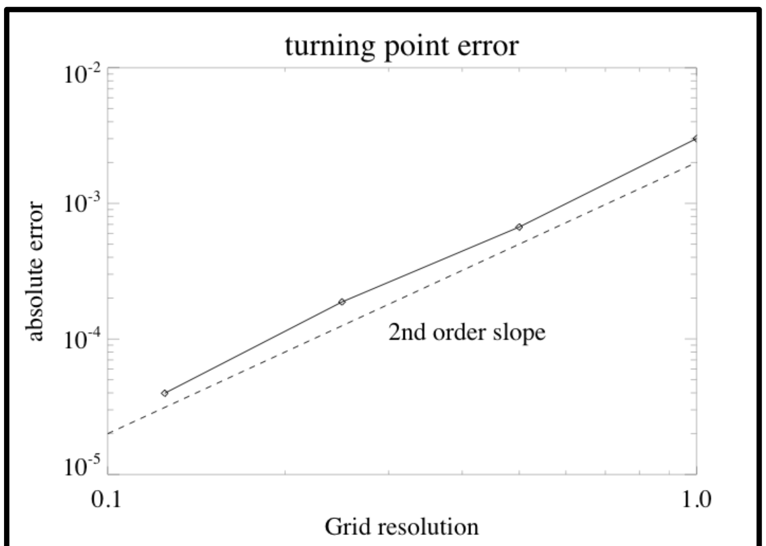
- Radiative shocks occur throughout astrophysics
  - Supernovae, accretion, stars, supernova remnants, collisions
- Our experiments
  - have all three relevant dimensionless parameters in the regime of shocks emerging from supernovae
- This produces qualitatively similar profiles
  - We should see any important unanticipated physics
  - Good code test in any event



CRASH has a Laser Package to model energy deposition

- Laser energy transport via 3-D ray-tracing based on geometric optics
- Laser energy absorption via inverse bremsstrahlung
- Efficient parallel AMR implementation using block adaptive tree library (BATL)
- Verification tests based on laser ray turning point and energy deposition in simple analytic density distributions





CRASH Radhydro Code: Hydro and Electron Physics

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

laser energy deposition

radiation/electron momentum exchange

electron heat conduction

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

Compression work

collisional exchange

radiation/electron energy exchange

CRASH Radhydro Code: Multigroup diffusion

- **Radiation transport equation reduces to a system of equations for spectral energy density of groups.**
- **Diffusion is flux-limited**
- **For the gth group:**

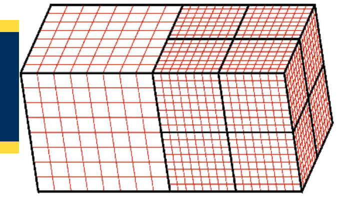
advection **compression work** **photon energy shift**

$$\frac{\partial E_g}{\partial t} + \nabla\cdot(E_g \mathbf{u}) - p_g \nabla\cdot\mathbf{u} - \frac{\nabla\cdot\mathbf{u}}{\Delta(log\ \varepsilon)}\Delta(p_g) = \text{diffusion + emission - absorption}$$

$$\text{diffusion} = \nabla\cdot(D_g \nabla E_g) \qquad \text{emission-absorption} = c\chi_{abs_g}(B_g - E_g)$$

$$\Delta(\cdot) = (\cdot)_{g+\frac{1}{2}} - (\cdot)_{g-\frac{1}{2}}$$

Overview of Solver Approach



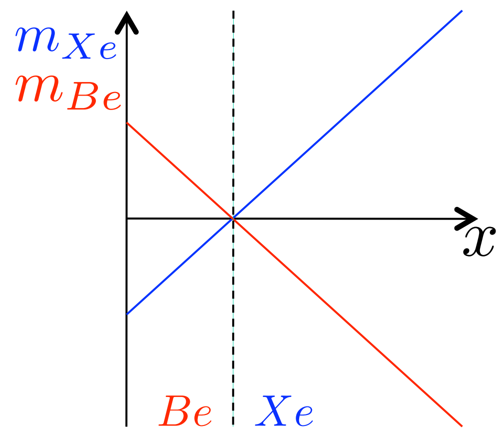
- Self-similar block-based adaptive grid
- Finite-volume scheme, approximate Riemann solver for flux function, limited linear interpolation
- Mixed Implicit/Explicit update
  - Hydro and electron equations
    - Advection, compression and pressure force updated explicitly
    - Exchange terms and electron heat conduction treated implicitly
  - Radtran
    - Advection of radiation energy, compression work and photon shift are evaluated explicitly
    - Diffusion and emission-absorption are evaluated implicitly
  - Implicit scheme is a preconditioned Newton-Krylov-Schwarz scheme

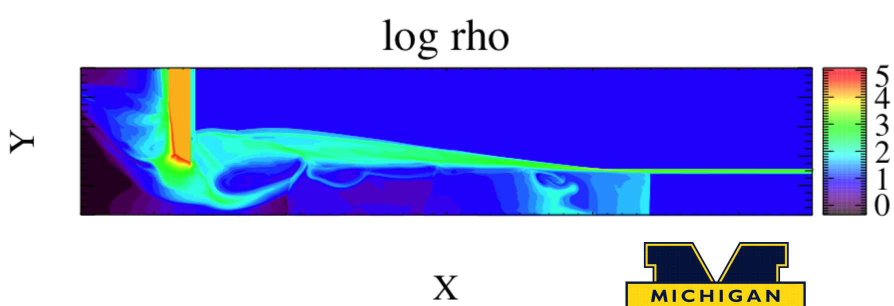
Material Interface treatment

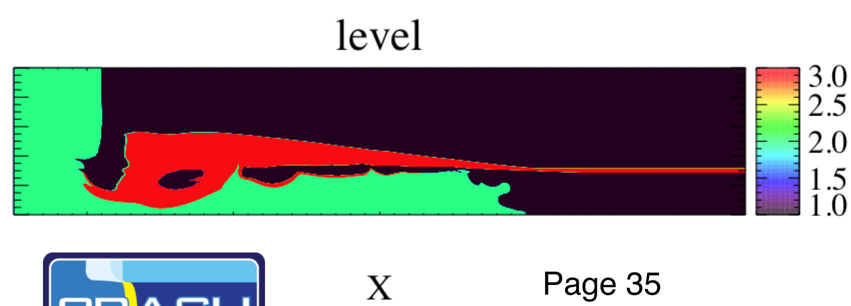
- For material α, level-set function m_α is initialized based on signed distance from interface.
- Level-set function propagated by

$$\frac{\partial}{\partial t}(\rho m_\alpha) + \nabla \cdot (\rho m_\alpha \mathbf{u}) = 0$$

- Cells are treated as a single material (that of the largest level-set function).
- Use AMR to resolve the interface







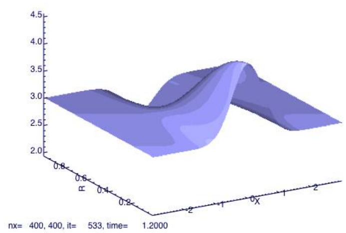
We extensively test our code

- New program units implemented with unit tests
  - Nightly execution of many unit tests for CRASH and its parent code
- New features implemented with verification tests
  - Daily verification & full system tests are run on a 16-core Mac.
  - Tests cover all aspects of the new feature, including restart, using grid convergence studies and model-model comparison.
- Compatibility & reproducibility checked with functionality test suite
  - Nightly runs. 9 different platforms/compilers on 1 to 4 cores: tests portability
- Parallel Scaling Tests
  - Weekly scaling test on 128 and 256 cores of hera.
  - Reveals software and hardware issues, and confirms that results are independent of the number of cores.

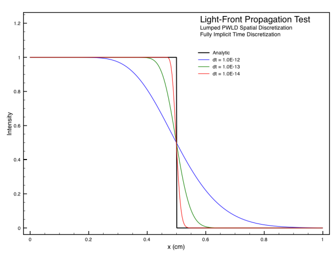
Multiple classes of tests are in our suite

- Hydrodynamics
- Radiation transport
- Radiation hydrodynamics
- Heat conduction
- Simulated radiography
- Material properties (EOS and opacities)
- Laser package
- Unit tests
- Full-system tests

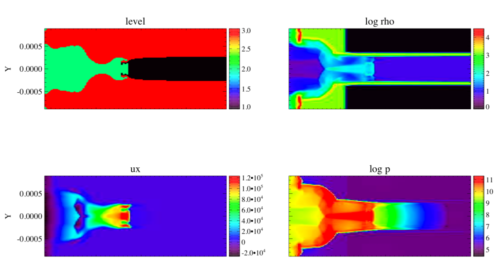
HEAT CONDUCTION



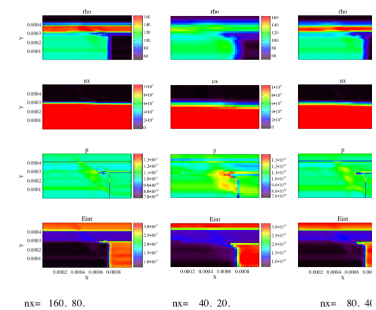
RADIATION TRANSPORT



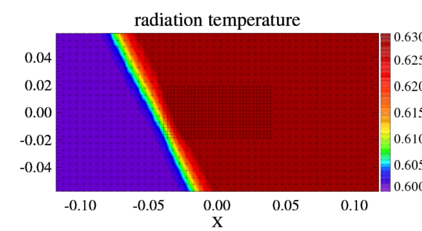
FULL SYSTEM



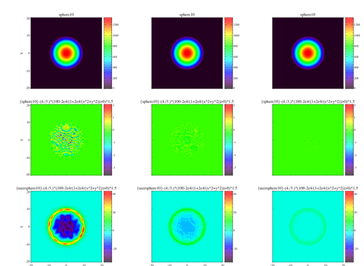
HYDRODYNAMICS



RADIATION HYDRODYNAMICS

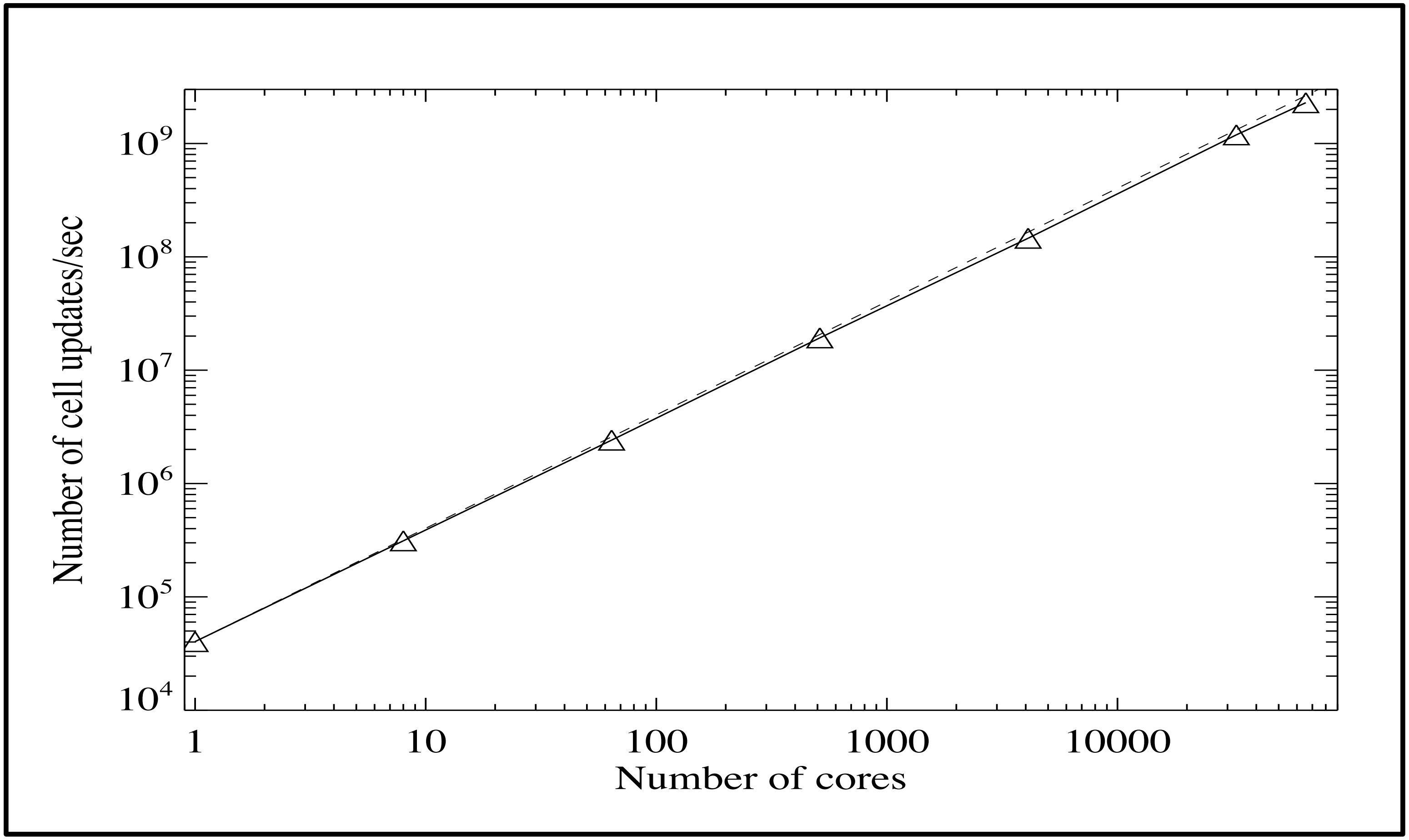


SIMULATED RADIOGRAPHY



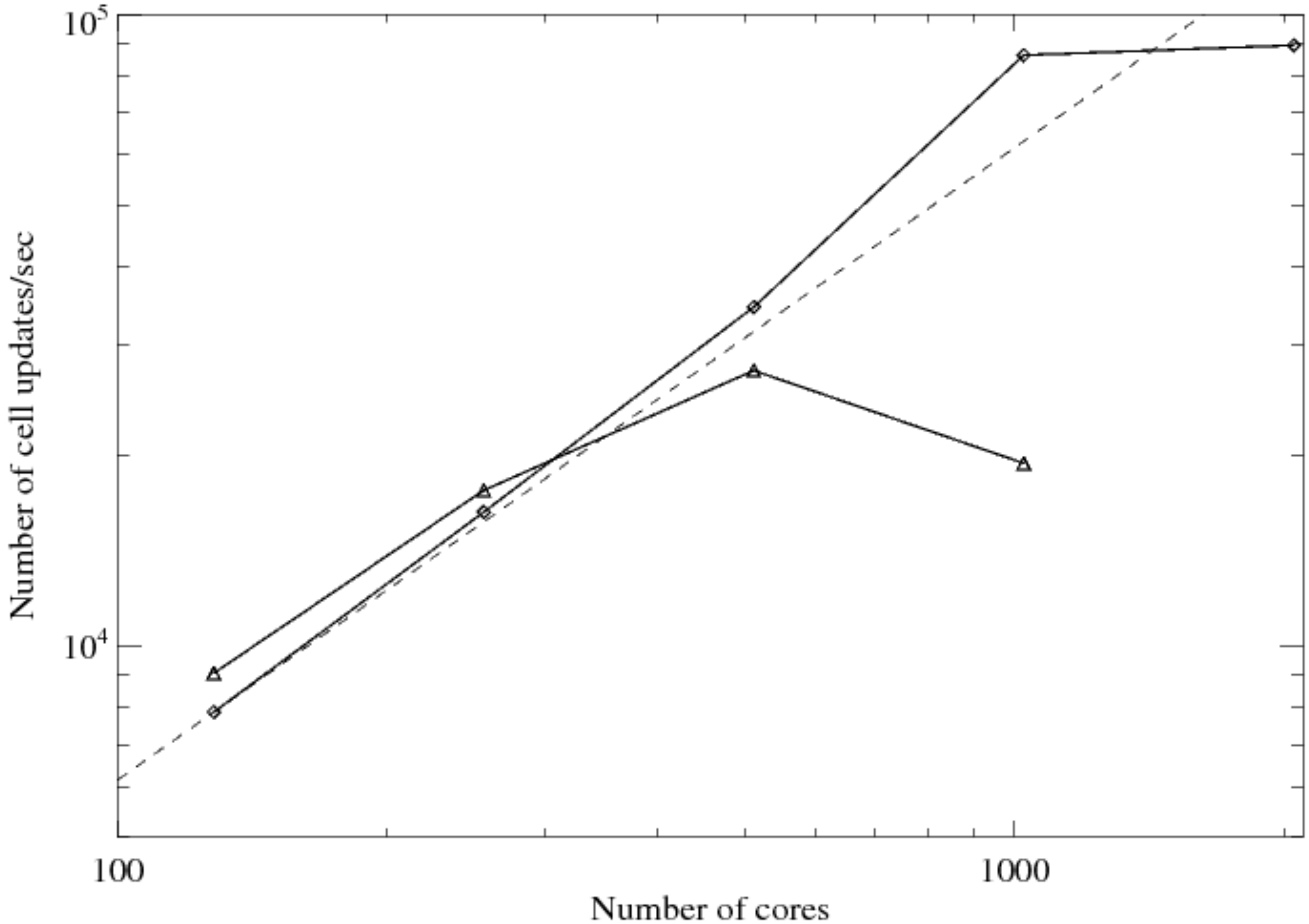
The hydro portion of the code scales very well

(CRASH hydro Weak Scaling on BG/L)

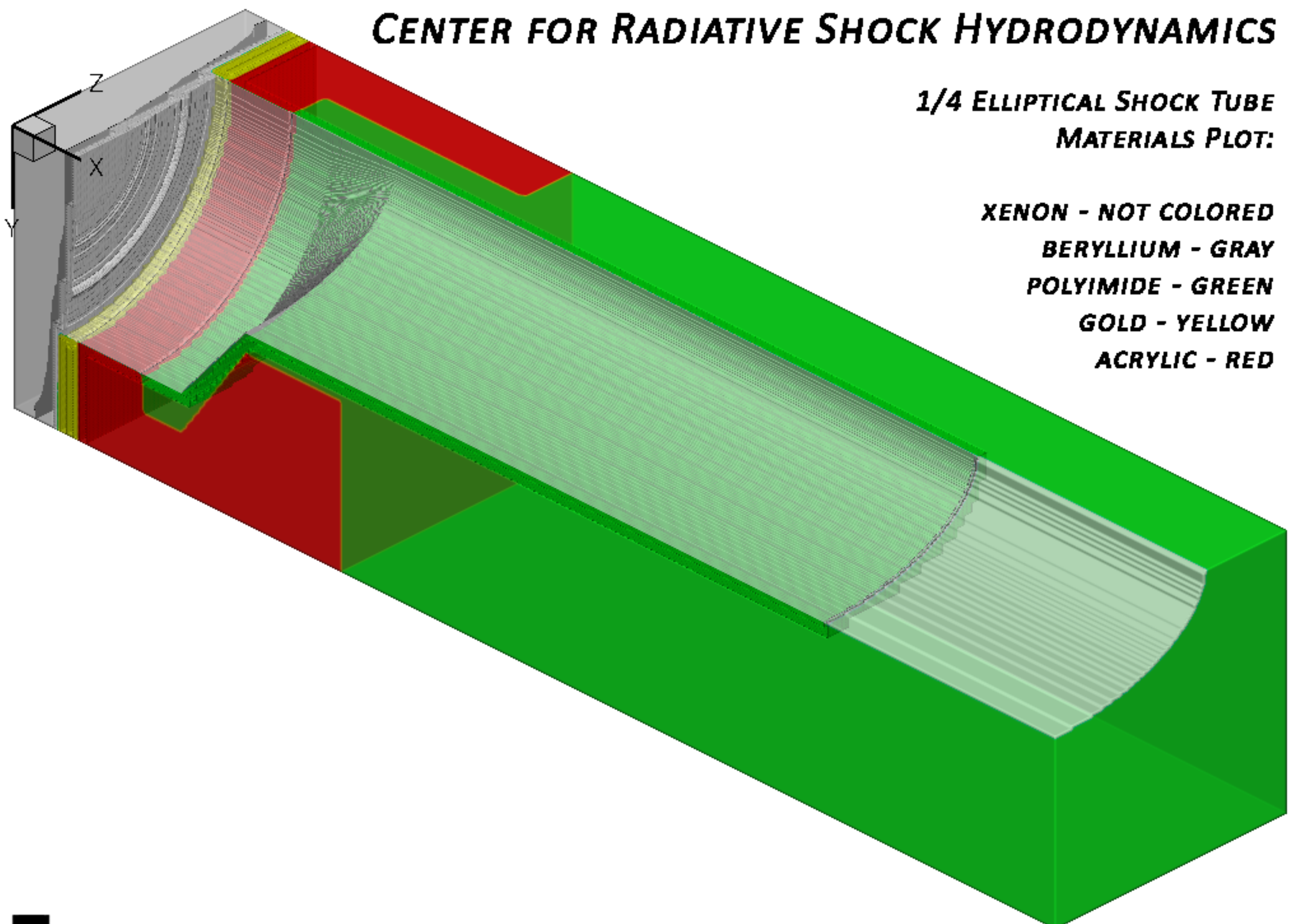


The full-system scaling is more communication-intensive

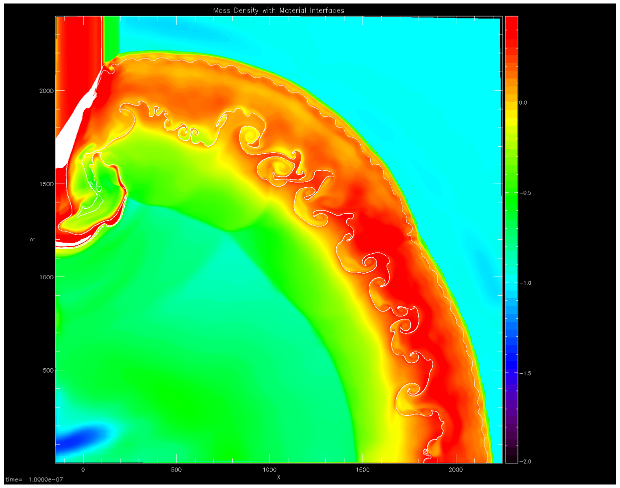
CRASH rad-hydro strong scaling on Hera and Pleiades



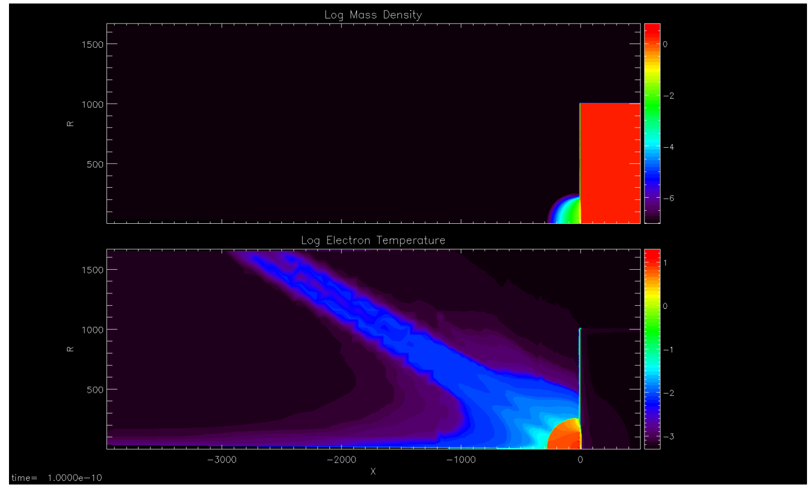
Simulation of the CRASH Experiment



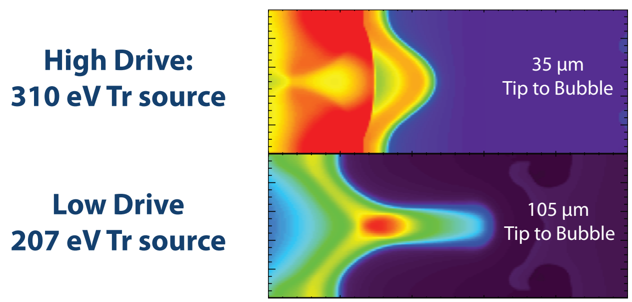
CRASH has been used to model several HED experiments



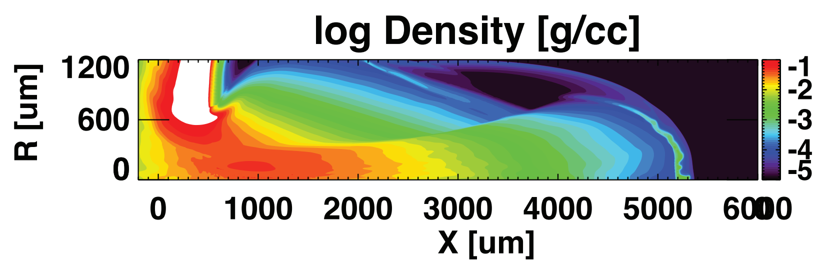
Rayleigh-Taylor growth in a diverging system



Ablative flow of laser driven foil for collisionless shock experiments



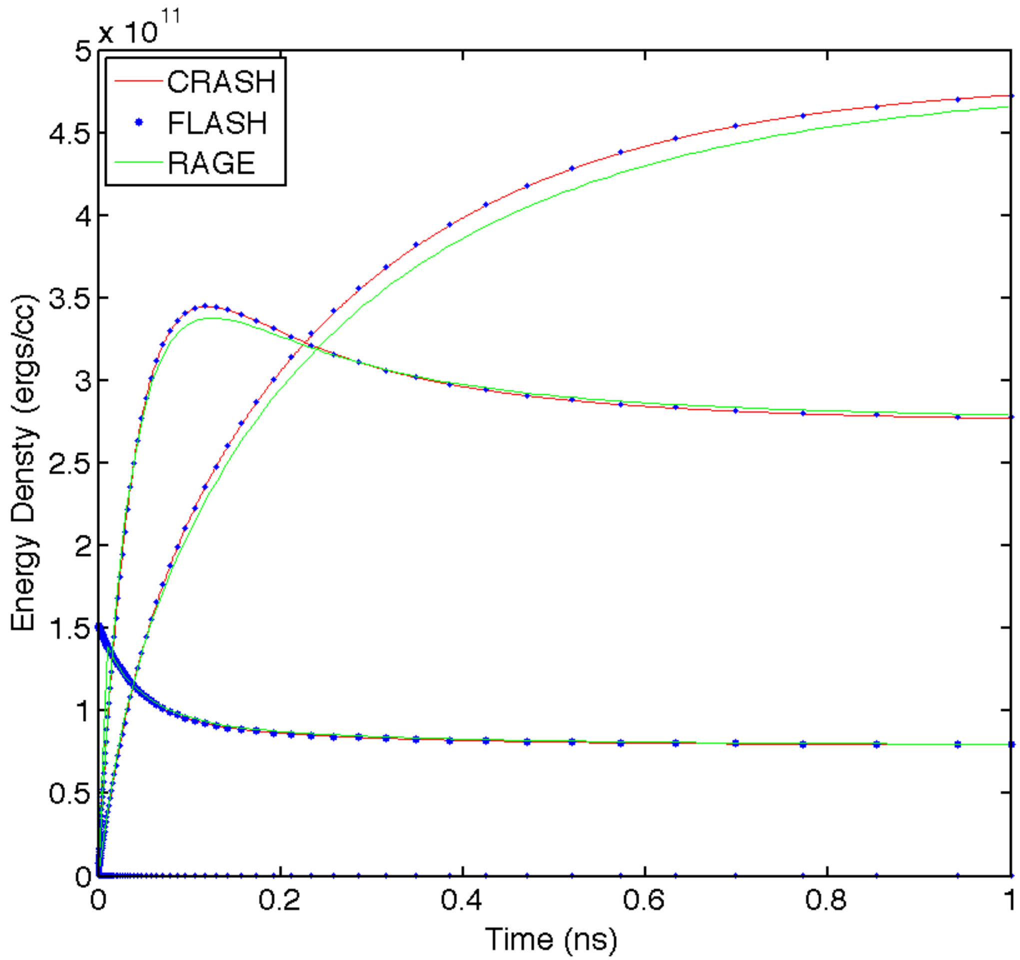
Rayleigh-Taylor growth in the presence of a radiative shock



Creation of plasma jets using laser irradiation of conical foils

Code comparison studies are not trivial but have proven useful

Infinite medium temperature relaxation
- **4 Energy groups**
- **Constant opacities**
- **Different in each group**



Study participants
- **FLASH:**
  - **Don Lamb**
  - **Milad Fatenejad**
- **CRASH**
  - **Bruce Fryxell**
  - **Eric Myra**
- **RAGE**
  - **Chris Fryer**

Accuracy is hard to come by in radiation hydrodynamics

- **All methods have weaknesses**
  - IMC: noise
  - Discrete ordinates: ray effects
  - Diffusion: errors for systems not optically thick
    - Flux limiter as potential tuning parameter
- **We use diffusion for rad hydro**
  - Also are doing radtran studies of diffusion vs transport

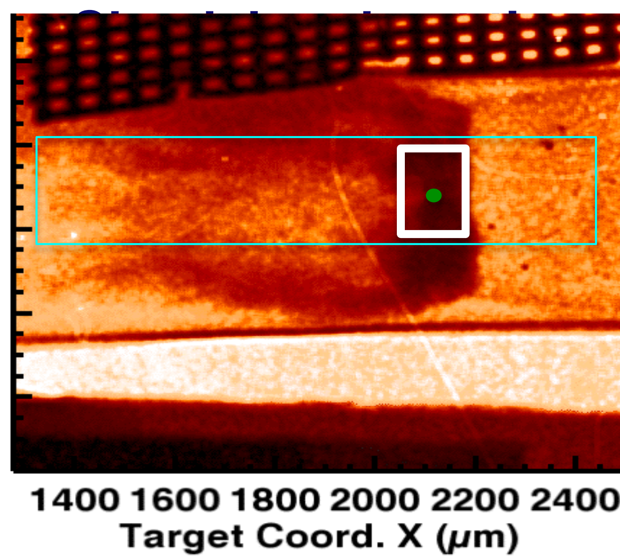
- **Current US policy puts us at an international disadvantage**
  - Only radhydro with diffusion is clearly not constrained
  - International groups in solar physics and astrophysics have already gone beyond this
  - There are no meaningful limitations: further sophistication by international researchers will be rapid

Our inputs and outputs for UQ reflect the specifics of our experimental system

Inputs

- Experimental (x)
  - Laser energy
  - Be disk thickness
  - Xe fill gas pressure
- Model parameters (θ)
  - Vary with model
  - Examples:
    - electron flux limiter, laser energy scale factor,
    - Opacity scale factor
- Form of model
  - e.g. 2D vs 3D

- Outputs (y)
  - Integrated Metrics
    - Shock location (SL)
    - Axial centroid of dense Xe (AC)
    - Area of dense Xe (A)
    - Radial moments
  - (BOT)



We use a model structure for calibration, validation & uncertainty assessment

Measured in calibration experiments with specific x and unknown theta (few of these)

Fits code over input space

x : **experimental input**

θ : **physics or calibration input**

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

$$\Rightarrow \begin{cases} \eta(x,\theta) \\ \delta(x) \quad \epsilon \\ \pi(\theta | y_m, y_c) \end{cases}$$

Replication error

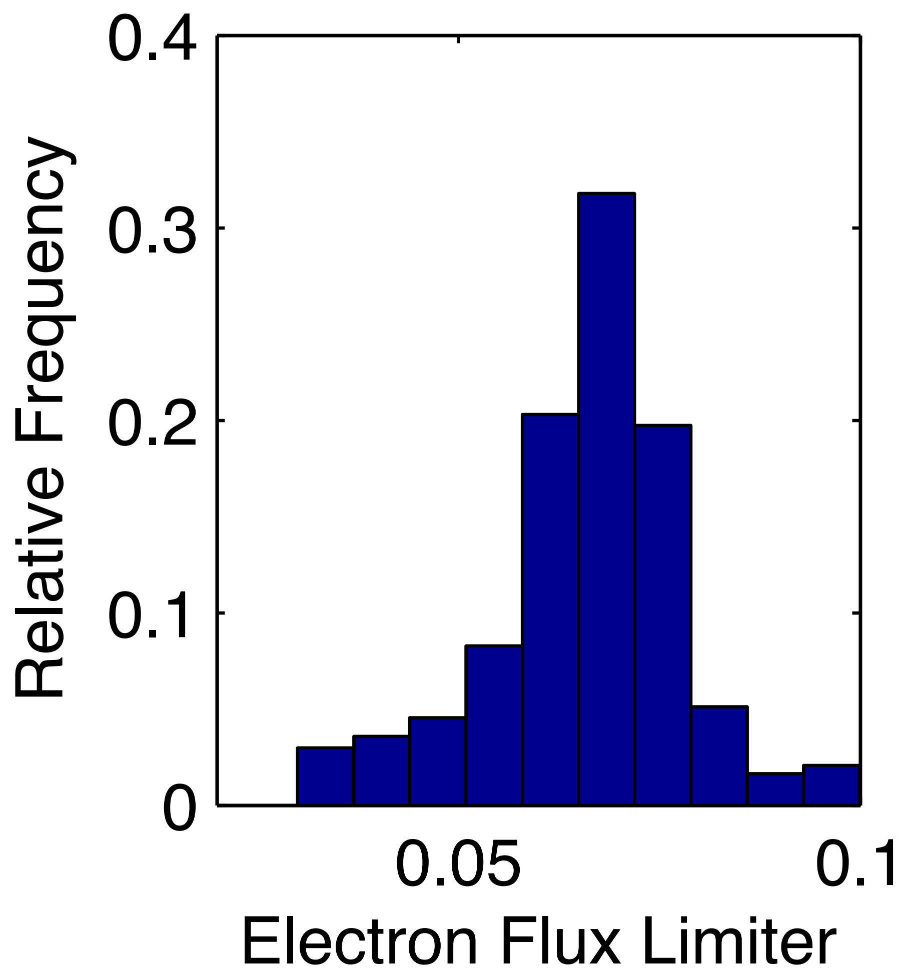
Computed with specific values of x and theta (lots of these)

Models discrepancy between reality and code – speaks to validation

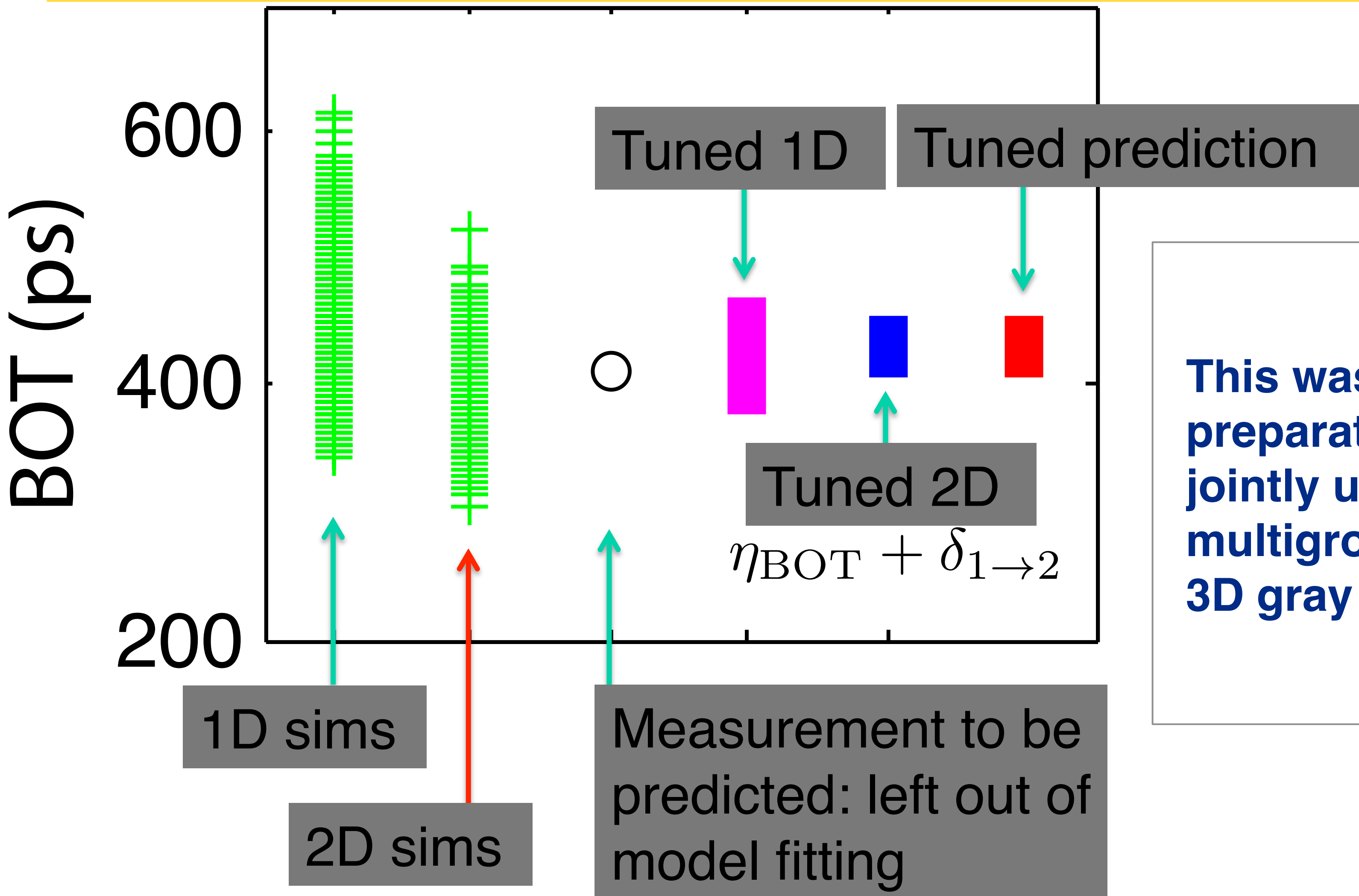
First CRASH application: Holloway et al RESS 2011

Flux limiter is an uncertain model parameter

- **Need to evaluate probability distribution of such parameters**
- **This can represent calibration or tuning**
- **If the residual discrepancy is small, we get calibration**
- **If not, we get tuning**



Using this structure we predicted shock breakout time (BOT) using 1D & 2D codes



This was preparation for jointly using 2D multigroup and 3D gray

Some comments on quantifying predictive capability

- This is really hard
- It needs deep thought and lots of work at every level
  - Experimental uncertainties are far more than just “error bars”
  - Computational uncertainty is enormously complex
    - The problem is not linearly decomposable
      - Numerics
      - Resolution (not just spatial)
      - The problem of high dimensionality
      - Quantifying uncertainty for wrong models
  - Statistical analysis does not stand alone
    - Extrapolation will always require expert judgment and analysis
    - Calibration vs discrepancy for limited data
- I see no way to do this remotely well without making it a dedicated, long-term, milestone-driven activity
  - You can’t hang a UQ bag on your technical donkeys

Acknowledgments

The Center for Radiative Shock Hydrodynamics, which developed the CRASH code, is funded by the Predictive Sciences Academic Alliances Program in NNSA-ASC via grant DEFC52- 08NA28616.

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Concluding Remarks

- **SWMF/BATSRUS/CRASH is publicly available**
  - It is downloadable from http://csem.engin.umich.edu after registration
  - However,
    - There is learning curve
      - ~1 month for a good PhD student
      - ~3-6 month for an active researcher
      - ∞ for senior Professors/administrators
    - We welcome collaborators who want to install/run the codes
- **SWMF/BATSRUS/CRASH are continuously evolving**
  - We typically provide 1 or 2 major upgrades a year
  - User feedback is very important for further development