Predicting Radiating Shock Experiments: Theory, VV/UQ, and more at CRASH

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ASC's Predictive Science Academic Alliance Program funds five university centers.

- Each PSAAP center focuses on a a multi-scale multi-physics problem.
- Each defines a 5th-year experiment (that hasn't been done before)
  - ⇒ *Predict outcome every year*
  - ⇒ *Each year, quantify how close prediction is expected to be.*
  - ⇒ *Focus of the project is to build confidence in the predicted outcome of this experiment*

- Stanford: hypersonic vehicles
- Caltech: dynamic response of materials
- Purdue: micro-electromechanical systems
- Texas (with Texas A&M): space-vehicle re-entry
- Michigan (with A&M): radiative shock hydrodynamics
  - ⇒ *This talk will introduce this center's problem and*
  - ⇒ *Detail some results from theory, verification, and uncertainty quantification*

The Center for Radiative-Shock Hydrodynamics deals with challenges similar to yours.

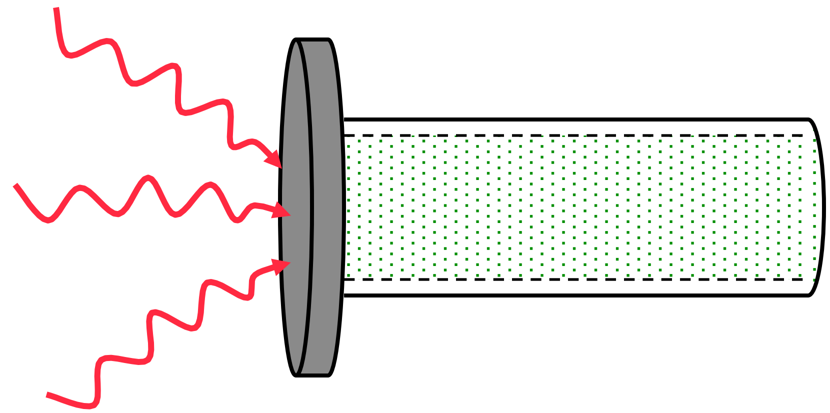
- *Similar ≠ The same (we have many fewer challenges)*
- We must develop and assess our predictive capability for a class of experiments with interesting characteristics:
  - ⇒ *High energy density*
  - ⇒ *Strongly coupled radiation and multi-material hydrodynamics*
  - ⇒ *Simulations with questionable resolution*
- There are needs to better develop
  - ⇒ *Theory*
  - ⇒ *V&V*
  - ⇒ *Computational Tools*
- We must quantify all aspects of predictive capability arising from many sources, including:
  - ⇒ *Uncertainty in constants of nature*
  - ⇒ *Errors in mathematical models (missing physics)*
  - ⇒ *Experimental errors, numerical errors, bugs, etc.*

This talk will cover several particular aspects of the CRASH's research program.

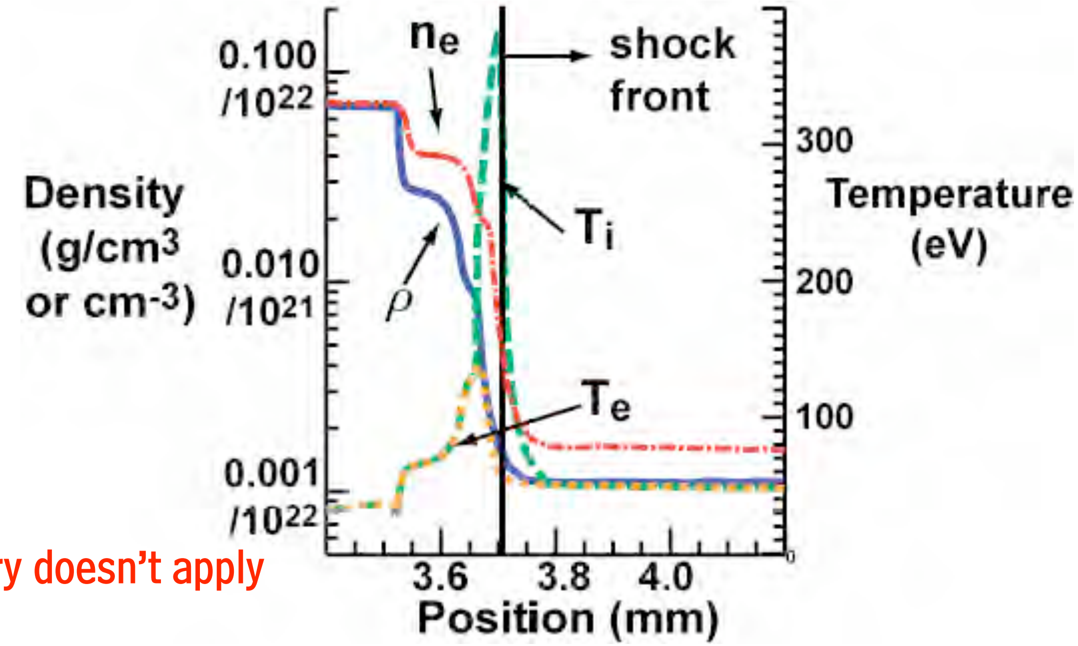
- I will
  - ⇒ *Describe the CRASH experiments and simulation strategy.*
  - ⇒ *Discuss a new theory for radiating shocks relevant to the CRASH experiment*
    - Including some interesting results for "uphill" radiation flow behind a strong shock.
  - ⇒ *Present new verification solutions for 3-T radiation-electron-ion coupling.*
  - ⇒ *Detail some uncertainty quantification work regarding the coupling of Lagrangian and Eulerian rad-hydro codes*
- These just happen to be some of the areas at CRASH that I have been involved with.
- There is a lot more work going on at CRASH that I won't have time to cover.

CRASH experiments induce radiating shocks

- Basic experiment:
  - ⇒ *10 laser beams blast a Be disk*
    - 5 kJ in 1 ns (5E12 W)
    - Be vaporizes
    - Slug of Be plasma reaches 200 km/s
  - ⇒ *Strong shock drives into Xe gas*
    - starts at 1 atm and room temp
    - pressure reaches 1,000,000 atm
    - ion temps reach 5,000,000 K (400+ eV)
  - ⇒ *Hot plasma radiates strongly*
    - thermal emission rate = acT^4
    - radiation perturbs "quiescent" Xe, altering shock propagation
    - radiation affects plastic wall, launching a radial shock inward.

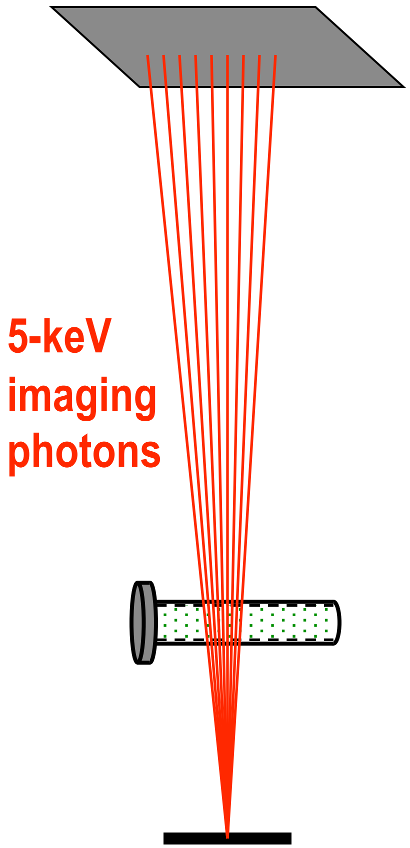


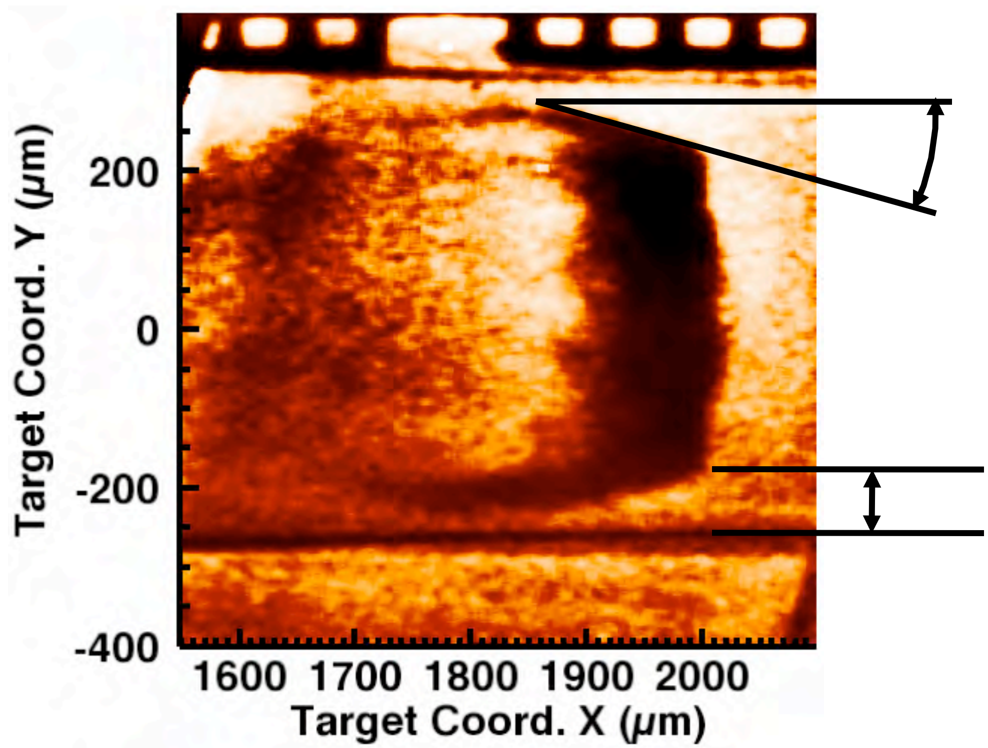
Simulation is challenging but not impossible.



- Challenges:
  - ⇒ *Large range of scales*
  - ⇒ *Complex hydrodynamics*
    - Standard radiating shock theory doesn't apply
  - ⇒ *Complex radiation flow*
    - Radiation deposition in wall drives radial shock
  - ⇒ *3T physics / possible NLTE effects*
  - ⇒ *Software development & QA*
- Not impossible:
  - ⇒ *Mathematical models (Navier-Stokes, Boltzmann, conduction, energy exchange) should be close to reality*
  - ⇒ *Should have access to significant computing power*

We are trying to quantitatively predict features of radiographs.

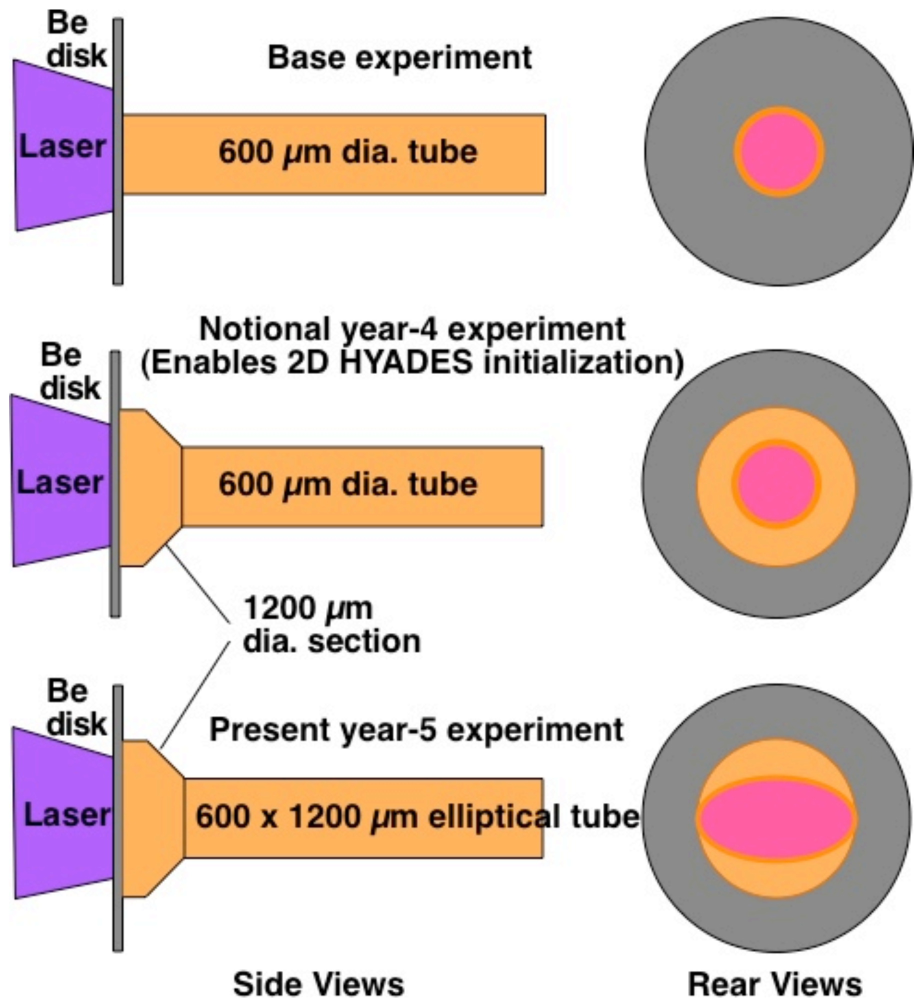




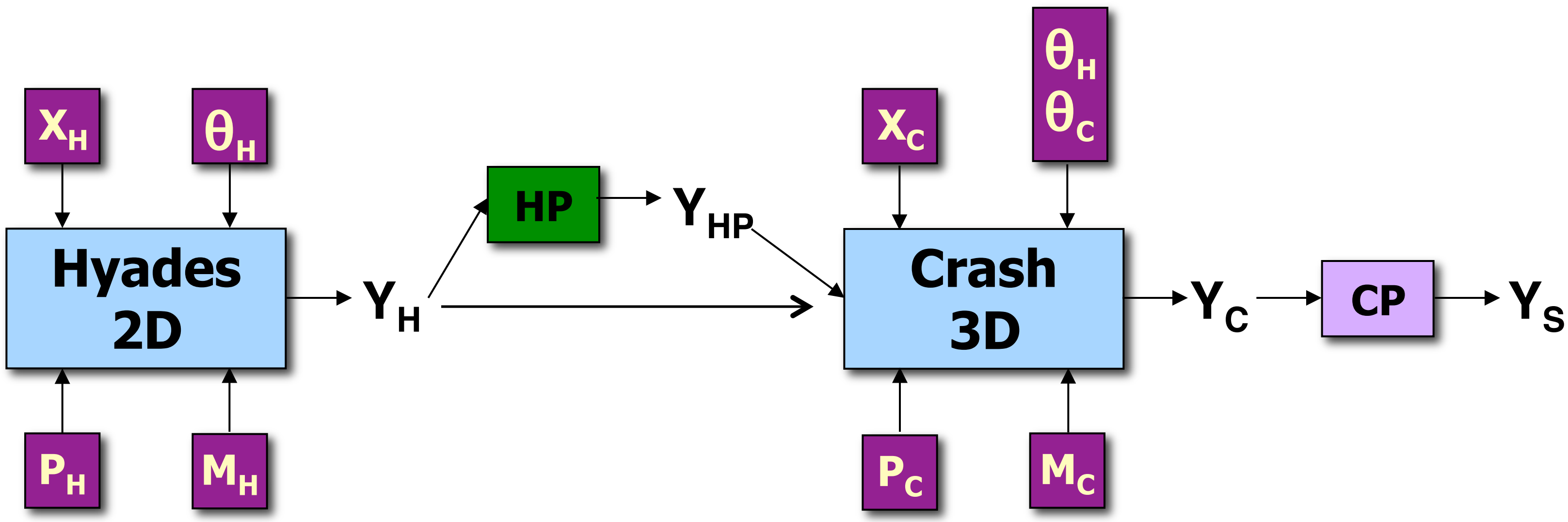
- x-ray snapshot shows dense Xe layer
- Must simulate this radiograph and compare to experiment
- Try to predict shock position, wall angle, Xe entrained behind shock

The Experiments get more complicated in years 4 and 5.

- The year four experiment involves a larger cylindrical tube that necks down into a smaller cylindrical tube.
- Year five has a cylinder neck down into an elliptical tube.
- Idea is that year four experiment will inform our understanding of rad-hydro flow in transition regions.
- No new physics between year 4 and 5
  - Year 5 is a 3-D problem though
- Experiments with reduced physics might be done on the year 5 geometry
  - Hydro only (low temperature)
  - Rad "only" (remove Be and shine x-rays down tube)



CRASH simulations employ multiple codes.



- Hyades 2D, a Lagrangian rad-hydro code, handles laser energy deposition
- Then using a pre-processor (or an emulator for Hyades) CRASH 3D is initialized
    - 3-D AMR Eulerian rad-hydro code
    - Built-in radiation diffusion, electron heat conduction, EOS/Opacity generation.
    - Radiation transport option via PDT (TAMU's S_n code)
- Post-processor produces simulated radiographs and extracts features.

Radiation Transport is the biggest computational hurdle at this point.

- For a typical 3D calculation back of the envelope calculation gives 10 trillion unknowns for radiation.
- Using the rule of thumb of 1 μs per unknown per iteration per time step
  - ⇒ *6,000 to 20,000 cpu hours per time step*
- Right now on rad only calcs we get better than 1 μs per time step on up to 10,000 cpus
- Might be able to reduce unknown count via
  - ⇒ *Biased quadrature sets*
  - ⇒ *Smart group choices*
  - ⇒ *Different meshes for rad and hydro*
- We also need to do a lot of runs for UQ purposes
  - ⇒ *1 heroic calculation won't do it*
  - ⇒ *Thinking about low-order/high-order strategies*

$$8 \times 30 \times 10^{9} \times 10^{2} = 2.4 \times 10^{13} \text{ unknowns}$$

Number of groups (30); Number of angles (10^2); Unknowns per cell (8); Number of cells (10^9)

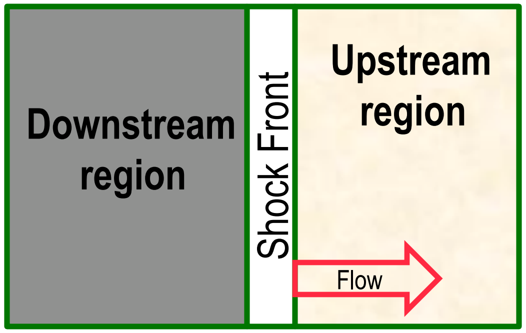
Thick-Thin Radiative Shocks

R.G. McClarren, R.P. Drake, J.E. Morel, and J.P. Holloway, "Theory of Radiative Shocks in the Mixed, Optically Thick-Thin Case", Physics of Plasmas, submitted April 2010.

R.G. McClarren and R.P. Drake, "Anti-Diffusive Radiation Flow in the Cooling Layer of a Radiating Shock", Journal of Quantitative Spectroscopy and Radiative Transfer, Accepted May 2010.

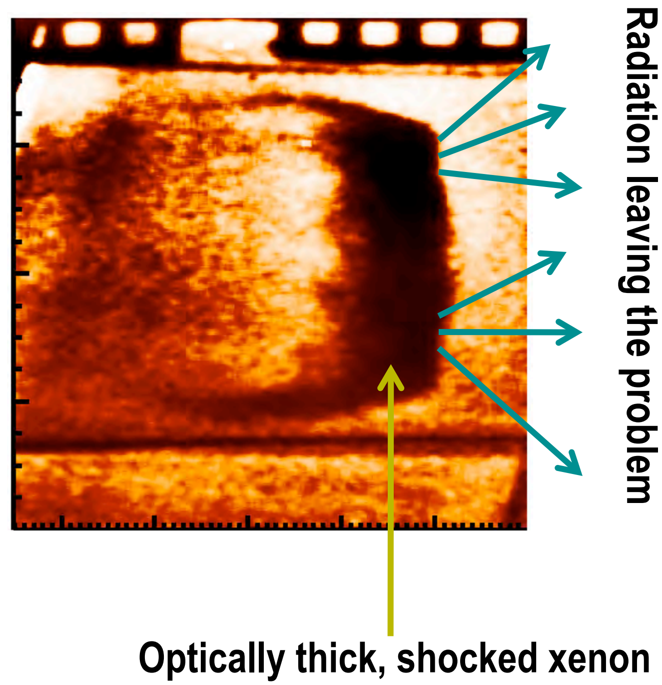
Radiating shocks can be classified based on two types of regimes.

- There are two energy-density related regimes of radiating shocks
  - ⇒ *Flux-dominated regime where the radiation energy flux ($c E_r$) is comparable to the material energy*
  - ⇒ *Pressure-dominated regime where radiation pressure is comparable to mechanical pressure*
- The optical depth of the material upstream and downstream of the shock
  - ⇒ *Optically thick (many radiation mean-free paths between the shock-front and the system boundary)*
  - ⇒ *Optically thin (a few or zero mean-free paths between shock-front and system boundary)*
- We use a two word-designation with the optical thickness of the downstream medium followed by the optical thickness of the upstream medium
  - ⇒ *Example: A shock that is thick downstream and thin upstream is a thick-thin shock*
- The main shock in the CRASH experiment is a thick-thin shock in the flux-dominated regime.



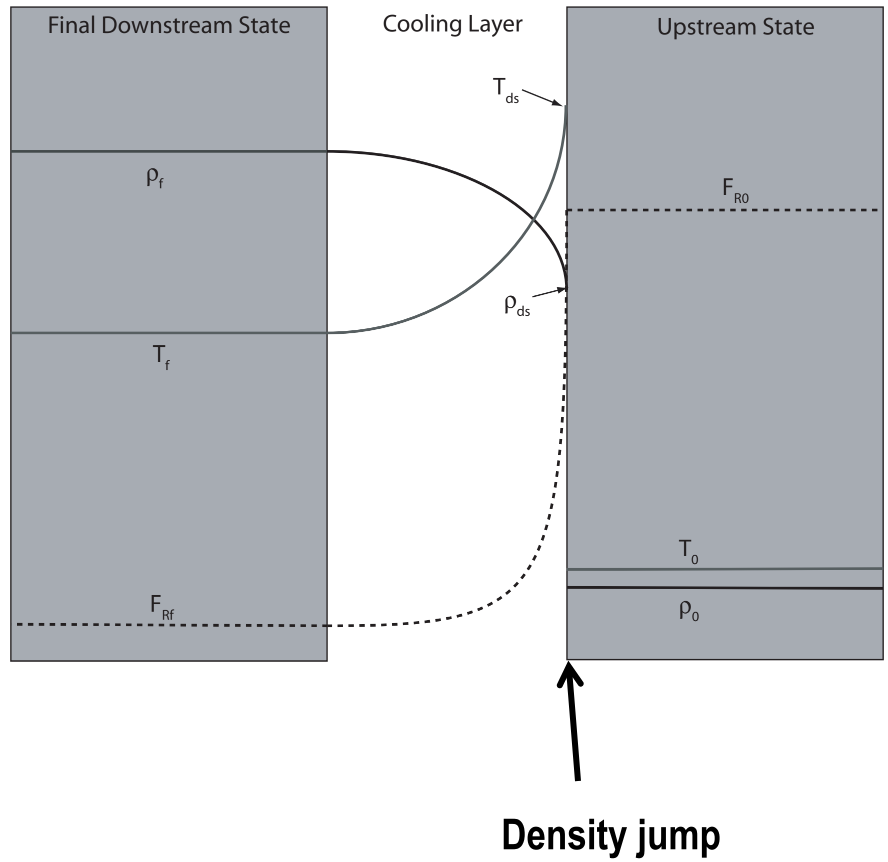
Previous radiating shock theories have dealt with the Thick-Thick or Thin-Thin case.

- Zel'dovich and Raizer and Mihalas[2] discuss the theory of thick thick shocks.
- In such a shock all energy that is radiated by the material remains in the system
  - ⇒ *This make the shock have a maximum compression of* $(\gamma+1)/(\gamma-1) \approx 4$
- Thin-Thin shocks where all the radiation leaves the problem has also been studied.
- In the CRASH experiment the xenon upstream of the shock is both finite and not optically thick
  - ⇒ *A significant fraction of radiation that moves upstream leaves the problem either out the walls or the end of the tube*
- The downstream xenon is optically thick to radiation
- Compressions of about 100 observed in experiment



We treat these shocks with a three-layer model.

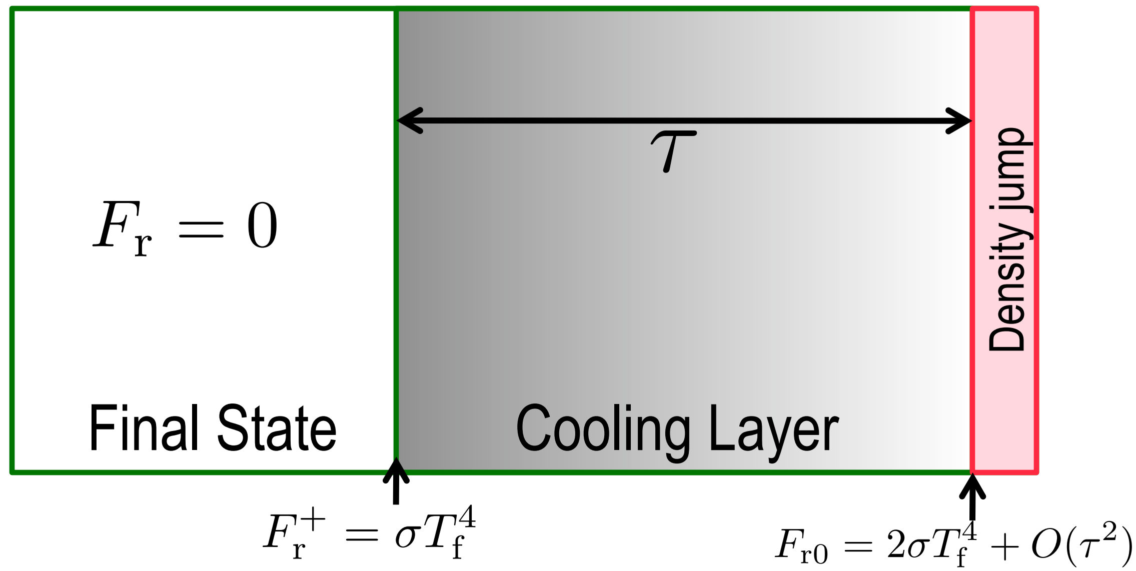
- All radiation that moves upstream of the density jump leaves the problem.
- The upstream state is quiescent with a constant temperature, density, and radiation flux.
- In the cooling layer the shocked material radiatively cools, and the density increases.
- At the final state there is no net radiation flux.
- This model ignores the effect of the "transition region" between the cooling layer and the final state.



For a steady shock we can get a simple relation between compression and radiation flux.

- Using the inverse compression $\eta = \rho/\rho_0$ we can manipulate the Euler equations to get a relation between the inverse compression and the radiation flux
$$F_{\rm rn} - F_{\rm rn0} = -1 + \frac{2\gamma}{\gamma - 1}\left[\eta - p_{0\rm n}(1-\eta)\right] - \frac{\gamma+1}{\gamma-1}\eta^2.$$
- The "0" subscript denotes upstream values, "n" means a normalized quantity.
- Therefore, if we know the radiation flux, Fr, everywhere we know the shock profile.
- The challenge is to find values for Fr everywhere.
- The inverse compression can be related to the temperature of the material as well.

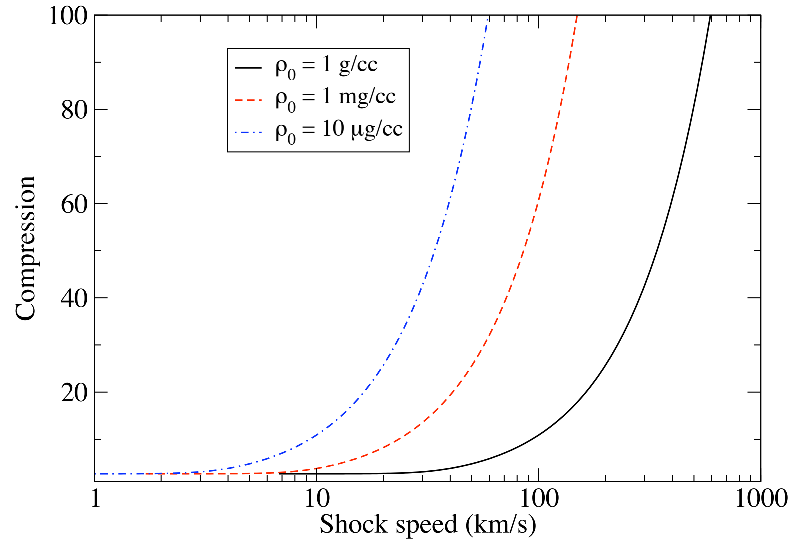
The radiation moving upstream of the density jump is twice the radiation flux from the final state.



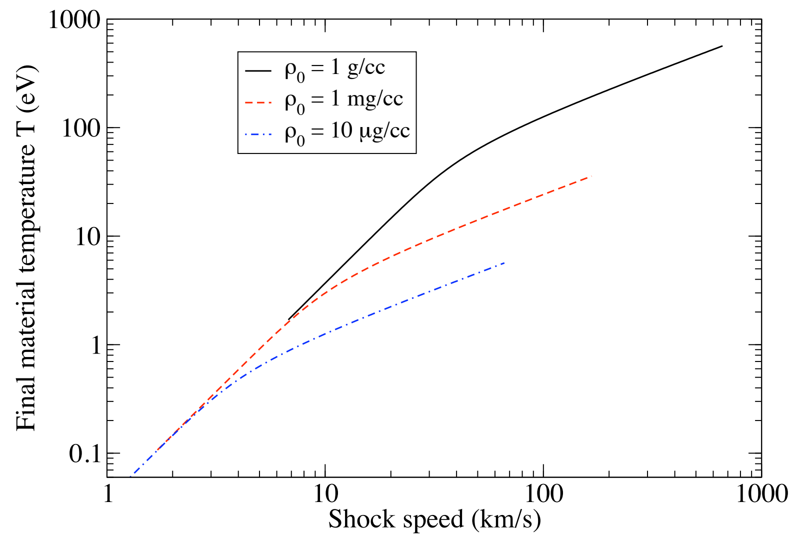
- The final state has no net radiation flux.
- A flux moving upstream from the final state is proportional to the final temperature to the fourth power.
- The radiation flux towards the final state from the cooling layer, must equal σT_f^4
- To second order in the cooling layer width, measured in optical depths, the radiation flux moving upstream from the cooling layer is equal to that moving downstream.
- This makes to the total radiation flux moving upstream to be $2\sigma T_f^4$

Final Compression and Temperature for Xenon

- The relation between the upstream radiation flux and the final temperature
  - ⇒ *Gives a quartic equation for the final inverse compression*
- The graphs on the right are for xenon with
  - ⇒ *$Z=9$ (nine times ionized)*
  - ⇒ *$\gamma = 5/3$*
- We can see the transition from a non-radiative to radiative shock.



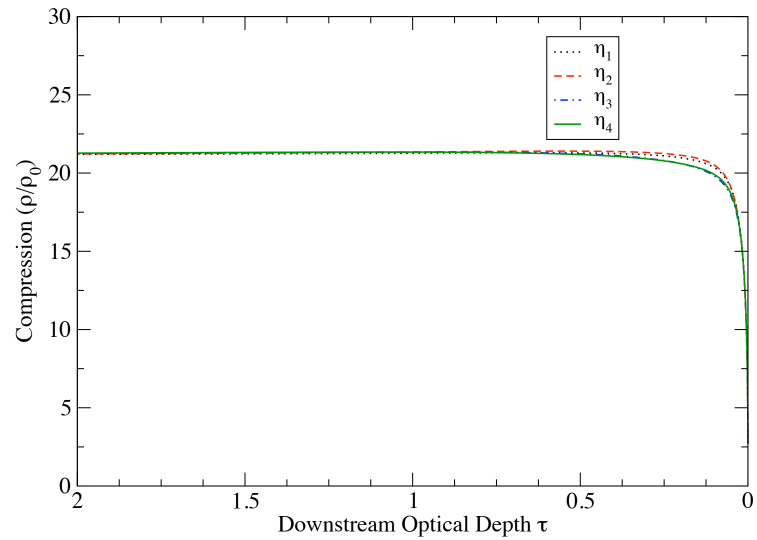
(a) Final compression



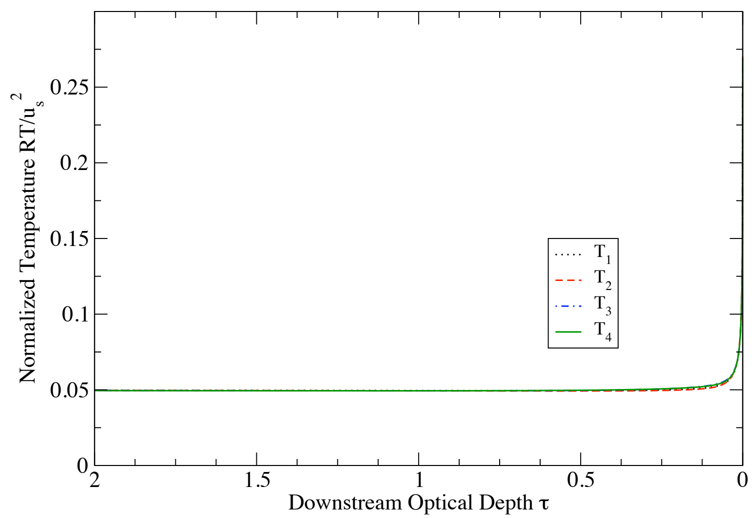
(b) Final Temperature

We compute shock profiles by iterating on the radiation mean intensity.

- We can derive an ODE for the inverse compression in terms of the radiation mean intensity, J_r.
- We then integrate this ODE from the density jump towards the final state using a postulated form for J_r
  - ⇒ *Then using the new value for the inverse compression we compute a new value of J_r and repeat until convergence.*
- This method will include the transition region between the cooling layer and the final state.
- It is important to note that we do not assume the radiation in the cooling layer is diffusive.



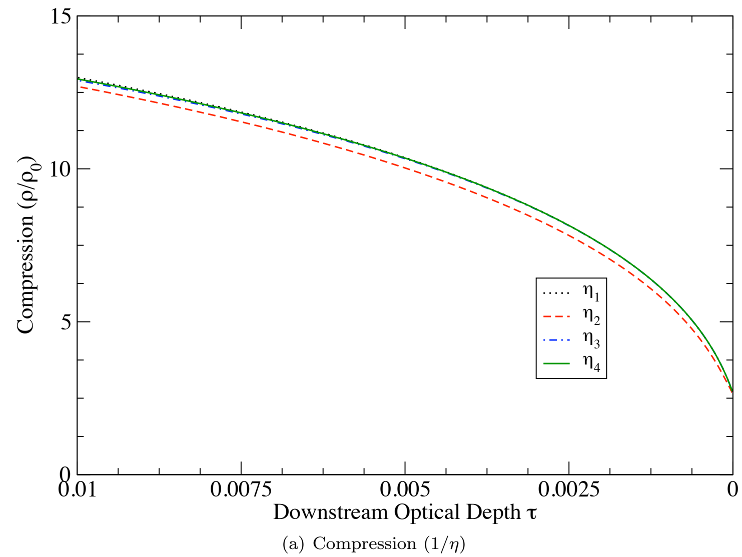
(a) Compression $(1/\eta)$



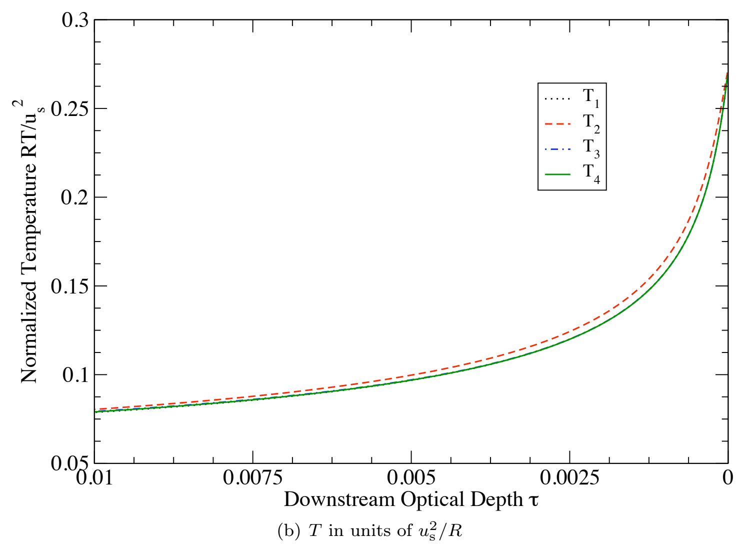
(b) T in units of u_s^2/R

We compute shock profiles by iterating on the radiation mean intensity.

- These profiles are for a particular shock strength ($Q=10^5$) and $\gamma=5/3$.
- The density jump is at $\tau=0$
- These results agree with our three layer model
  - ⇒ *Cooling layer is much smaller than a mean-free path*
  - ⇒ *The final values for compression and temperature agree with predictions.*
- Four iterations is sufficient to compute these profiles.



(a) Compression ($1/\eta$)



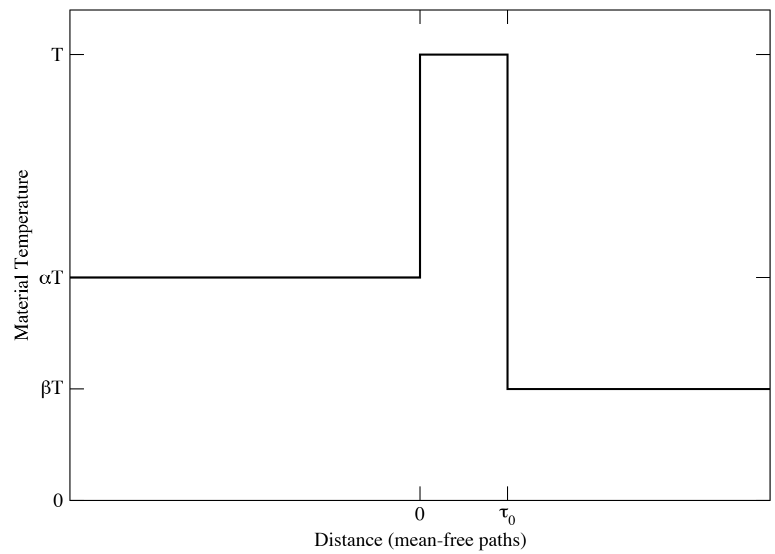
(b) T in units of u_s^2/R

This isn't the whole story of thick-thin shocks.

- There are several aspects that are present in the CRASH experiment that are not in our model
  - ⇒ *The radiation flux is not constant upstream of the shock due to losses out the side of the tube.*
  - ⇒ *There is some absorption of radiation in the upstream region.*
- We are also thinking about how these shocks will behave in other geometries
  - ⇒ *Convergent geometries could be thick-thin or thin-thick depending on the shock direction*
- Work needs to be done to understand the wall shocks in the CRASH experiment.
  - ⇒ *This could be significantly harder.*

Diffusion methods can qualitatively fail in the cooling layer of a radiative shock.

- Diffusion methods (including FLD) assume that the gradient of the rad energy density is in the opposite direction of the rad flux
  - ⇒ *Radiation flows downhill locally*
- Transport has no such restriction.
- Through exactly integrating the radiative transfer equation for a simple model problem
  - ⇒ *We can prove that radiation will flow uphill under certain constraints*
  - ⇒ *The problem resembles a rad shock*
- When this is the case, diffusion will be qualitatively wrong.



Conditions for uphill rad flow

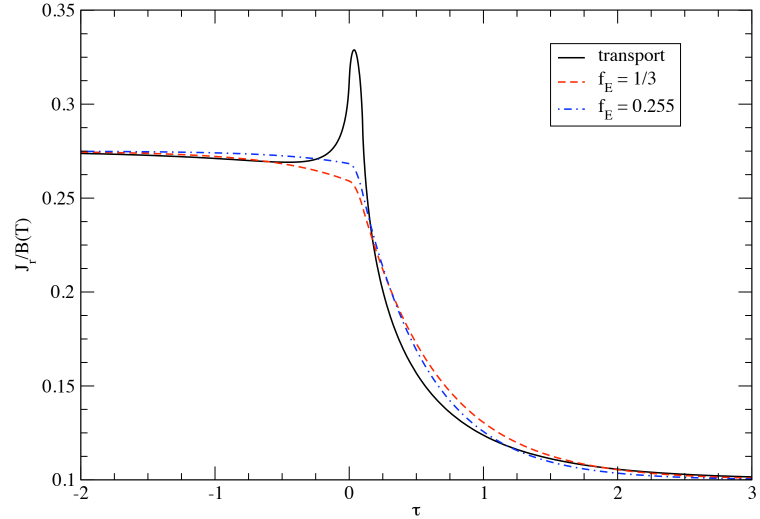
$$a = \alpha^4, \qquad b = \beta^4$$

$$(1-a)(1-b) > 0$$

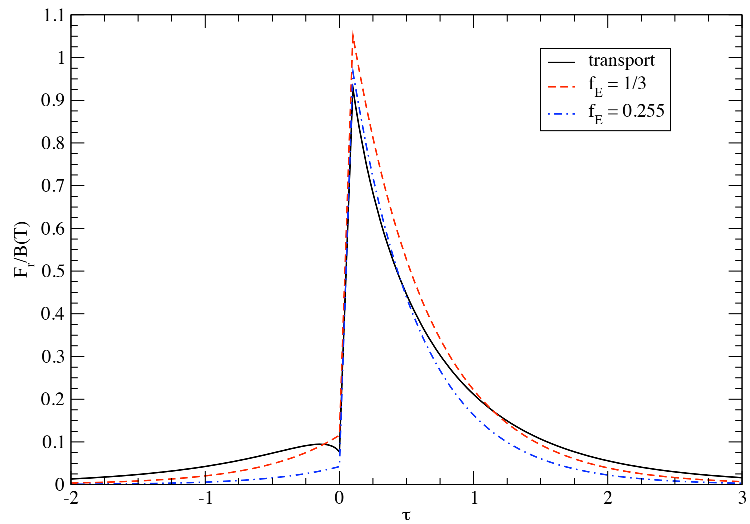
$$\frac{(1-a)(1-b)}{(1-a)^2 + (1-b)^2} < \frac{1}{3} - \frac{2}{9}\tau_0 + O(\tau_0^2)$$

Numerical results demonstrate anti-diffusive rad flow.

- Transport results from integrating the radiative transfer equation.
- Diffusion results with several Eddington factors.
- $E_r = J_r/c$
- Note "spike" in transport solution, not present in diffusion solutions.
- This monotonic behavior of the radiation energy in the cooling layer has been observed before.
- Note that these results do not mean that diffusion can never get a spike in the cooling layer.
- Transport solution is linear comb. of exponential integral functions
  - ⇒ *Diffusion solution is comprised of simple exponentials.*



(a) J_r



(b) F_r

Verification Solutions for 3-T Physics

R.G. McClarren and J.G. Wohlbier, "Analytic Solutions for Ion-Electron- Radiation Coupling With Radiation and Electron Diffusion", Journal of Quantitative Spectroscopy and Radiative Transfer, submitted April 2010. LA-UR 10-01969

Verification solutions to the 3-T equations

- This work was motivated by a desire to verify that CRASH 3D and other codes are solving the 3-T (radiation, electron, ion) equations correctly.
- Previously, Su and Olson presented solutions for 2-T (radiation and material) problems under the assumption that $C_{\mathrm{v}} \propto T^3$
  - ⇒ *They solved the 2-T equations for both transport and diffusion in slab geometry*
  - ⇒ *The idea is that with this dependence of the heat capacity the equations are linear and integral transforms can be used to solve the equations*
- Previously, have used this linearization to solve the P_1 and S_2 equations in several geometries.
- This work extends their solutions to the 3-T case
  - ⇒ *Different assumptions need to be made to linearize the equations*

3-T Equations and Linearization

- We use a radiation diffusion model for the 3-T equations and include electron heat conduction

$$\frac{\partial E_\mathrm{r}}{\partial t} = \frac{\partial}{\partial x}\frac{c}{3\sigma_\mathrm{t}}\frac{\partial E_\mathrm{r}}{\partial x} + c\sigma_\mathrm{a}(aT_\mathrm{e}^4 - E_\mathrm{r}),$$

$$C_\mathrm{ve}\frac{\partial T_\mathrm{e}}{\partial t} = \frac{\partial}{\partial x}D\frac{\partial T_\mathrm{e}}{\partial x} + \gamma_\mathrm{ei}(T_\mathrm{i} - T_\mathrm{e}) - c\sigma_\mathrm{a}(aT_\mathrm{e}^4 - E_\mathrm{r}),$$

$$C_\mathrm{vi}\frac{\partial T_\mathrm{i}}{\partial t} = -\gamma_\mathrm{ei}(T_\mathrm{i} - T_\mathrm{e}).$$

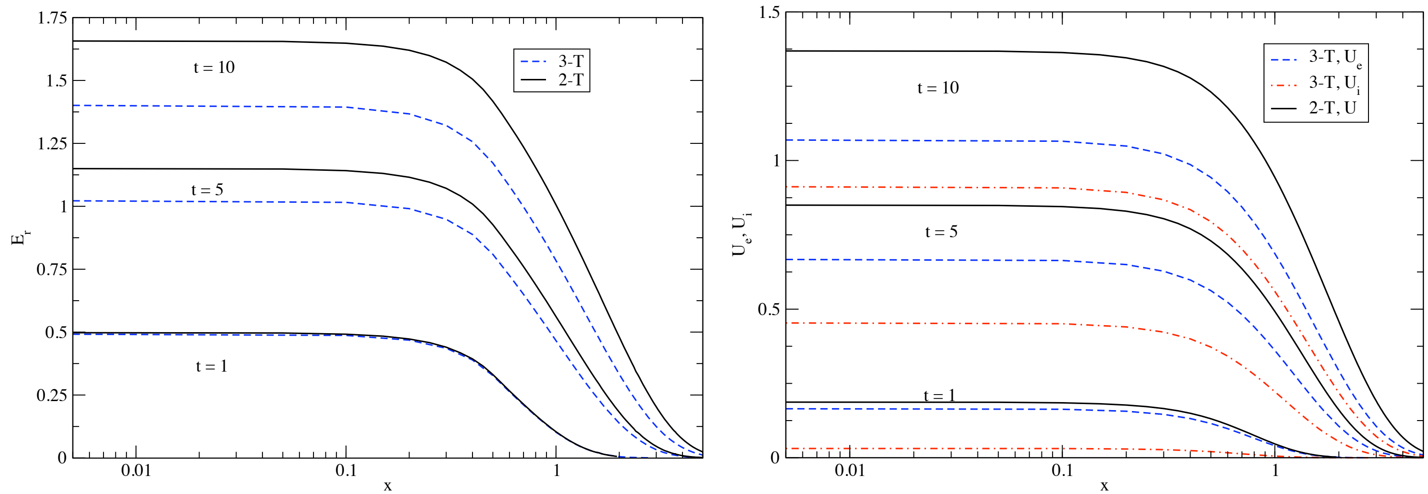
- To make these equations linear we need

$$C_{v\alpha} = \beta_\alpha T_\alpha^3, \quad D = 4a\kappa T_\mathrm{e}^3, \quad \gamma_\mathrm{ei} = a\gamma\frac{T_\mathrm{i}^4 - T_\mathrm{e}^4}{T_\mathrm{i} - T_\mathrm{e}}.$$

- Once we have linearized the equations we can solve using Fourier and Laplace transforms.
- It turns out we can analytically invert the Laplace transforms
  - $\Rightarrow$ *The Fourier transforms are computed numerically.*

Results for Su-Olson problem

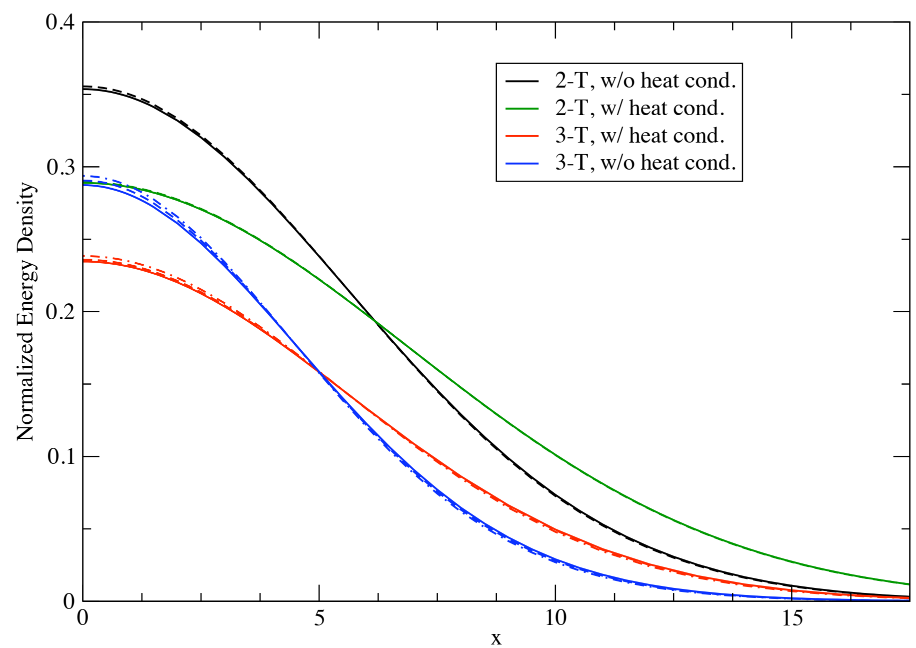
- Su and Olson solved the problem of a material with a radiation source turned on in a cold material.
- The source extends over $x \in [-1/2, 1/2], \qquad t < 10$
- Solutions below are in dimensionless variables, Er, Ue, Ui
- The maximum energy density in the 3-T problem is below that from the 2-T solution.



(a) Radiation Energy (b) Material Energy

Turning on a new physics decreases energy density.

- The comparisons at t=100 (long after the source is turned off) show each new physics decreases the maximum energy density.
- Solid lines are Er
  - ⇒ *Dashed lines are Ue*
  - ⇒ *Dash-dot lines are Ui*
- Not unexpected
  - ⇒ *Each new physics gives the energy a new place to go*



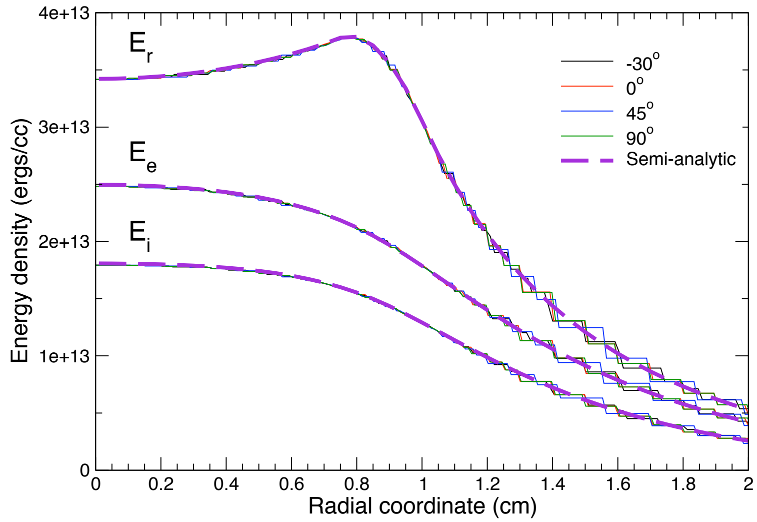
Due to linearity we can transform the planar geometry solution to other geometries.

- The solution from a planar source can be related to the solution from a point source
  - ⇒ *Consider the plane source is made up of an integral over point sources, and invert:*

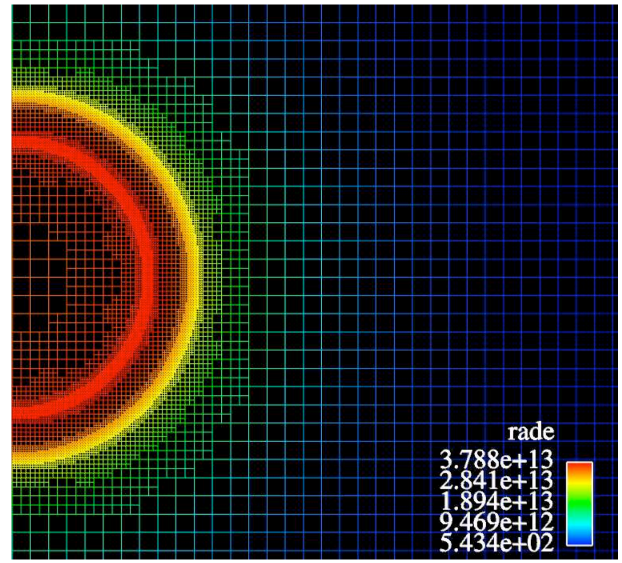
$$G_{\text{point}}(r,t) = -\frac{1}{2\pi r}\frac{\partial}{\partial x}G(x=r,t),$$

- Then using this point kernel solution, we can integrate to get the solution from any source we like.
  - ⇒ *Only constraint is how complicated of integrals we want to do.*
- Integrals over spheres are easy to carry out
  - ⇒ *This will give us solutions to the 3-T equations with a spherical source.*
- Using linearity again we can subtract spheres of different radii to get a spherical shell source.
- The inverse transforms for this case are no harder than before.
- Cylinders are more difficult than spheres, though possible.

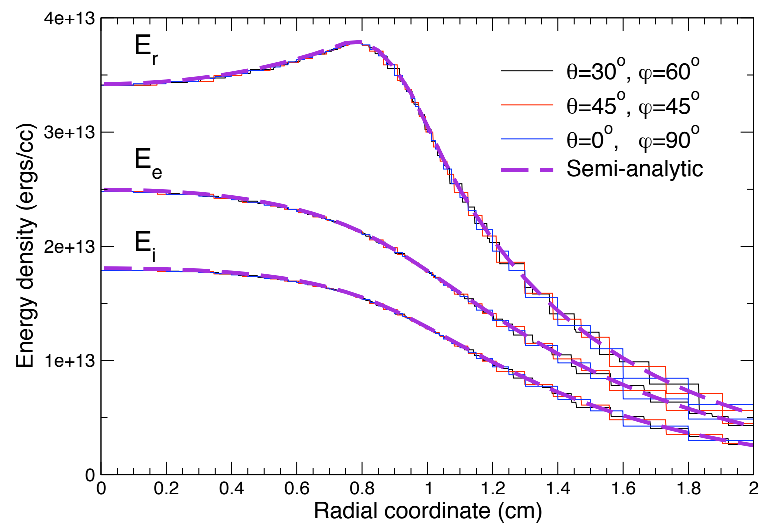
3-T xRage results for a spherical cell source



2-D ⟷



- John Wohlbier (CCS-2) used xRage to solve the problem of a shell radiation source
- Solved in several geometries
  - ⇒ *1-D (r) – not shown*
  - ⇒ *2-D (rz)*
  - ⇒ *3-D (xyz)*
- Results agree well with analytic solution
  - ⇒ *Not a true verification study at this point*



3-D

Next step is to solve this problem with rad transport and/or a nonlinear material.

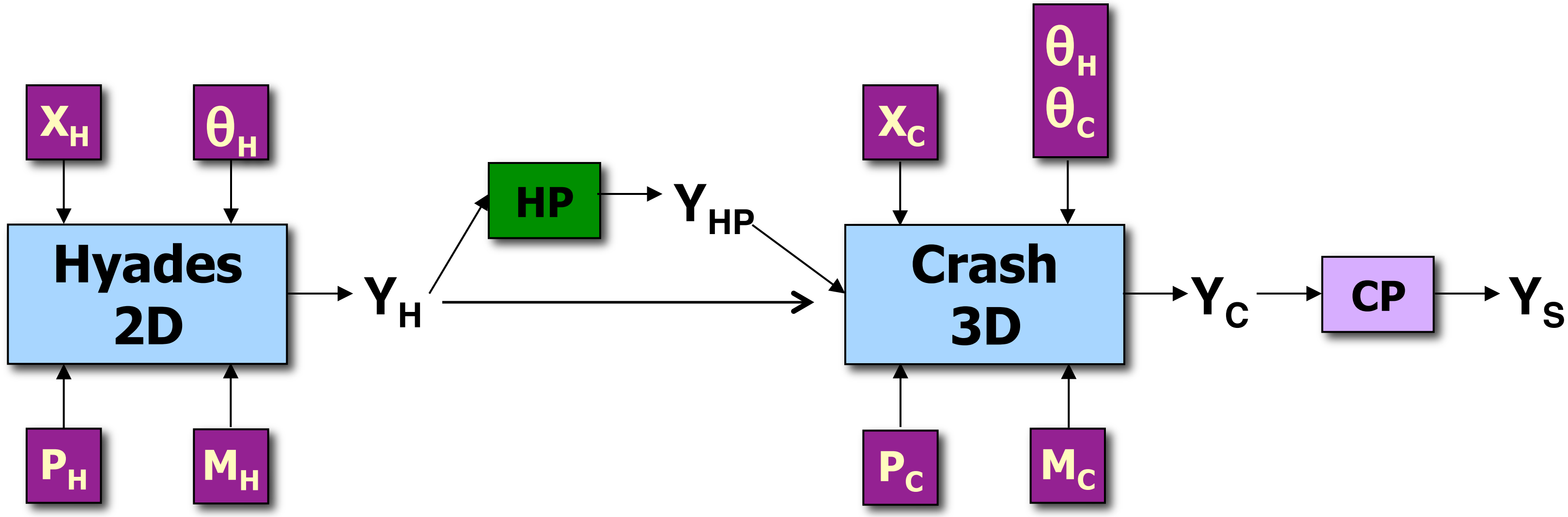
- Extending these results to radiation transport (as opposed to diffusion) should be straightforward
  - ⇒ *Just more integrals to compute*
  - ⇒ *Useful to test 3-T IMC or S_n*
- Two paths available for nonlinear equations
  - ⇒ *Solve a 0-D problem with real C_v and electron-ion coupling coefficients*
    - This is just solving an IVP for a system of ODE's
    - Already done for 2-T equations (Mosher 2006)
  - ⇒ *Not solve for pointwise values of the rad, electron, and ion energies*
    - Rather solve for spatial moments of these energies as a function of time
    - Just as useful for verification as an analytic function of space
- Multigroup extensions also possible.

A Physics-Informed Emulator

For UQ Analysis on Coupled Rad-Hydro Codes

R.G. McClarren, D. Ryu , R.P. Drake, et al., "A Physics Informed Emulator for Laser-Driven Radiating Shock Simulations", Reliability Engineering and System Safety, submitted March 2010.

The coupling of two codes makes UQ for CRASH challenging



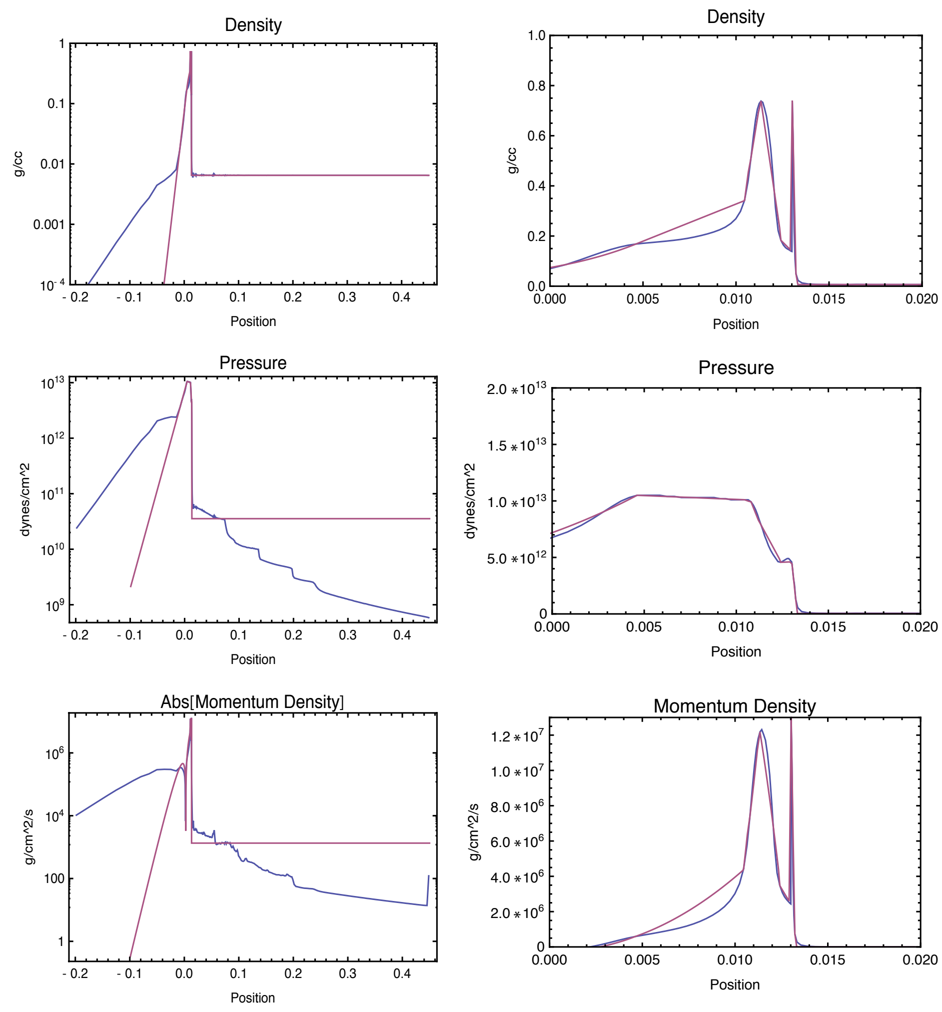
- Hyades 2D is a commerical, Lagrangian rad-hydro code
  - ⇒ *We use for laser energy deposition*
  - ⇒ *A gray box (at best)*
- We desire to rely on this code as little as possible for success
  - ⇒ *Semi-reliable*
  - ⇒ *Expensive (in terms of human time) to get solutions*
- To do UQ studies on CRASH 3D, we need to know sensitivity of CRASH output on Hyades input
  - ⇒ *This would easier with an emulator for Hyades*

We first attacked a 1-D problem with real experimental data.

- The Hyades output data at 1.2 ns, even in 1-D, is thousands of degrees of freedom
- We first tried to reduce this data using purely statistical means
  - ⇒ *Bayesian partition model, and other methods were used*
- These methods reduced the number of degrees of freedom to about 400
  - ⇒ *Still too many to do a dense Latin-Hypercube sampling of the space*
- Statistical methods have no physical judgment
- Using physics reasoning we were able to reduce the Hyades output to 40 DOFs.
- These 40 points were arrived at by looking at which parts of the data really matter to what we are trying to compute
  - ⇒ *Shock location at ∼13 ns*

We used a piecewise linear/exponential fit between important features.

- Looking at the Hyades output we were able to pick out 10 points that are important.
- Between these points we use a linear fit, perhaps on a log-scale.
- Some features are obvious
  - ⇒ *Shock location*
  - ⇒ *Be/Xe interface*
  - ⇒ *Edge of precursor*
- Others are just features in the solution
  - ⇒ *Where the pressure derivative goes negative*

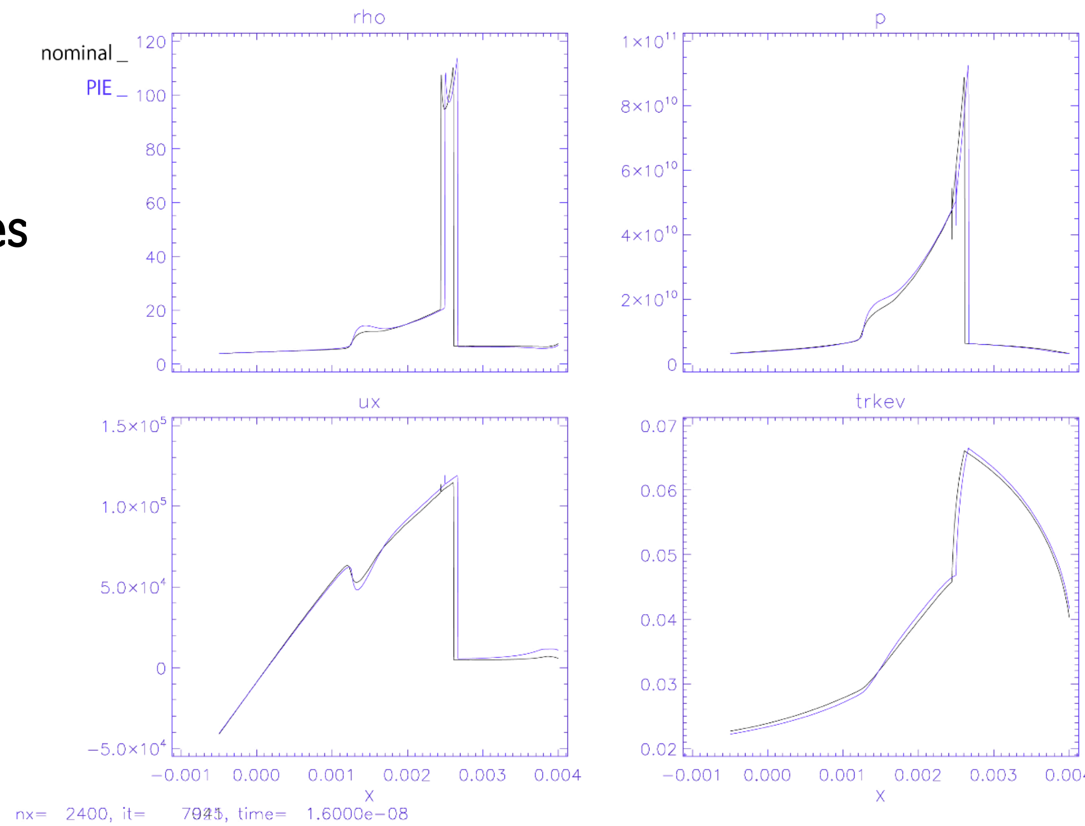


(a) Hyades Results

(b) Detail

Initializing CRASH with PIE or Hyades affected shock location less than experimental error.

- Our dimension reduction was successful to point that it didn't affect shock location.
- We call the reduction of the Hyades data + the emulator for those 40 points the Physics-Informed Emulator (PIE)

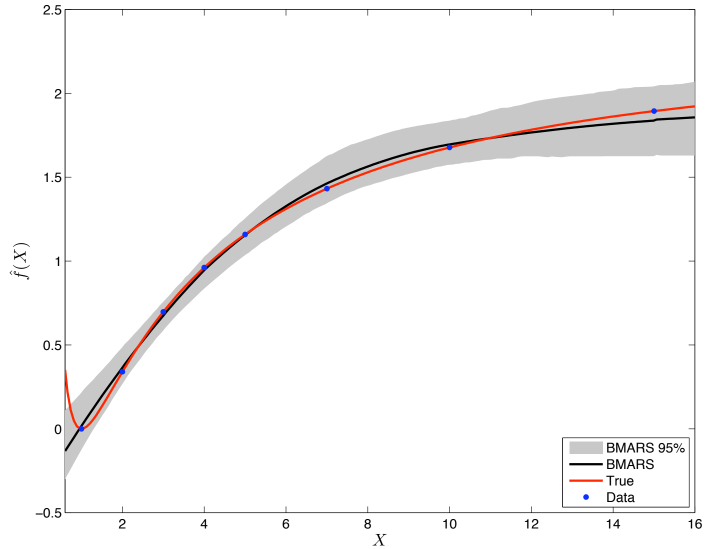


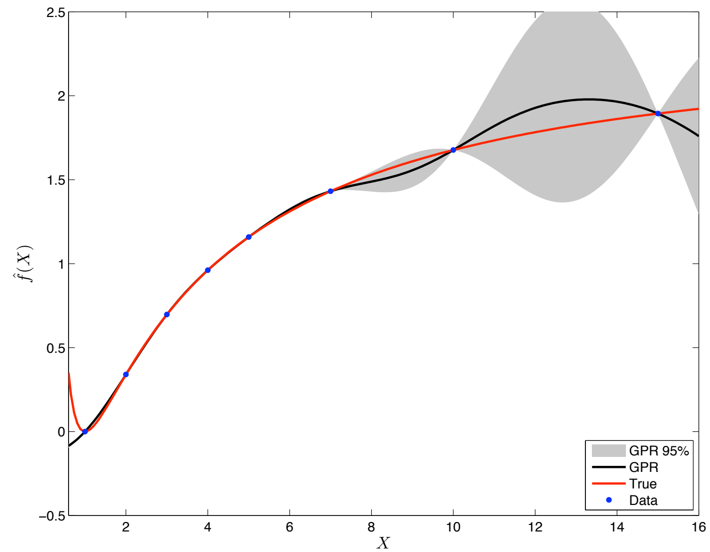
We used Bayesian MARS and Gaussian Process Regression to build an emulator.

- Bayesian MARS (multiple adaptive regression splines) tries to build the smallest system of splines to interpolate the data.
  - ⇒ *Uses a probabilistic approach to find the best regression.*
- Gaussian process models generates a distribution of functions that interpolate the data
  - ⇒ *The functions that interpolate the data are the most likely in this distribution.*
- For demonstration, models compared on function

$$f(x) = (\log x)^2/\sqrt{x}$$

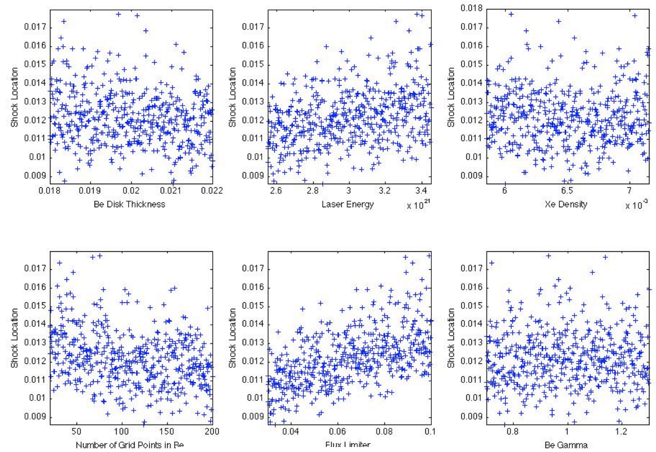
- Neither model is perfect.



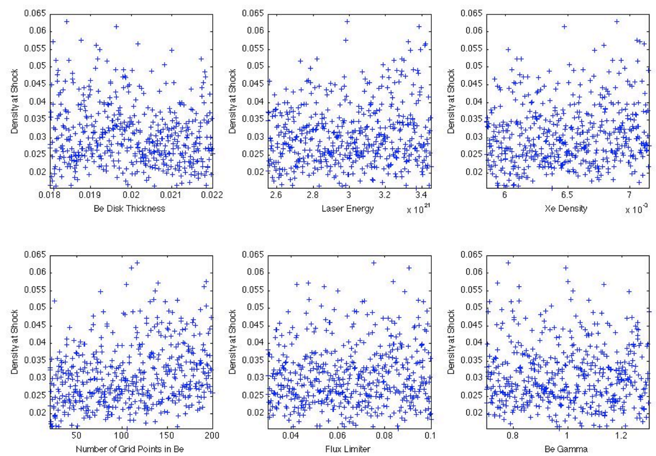


PIE built with 512 runs of Hyades

- Hyades runset varied 15 parameters
  - ⇒ *8 for experiment configuration*
    - Be thickness
    - Laser energy
  - ⇒ *7 numerical parameters*
    - Number of energy groups
    - Xenon gamma
    - Electron flux limiter
- Results for shock location and density at shock as function of six inputs shown at right.



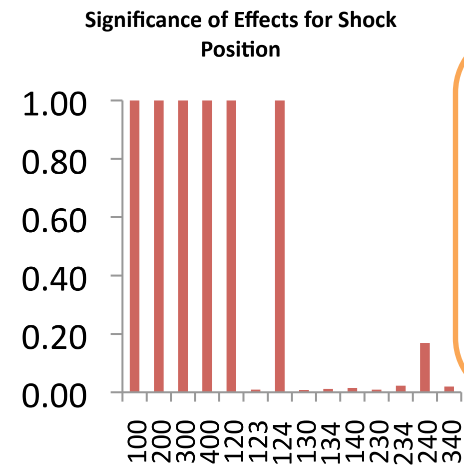
Shock Location



Density at Shock

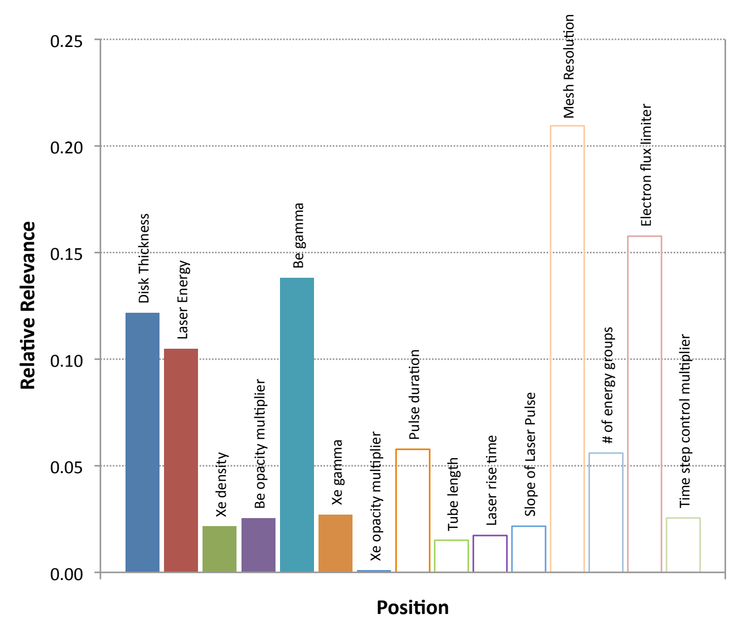
Emulator also allowed use to determine which inputs to Hyades are most important.

- From BMARS we can tell which inputs affect each output the most
  - ⇒ *Which fraction of my regressions don't have a particular interaction.*
- GPR has relative relevance parameters that tell how important each input is.
- This lead us to study how to reduce uncertainties in the important parameters.

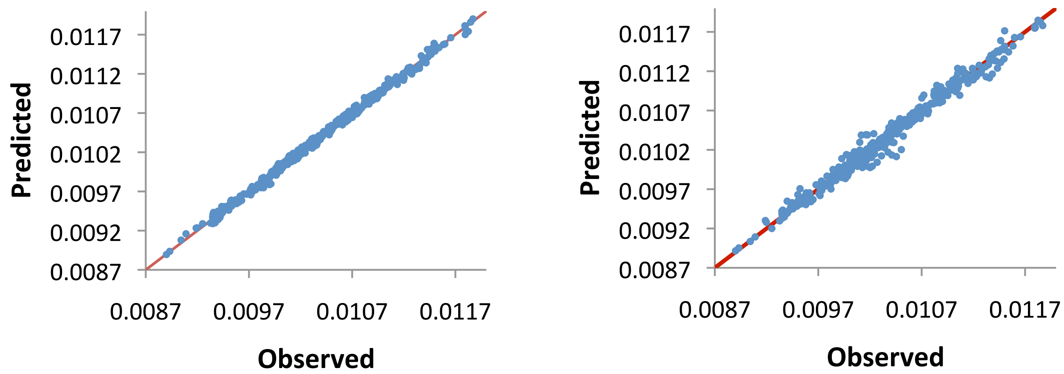


Effects in Graph

0	none
1	Laser Energy
2	Pulse Duration
3	Xe Density
4	Be Thickness



Emulation accuracy is comparable for both methods.



(a) BMARS

(b) Gaussian Process Regression

- Straight line of x=y would be perfect emulation.
  - ⇒ *Predicted is emulator value*
  - ⇒ *Observed is Hyades value.*
- This data is for shock location.
- Both predict shock location within 3%
  - ⇒ *Comparable for other methods.*
- The GPR emulator was used in a Kennedy-O'Hagan model to predict shock location on a series of experiments.

Emulator in 2-D is more complicated.

- Work is ongoing to understand 2-D Hyades output.
- Inside the tube the PIE approach seems to work.
  - ⇒ *Interaction with walls is more complicated.*
- We are considering building thousands of GPR emulators to describe this data.
  - ⇒ *Easy to do in parallel when one assumes that each output point is uncorrelated to the others.*
- Might even add a laser package to CRASH to avoid Hyades altogether.

There is a lot of interesting work going on at CRASH.

- Ongoing work includes
  - ⇒ *Radiating shock physics*
  - ⇒ *UQ and Assessing Predictive Capability*
  - ⇒ *Numerical Methods*
  - ⇒ *Verification and Validation research*
- I’ve given you a taste of some of the projects I have worked on.
  - ⇒ *Thick-Thin Shock Theory*
  - ⇒ *3-T Verification Solutions*
  - ⇒ *UQ on code coupling*
- I didn’t talk about other work that I have contributed to CRASH
  - ⇒ *Radiation transport numerical methods*
  - ⇒ *Developing test problems to compare diffusion vs.* S_n *transport*
- All of this work will, ideally, contribute to a successful prediction of the year five experiment.

A lot of people worked hard to get the results in this talk.

- CRASH at U of Michigan
  - ⇒ *Paul Drake, James Holloway, Ken Powell, Quentin Stout, Bruce Fryxell, Eric Myra, Bart van der Holst, Gabor Toth, Carolyn Kuranz, and Jason Chou, and others*
- Texas A&M
  - ⇒ *Marvin Adams, Jim Morel, Bani Mallick, Duchwan Ryu, Daryl Hawkins, Nancy Amato, Lawrence Rauchwerger, Timmie Smith, and others*
- Simon Fraser University
  - ⇒ *Derek Bingham*
- LANL
  - ⇒ *John Wohlbier and Rob Lowrie*
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Questions?