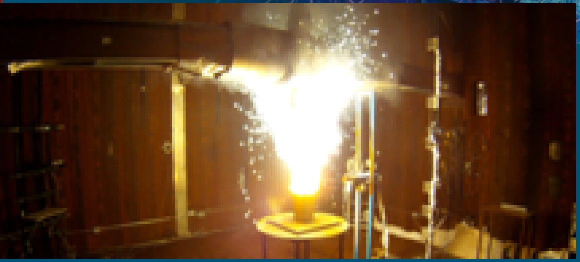
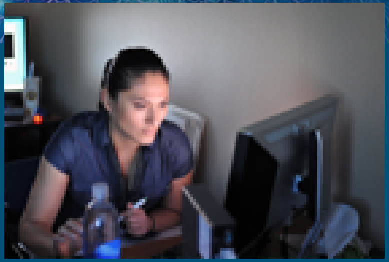
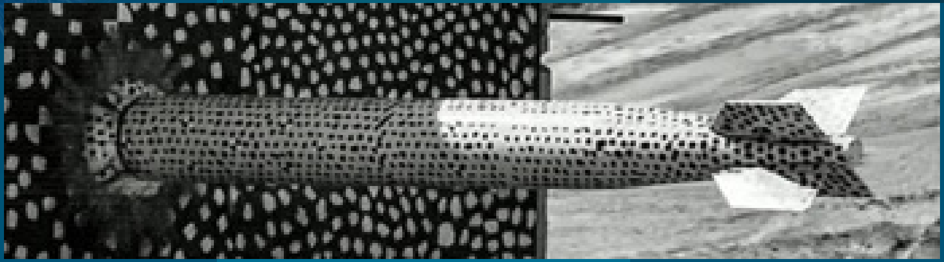
SAND2022-5817C

Sandia National Laboratories

Bayesian Parameter Estimation for Data Integration in ICF Experiments







PRESENTED BY

Patrick F. Knapp

November 7, 2018

Thanks to my many colleagues and contributors

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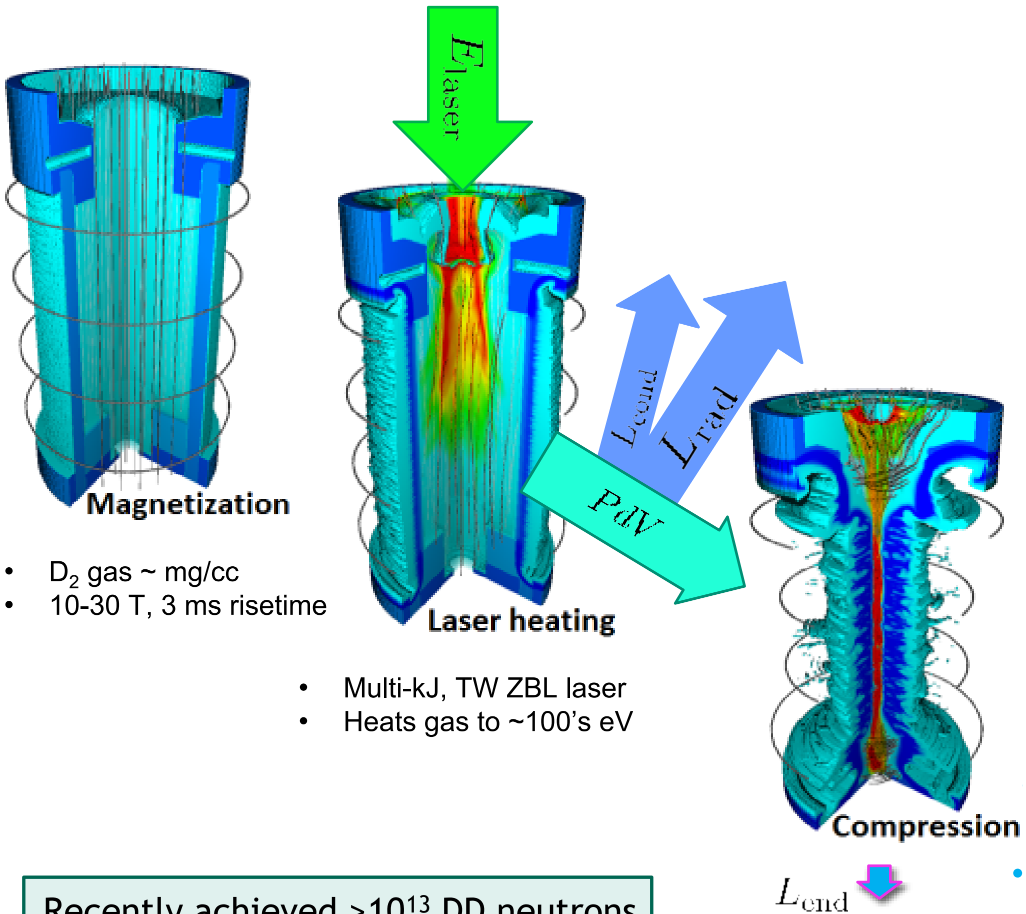
Goals

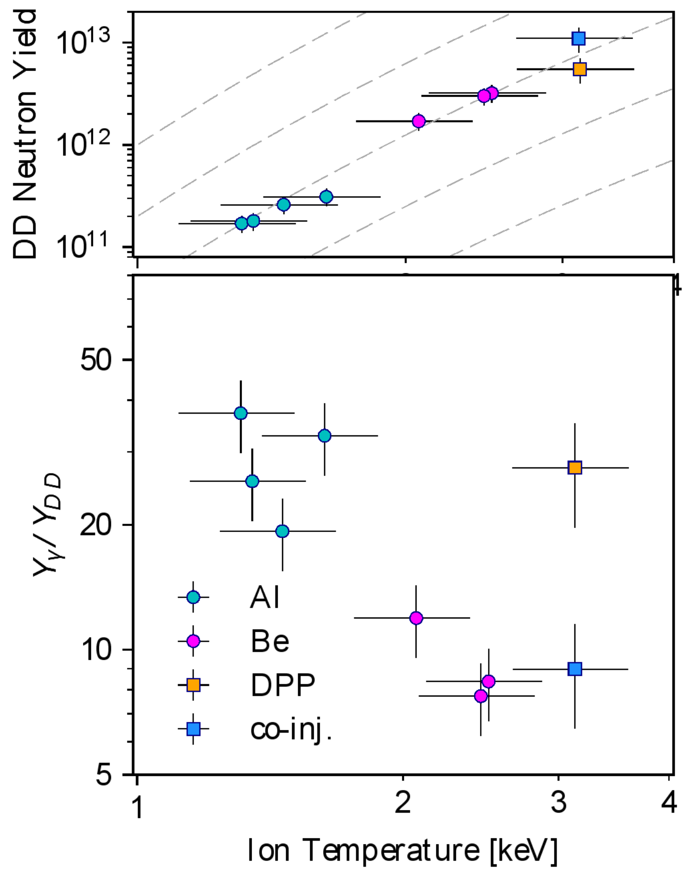
- Develop a methodology for integrating multiple, disparate diagnostics on a single experiment to better constrain the stagnation conditions and uncertainties
  - Leverage the power of multiple constraining measurements
- Use a physically-motivated model to interpret diagnostic data subject to physics-based constraints
  - Allow our intuition and knowledge to play a role in determining the solution (but not fully!)
  - The emphasis of the model is on clarity and transparency of parameters → give us answers that are easy to interpret
- Use a formalism that allows quantitative comparison of different candidate physics models
  - If we introduce a new model of the experiment we must be able to quantify its utility, particularly if it is more complicated
- Use a formalism that enables diagnostic designs to be tested for their utility

MagLIF uses preheat, magnetic insulation and adiabatic compression to achieve high pressure



- D_2 gas ~ mg/cc
- 10-30 T, 3 ms risetime

- Multi-kJ, TW ZBL laser
- Heats gas to ~100's eV



Recently achieved >10^{13} DD neutrons
E_{ph} > 1 kJ, P_{HS} > 1 Gbar
T_{burn} ~3 keV

Laser heating allows high pressures to be achieved with low implosion velocity (<100 km/s)

- Preheat energy is contained during implosion via magnetic insulation
- Flux compression allows confinement of fusion products with low fuel ρR
- Long dwell time between preheat and stagnation makes us sensitive to early time mix

Slutz et al., Phys. Plasmas 17, 056303 (2010)

We have developed a forward model that allows direct, quantitative comparison of the data with synthetic diagnostics

X-ray Emission:

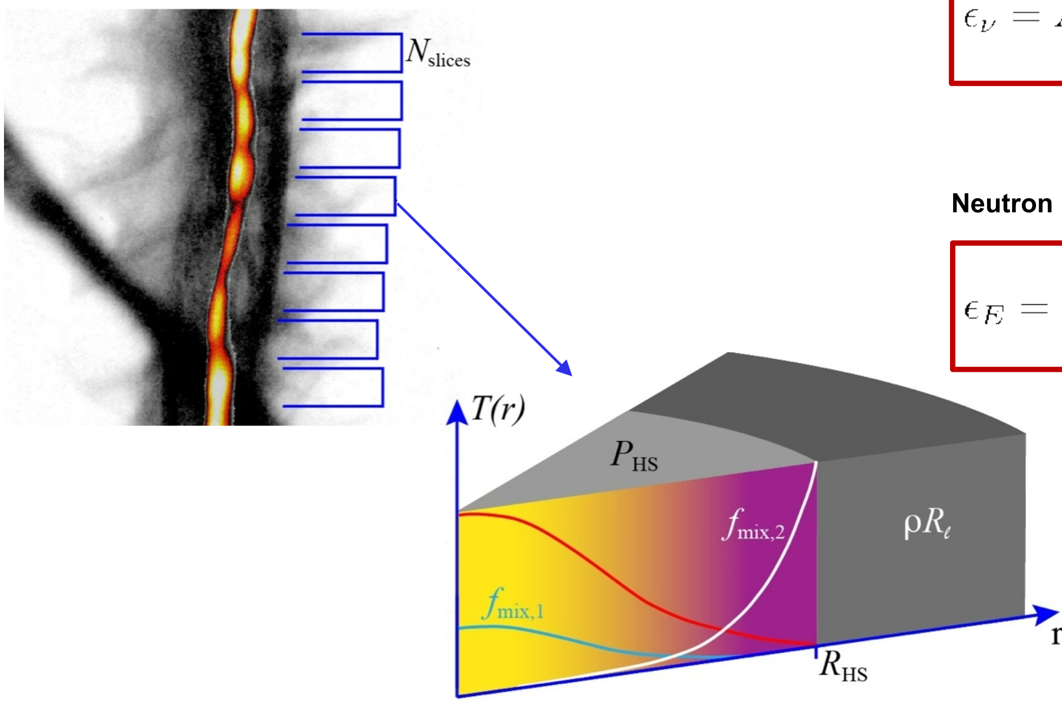
$$\epsilon_\nu = A_{f-f} e^{-\rho R_\ell \kappa_\nu} \tau_{\mathrm{b}} P_{\mathrm{HS}}^2 \frac{g_{\mathrm{FF}} \langle Z \rangle}{(1+\langle Z \rangle)^2} \sum_i f_i \tilde{j}_i \frac{e^{-h\nu/T}}{T^{5/2}}$$

$$\tilde{j}_i \equiv \frac{j_i}{j_{\mathrm{D}}} = Z_i^2 + \frac{A_{f-b}}{A_{f-f}} \frac{Z_i^4}{T} e^{Ry Z_i^2/T}$$

Neutron Emission:

$$\epsilon_E = \frac{P_{\mathrm{HS}}^2 \tau_{\mathrm{b}}}{1+\delta_{1,2}} \frac{f_1 f_2 \langle \sigma v \rangle}{(1+\langle Z \rangle)^2 T_{\mathrm{i}}^2} I_o(E)$$

$$^{*}I_o(E) = e^{\frac{-2\bar{E}}{\sigma^2}(\sqrt{E}-\sqrt{\bar{E}})^2}$$



Basic Model Parameters

$\{T_{\mathrm{i}}\} = \{T_{\mathrm{e}}\}$

$\{\rho R_\ell\}$

$\{P_{HS}\}$

$\{f_{\mathrm{mix}}\}$

$\{R_{\mathrm{HS}}\}$

Global/hyper Parameters

Z_{mix}

τ_{burn}

h_{HS}

T_{exp}

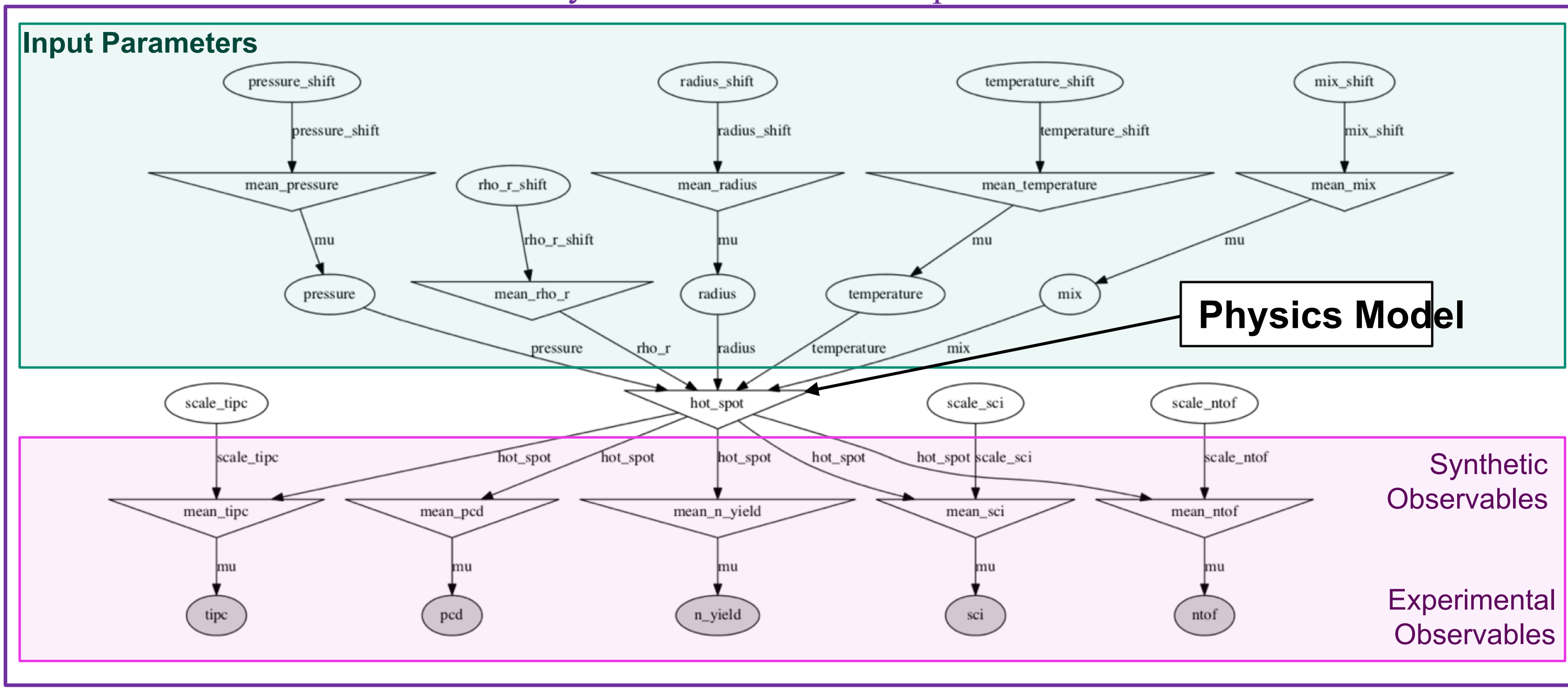
Assumptions:

- Each slice has its own independent parameters characterizing a static, isobaric hot spot surrounded by a liner $P_{\mathrm{HS}} = (1+\langle Z \rangle) n_{\mathrm{i}} k_B T$
- Ideal gas EOS:
- All elements have same burn duration
- Electron and ion temperatures are equal
- X-ray emission is dominated by continuum (BF & FF)

*Ballabio et al., NUCLEAR FUSION, Vol. 38, No. 11 (1998)

Analysis is performed using Bayesian Parameter estimation to determine the most likely hotspot parameters

Bayesian Hierarchical Graph Model



- Bayesian parameter estimation is a well-established technique used in a variety of fields*
- Analysis can be used to infer most likely parameters, correlations between model parameters and/or data
- Can compute value of information to determine which data constrain which parameters and how well

*U. Von Toussaint, Rev. Mod. Phys. Vol. 83 (2011)

Bayesian Parameter estimation is an iterative process that updates our assumptions based on observables

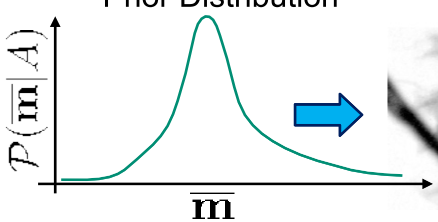
Bayes' Theorem

$$\mathcal{P}(\overline{\mathbf{m}}|\overline{\mathbf{d}}, A) = \frac{\mathcal{P}(\overline{\mathbf{d}}|\overline{\mathbf{m}}, A)\mathcal{P}(\overline{\mathbf{m}}|A)}{\mathcal{P}(\overline{\mathbf{d}}|A)}$$

Likelihood

$$\mathcal{P}(\overline{\mathbf{x}}|\overline{\mathbf{m}}, \mathcal{A}) \propto \prod_{i=1}^{N} \exp\left(-\frac{(\mathcal{F}_i(\overline{\mathbf{m}}) - x_i)^2}{2\sigma_i^2}\right)$$

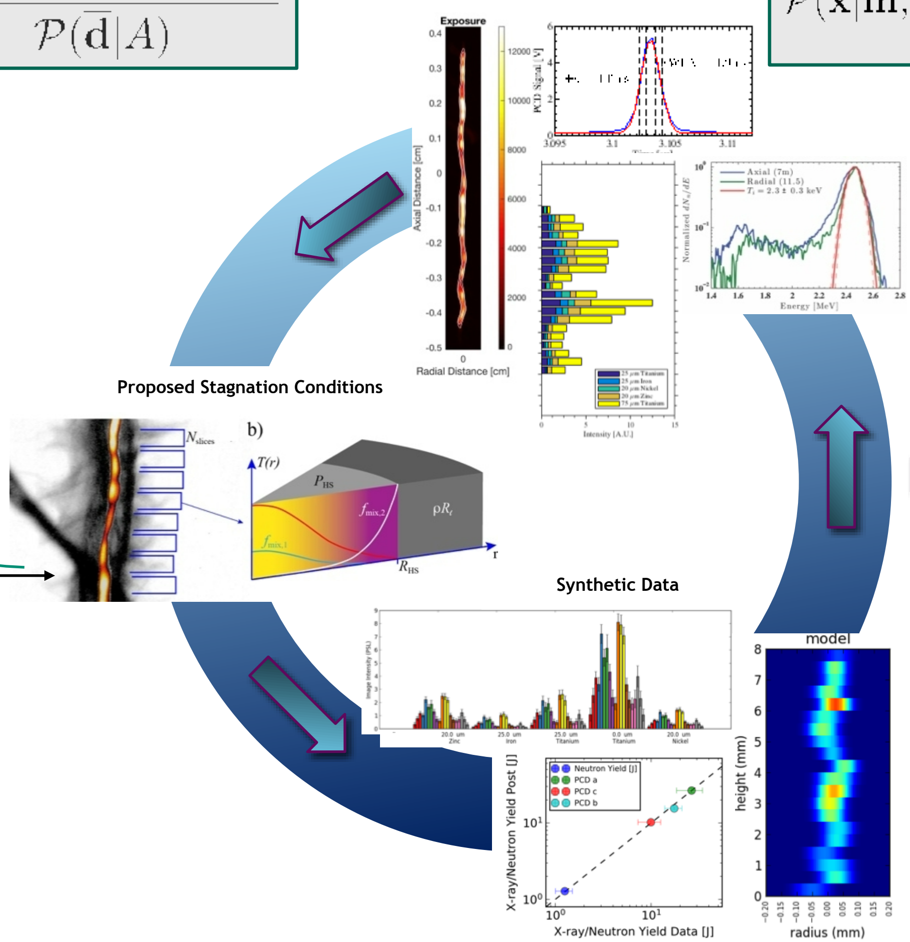
Prior Distribution



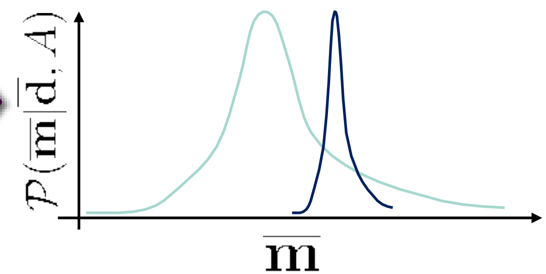
Experimental Data

Proposed Stagnation Conditions

Synthetic Data



Posterior Distribution



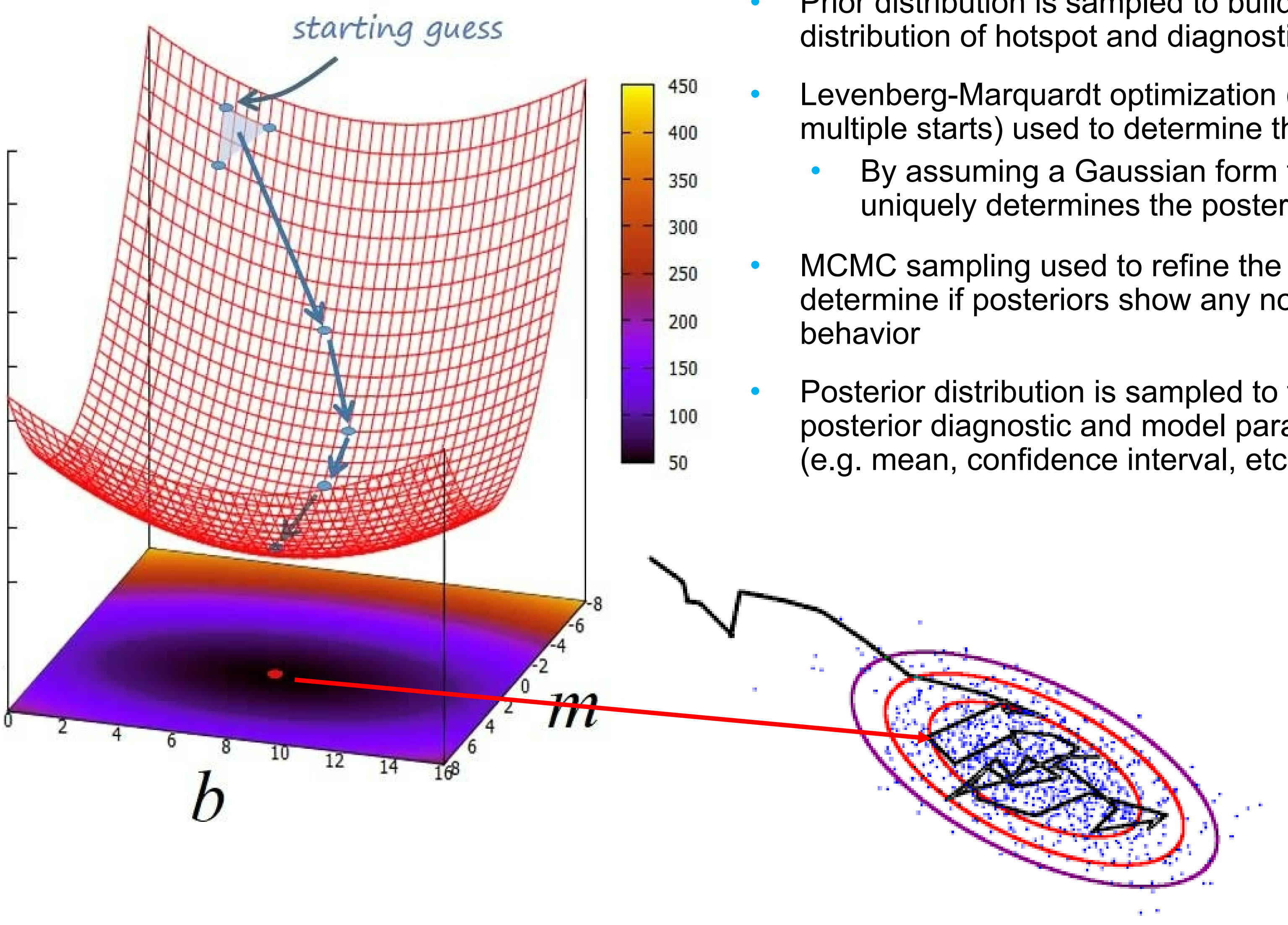
Model Parameters

$$\overline{\mathbf{m}} = \begin{cases} P_{\mathrm{HS}} \\ T \\ f_{\mathrm{mix}} \\ R_{\mathrm{HS}} \\ \rho R_\ell \end{cases}$$

Outputs/Benefits:

- **most likely parameter values**
- **confidence intervals**
- **correlations**
- **Value of information**

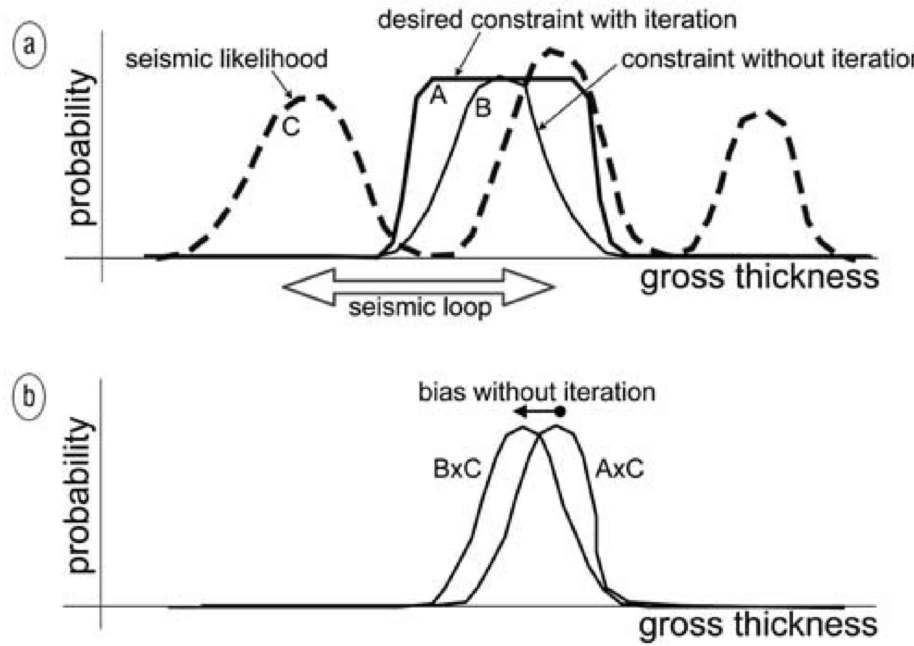
Optimization Procedure



- Prior distribution is sampled to build the prior distribution of hotspot and diagnostic realizations
- Levenberg-Marquardt optimization (with optional multiple starts) used to determine the MAP solution
  - By assuming a Gaussian form this solution uniquely determines the posterior
- MCMC sampling used to refine the solution and determine if posteriors show any non-linear behavior
- Posterior distribution is sampled to form the posterior diagnostic and model parameter statistics (e.g. mean, confidence interval, etc.)

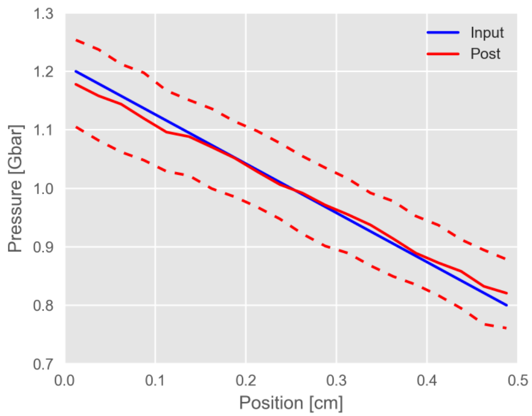
Combating bias introduced via the prior

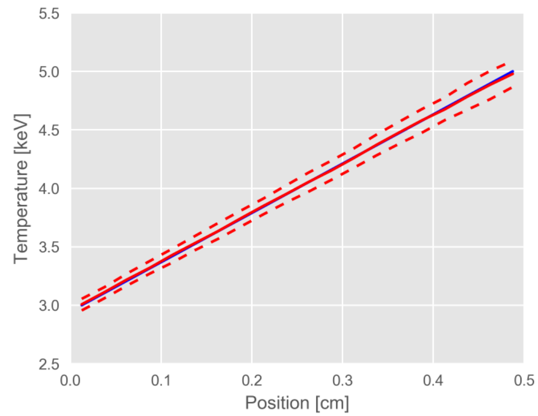
- In the case of a sufficiently peaked prior, and/or sufficiently weak pressure on the solution, the prior can bias the resulting solution
- If the prior is low, the solution will be low, and high if the prior is high
- A simple iteration over the procedure will effectively remove this bias, recovering the solution as if a constrained uniform prior were used
- The iteration loop simply replaces the prior mean with the posterior mean from the previous iteration, leaving the prior standard deviation untouched
- The loop consistently converges in just a few iterations, make this a cheap and effective means of removing bias

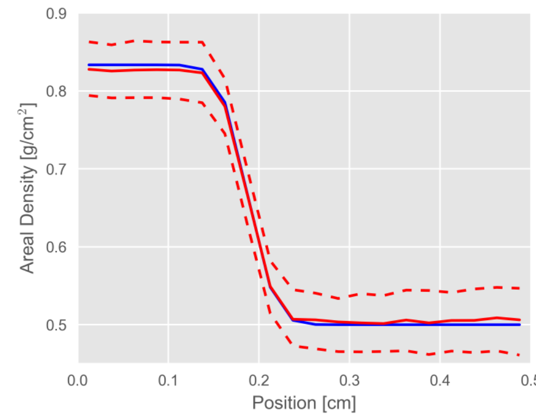


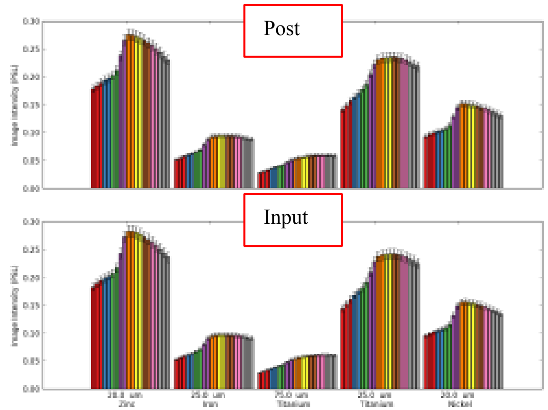
Glinsky et al., **Bayesian inversion whispers,** THE LEADING EDGE MA

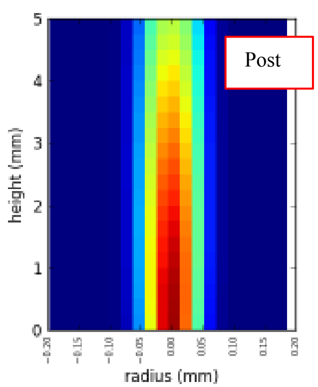
1D model Test case

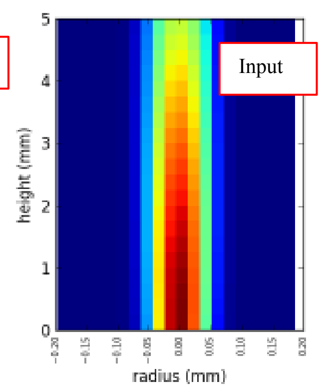


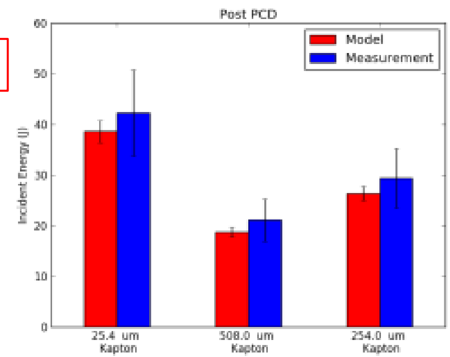








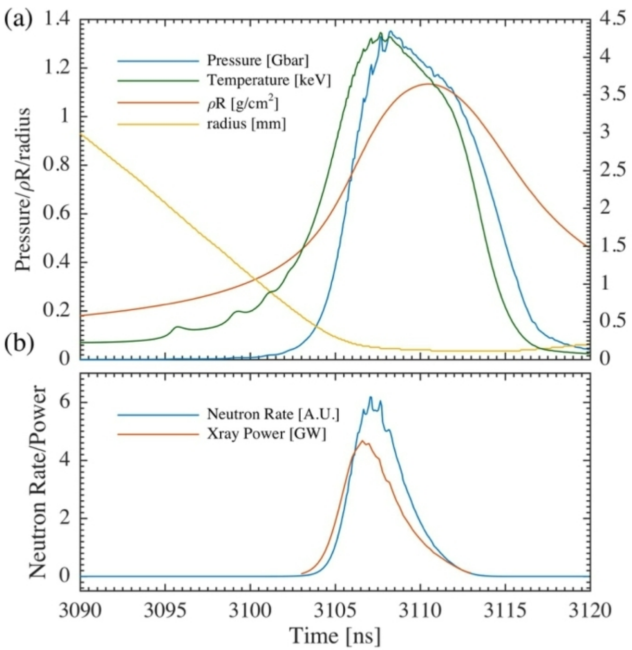


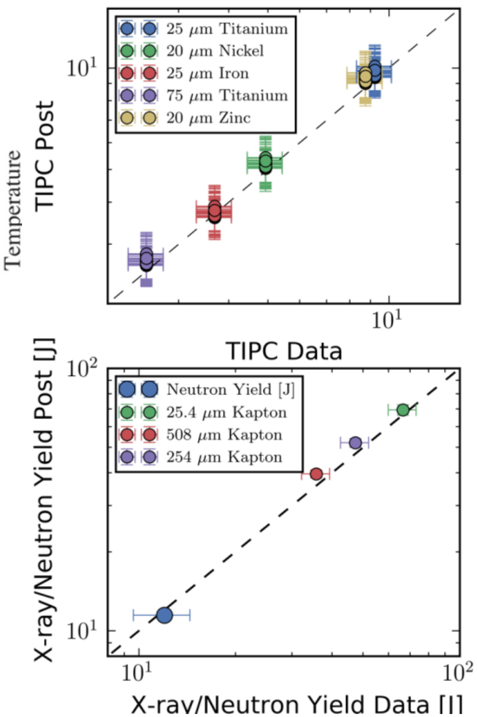


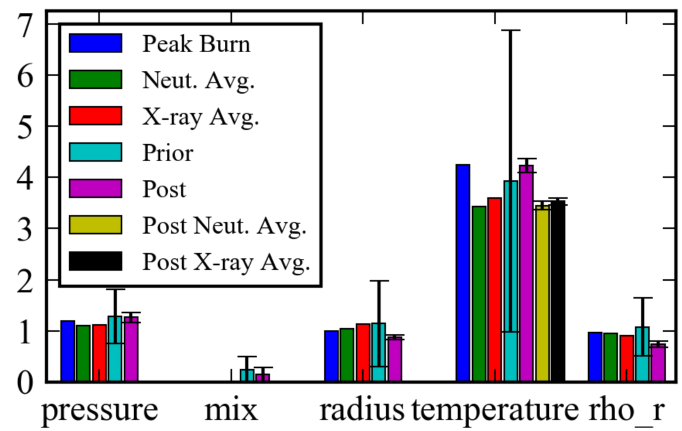
- Constructed a test case that exercises multiple parameters simultabneously
- Prescribed variations in P, T, and radius (all accurately determined)
- Mix and liner areal density are determined, but with large confidence intervals

Method has been successfully tested on 1D GORGON simulation data

What is the meaning of the model parameters in the presence of significant time evolution?

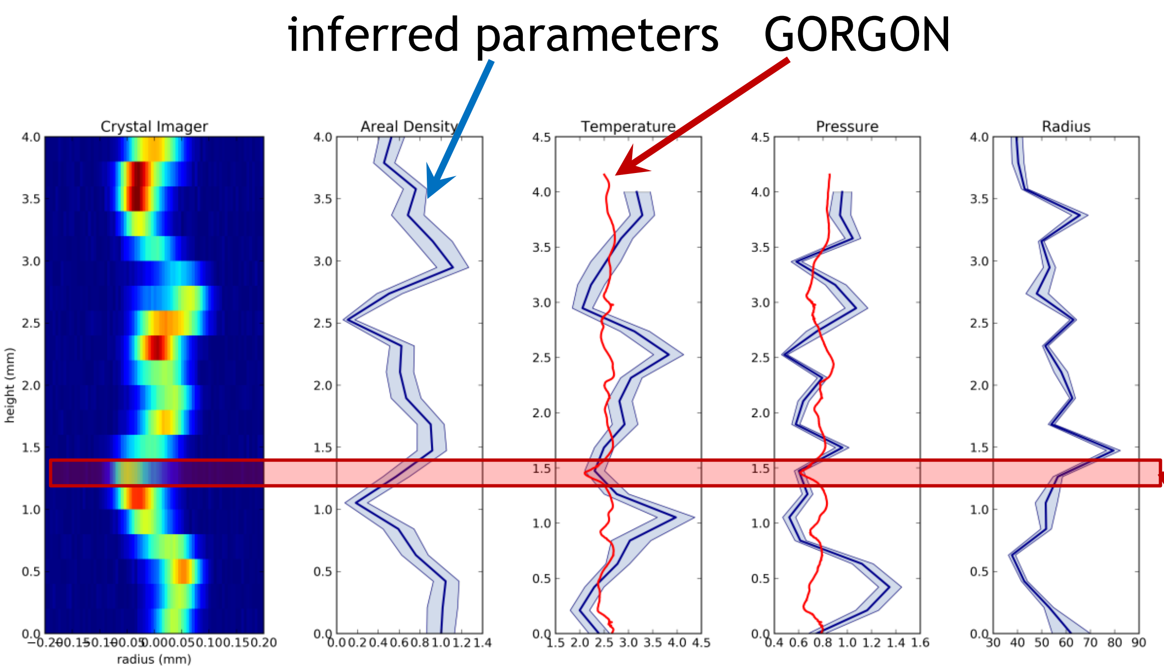


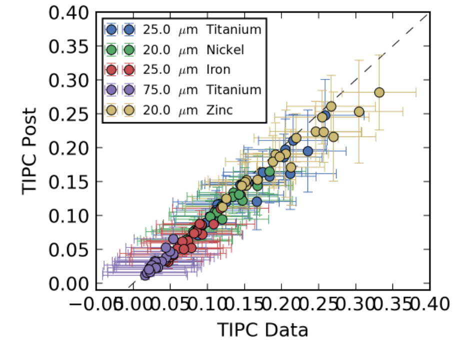


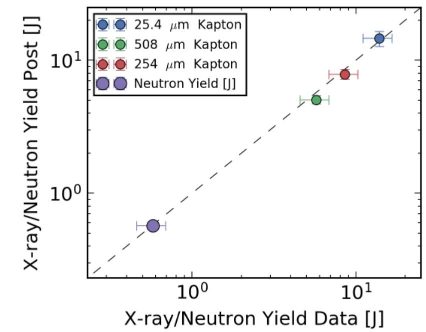


- The inversion is able to recover a high fidelity solution to the 1D GORGON simulation
- Inferred quantities correspond closely to simulated values at peak burn
- Inferred areal density is low, likely due to use of cold opacity in model

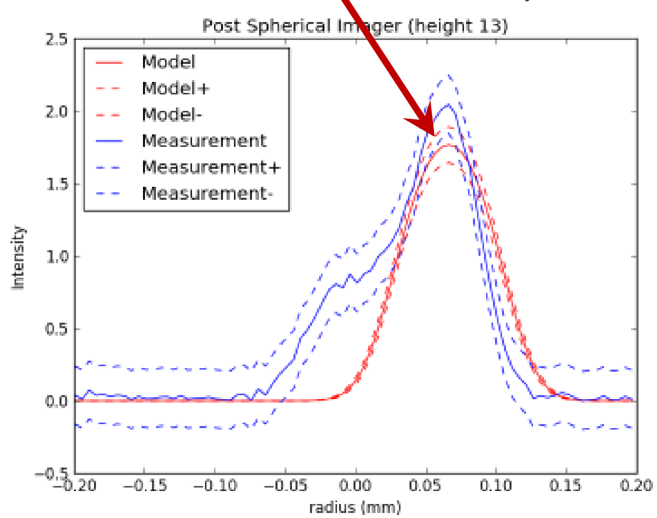
Running inversion on 3D Gorgon data reveals significant bias in the solution







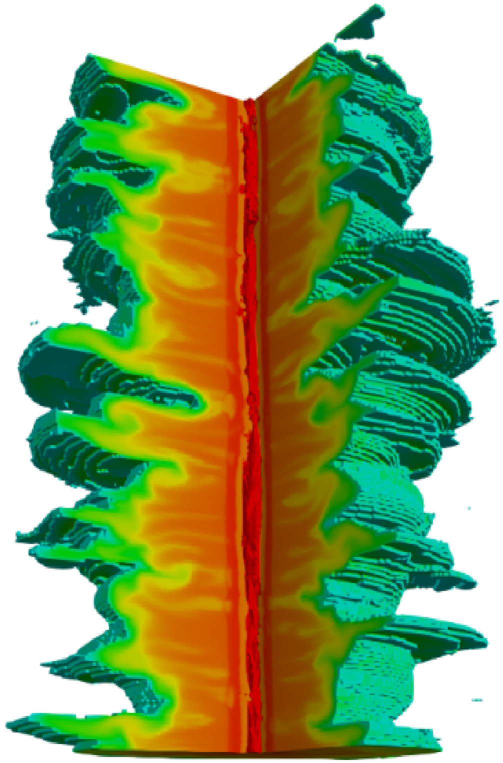
- Integrated diagnostic data is matched within uncertainties
- However, biases and excessive correlations appear in the solution parameters
- Poor fits to the crystal imager profiles ar observed in certain areas



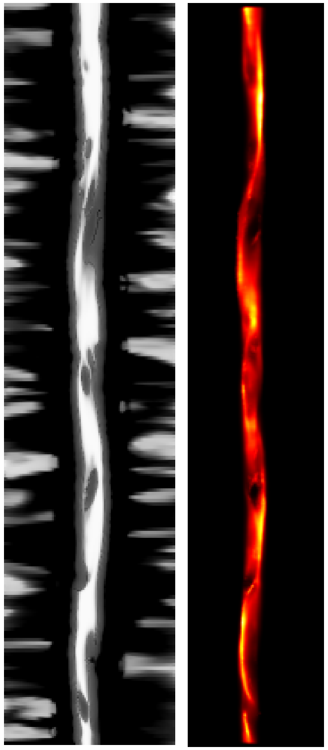
The biases are believed to be related to the three dimensional nature of the stagnation

Visualizations from GORGON Calculation at Peak Burn

Density Slice



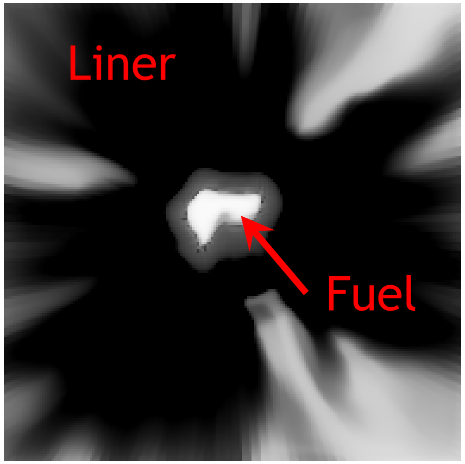
Density Map



Synthetic Image

- Inability to match asymmetric indicates deviation from cylindrical symmetry
- This puts an artificial bias on the volume, which cascades through the correlations in the model and diagnostics to bias all quantities
- The large, anti-correlated swings in areal density and temperature are symptoms of this

Cross Section

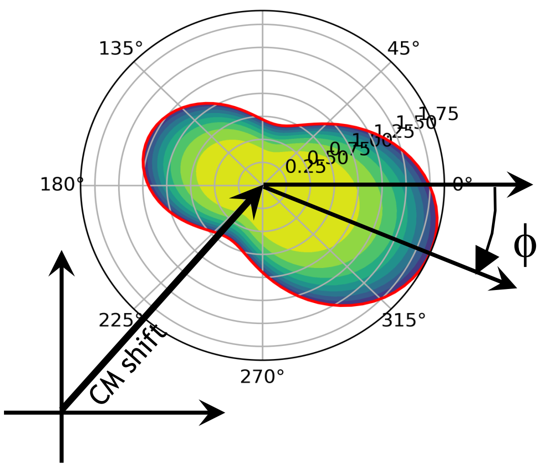


Significant asymmetries are seen in the fuel morphology

We have developed two 3D models with different shape parameterizations to overcome this bias

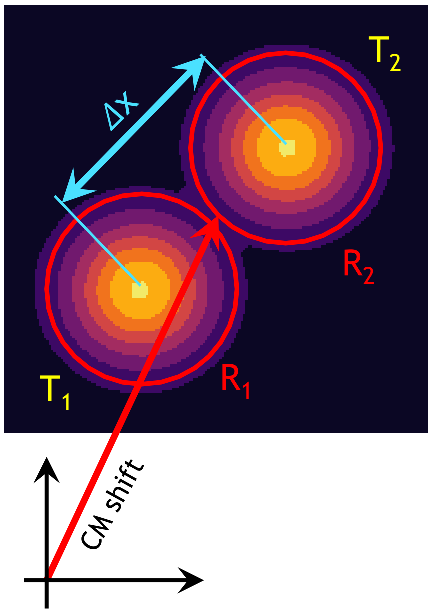
Legendre Expansion

$$R(\theta) = R_o \sum_{\ell=0}^{2} a_\ell P_\ell(cos(\theta - \phi)$$



$a_0 = 1$
a_1
a_2
ϕ
r_{CM}
θ_{CM}

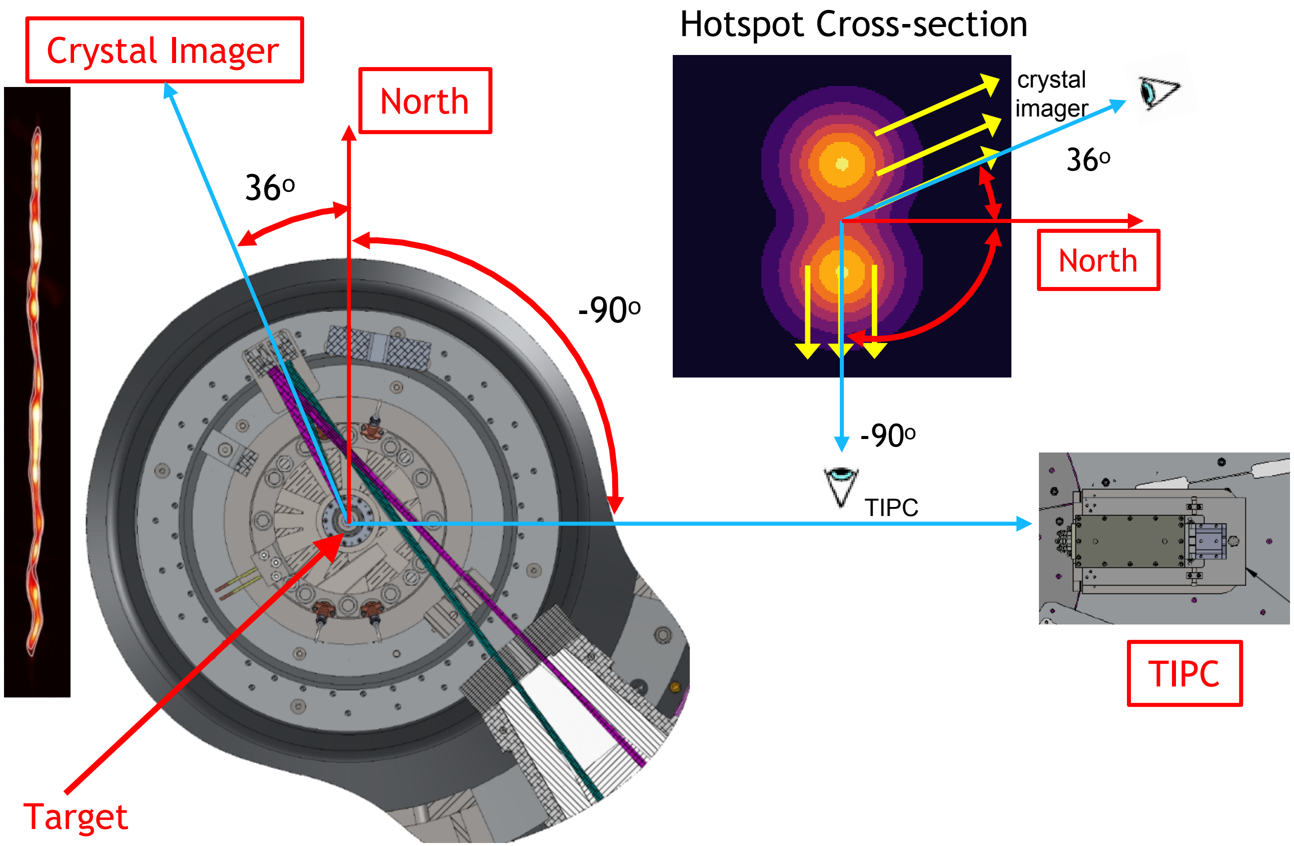
KDE Expansion



- Temperature parameters control the relative peaks of the two modes
- Radius parameters control the relative size of each mode

Temperature profile defined by one of two kernels	
Power-Law Kernel	**Super-Gaussian Kernel**
$K(\mathbf{x}\|\mathbf{X}, R) = 1 - T_{\text{frac}}\left(\frac{\sqrt{(\mathbf{x} \quad \mathbf{X})^2}}{R}\right)^p \quad T_{\text{frac}} = \frac{T_{\text{peak}}}{T_{\text{wall}}}$	$K(\mathbf{x}\|\mathbf{X}, R) = \exp\left(-\left(\frac{1}{2}\frac{(\mathbf{x} \quad \mathbf{X})^2}{\sigma^2}\right)^p\right) \quad \sigma = \frac{2}{3}R$

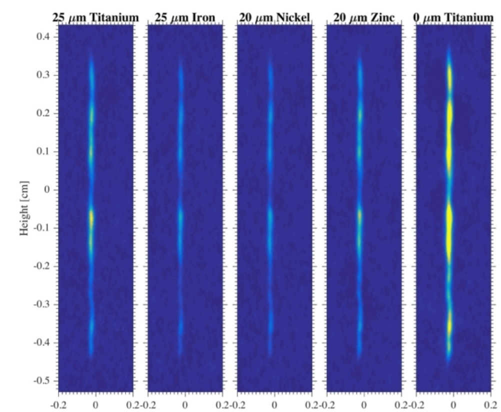
The addition of shape and CM shift parameters requires that we have an additional viewing angle in our diagnostics



Top view of Load Region

Original model treats TIPC as a 1D imager

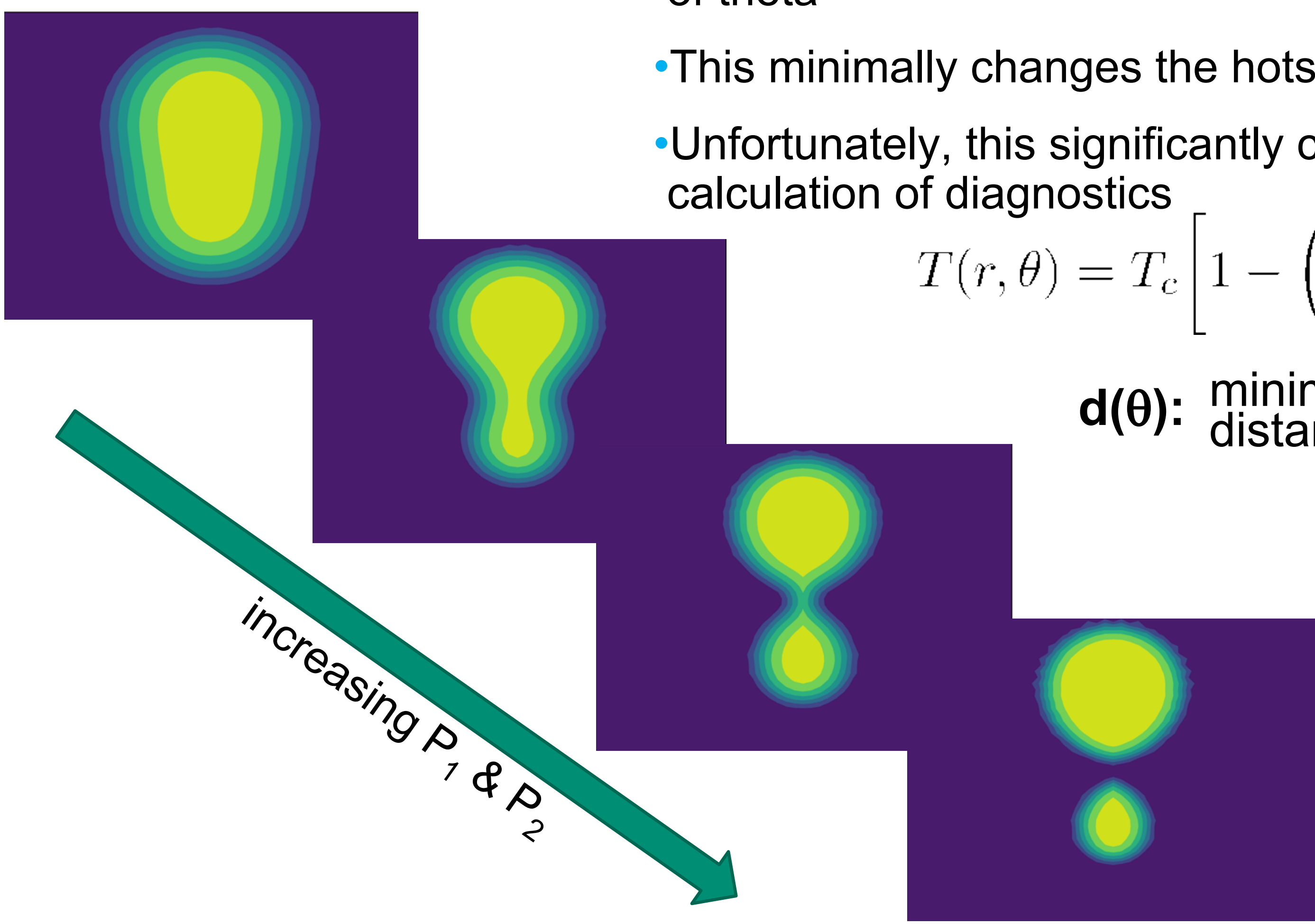
Now, we exploit the full images as well as the viewing angles of the crystal imager and TIPC



But TIPC has much worse resolution than the crystal imager

Legendre Polynomial expansion allows us to add a series of "shape" parameters to each slice

$$R(\theta) = R_o \sum_{\ell=0}^{2} a_\ell P_\ell(cos(\theta - \phi))$$

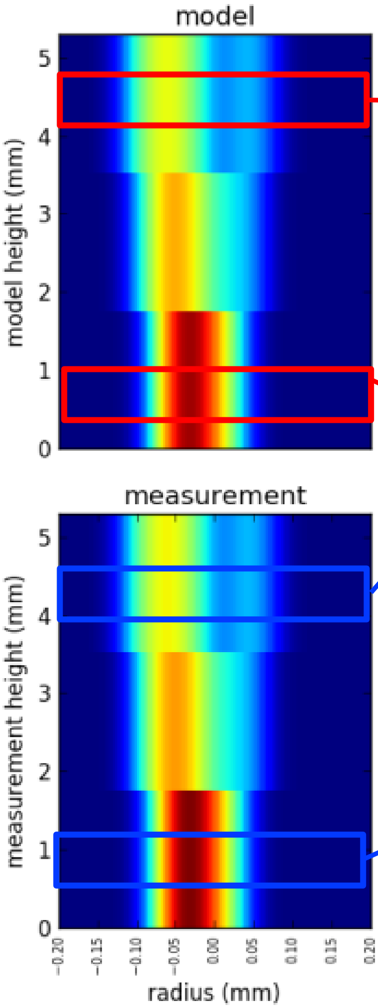


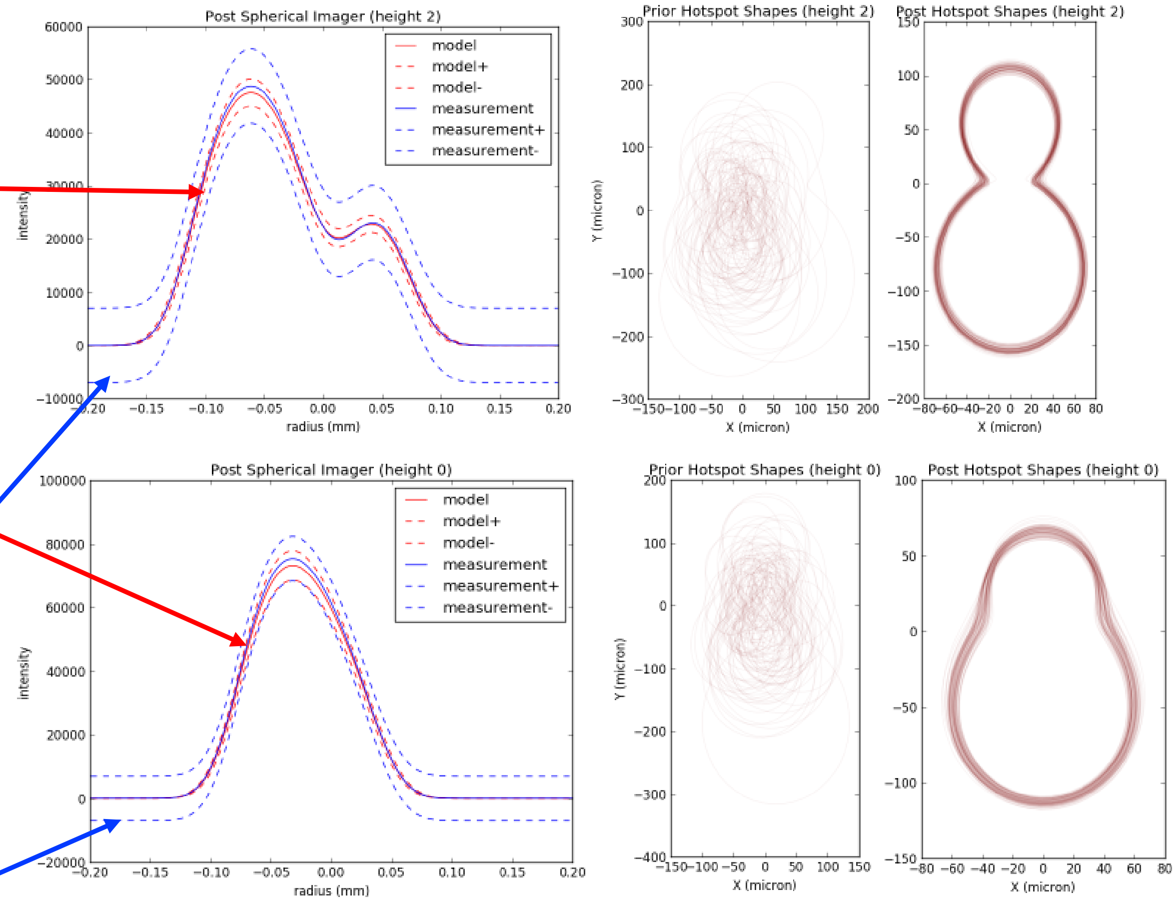
- We maintain the isobaric assumption and the same radial temperature profile, but R varies as a function of theta
- This minimally changes the hotspot model
- Unfortunately, this significantly complicates calculation of diagnostics

$$T(r,\theta) = T_c\left[1 - \left(\frac{T_w}{T_c}\right)\left(\frac{d(\theta)}{R(\theta)}\right)^{\nu}\right]$$

d(θ): minimum perpendicular distance to the boundary

The algorithm is able accurately match the shape parameters using the Legendre expansion

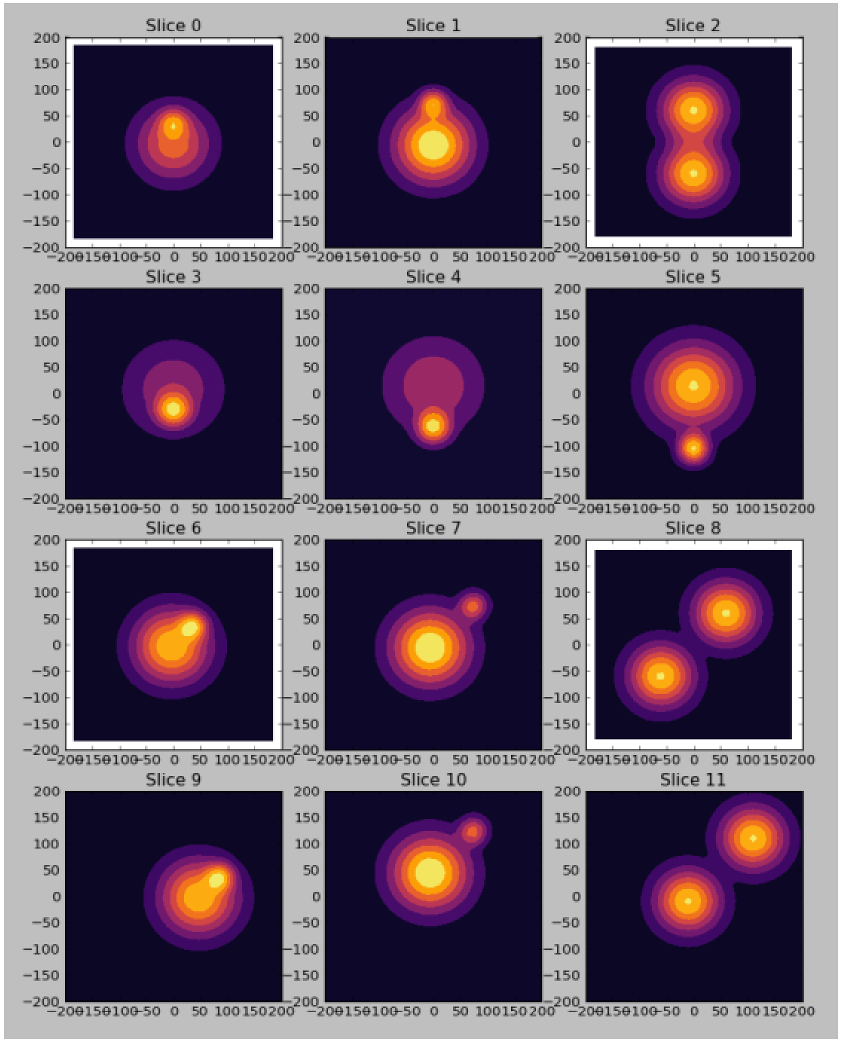




- The shape parameters (P1 and P2) are recovered exactly
- Algorithm is unable to simultaneously recover all parameters
  - Rotation angle is particularly difficult
  - This may be due to the use of an incomplete symmetry group
- Seeking a modified parameterization that will be better suited to inversion

Description of the Gaussian KDE model

Temperature Maps



- New model allows two independent modes to be separated and positioned arbitrarily
- Each mode has a temperature profile specified by either
  - Power law (as in original case)
  - Super-Gaussian (p=1 corresponds to Gaussian, **shown**)
- In addition to original 5 parameters (T_c, P_{HS}, R_{HS}, f_{mix}, ρR_ℓ) there are 6 new parameters
  - temperature ratio (defined as the log of the temperature ratio)
  - radius ratio (defined as the log of the radius ratio)
  - $\mathbf{X}_{CM}$
  - $\boldsymbol{\Delta}\mathbf{X}$
- As with the Legendre expansion, TIPC and Crystal Imager must be simultaneously used as full images, exploiting their near orthogonal views
- Currently NO azimuthal variations in liner areal density allowed
  - Need to take a hard look at this

Parameterizing a hotspot using a sum of circular kernels

Model Parameters

$$\overline{m} = \{P_{\mathrm{HS}}, f_{\mathrm{mix}}, \rho R_{\ell}, \overline{R}, a_i, \overline{T}, b_i, \mathbf{X}_{\mathrm{CM},i}, \delta \mathbf{X}_i\}$$

$$b_i = \log(T_i/T_0) \qquad a_i = 2\log(R_i/R_0)$$

Super-Gaussian Kernel

$$K(\mathrm{x}|\mathbf{X}, R) = \exp\left(- \left(\frac{1}{2}\frac{(\mathrm{x} \quad \mathbf{X})^2}{\sigma^2}\right)^p\right) \quad \sigma = \frac{2}{3}R$$

Power-Law Kernel

$$K(\mathrm{x}|\mathbf{X}, R) = 1 - T_{\mathrm{frac}}\left(\frac{\sqrt{(\mathrm{x} \quad \mathbf{X})^2}}{R}\right)^p \quad T_{\mathrm{frac}} = \frac{T_{\mathrm{peak}}}{T_{\mathrm{wall}}}$$

Defining the Parameters for each Kernel

$$R_i = \overline{R}\sqrt{\frac{2e^{a_i}}{\sum_i e^{a_i}}}$$

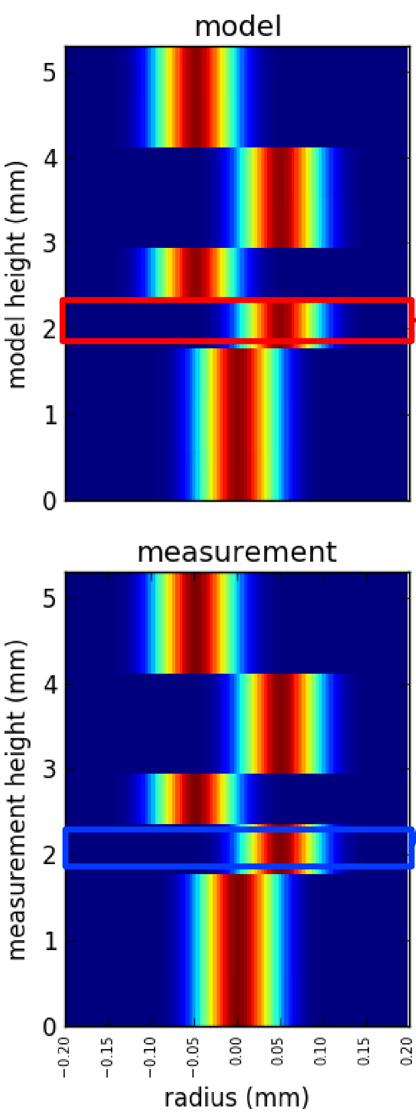
$$T_i = \overline{T}\frac{e^{b_i - a_i}\sum_i e^{a_i}}{2\sum_i e^{b_i}}$$

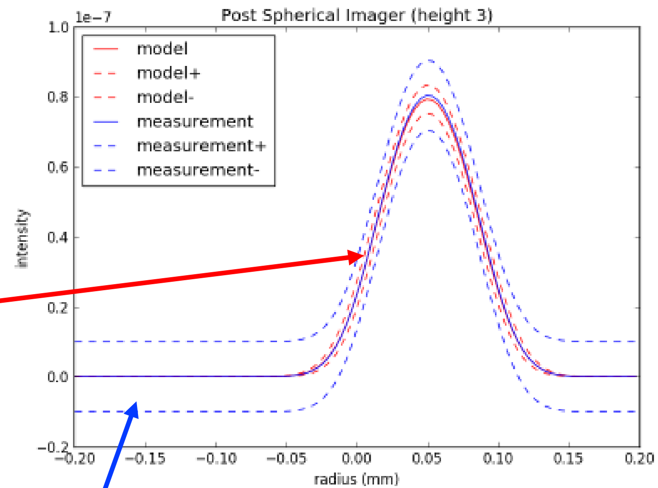
$$\mathbf{X}_{i\neq 0} = \mathbf{X}_0 + \delta\mathbf{X}_i$$

$$\mathbf{X}_0 = \mathbf{X}_{\mathrm{CM}} - \frac{\sum_i \delta\mathbf{X}_i e^{b_i}}{\sum_i e^{b_i}}$$

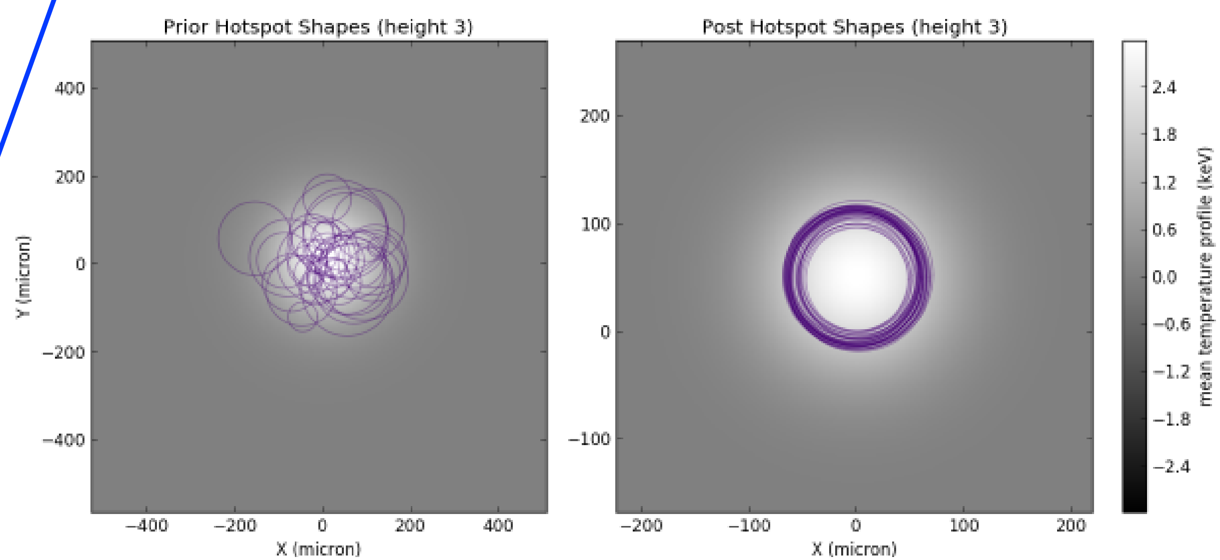
- Allows arbitrary number of kernels
- kernel radius and temperatures are defined as ratios to 0^{th} kernel parameters
- CM of ensemble is calculated as the emission weighted CM (~R^2T)
- for 2 kernels, 6 parameters are required beyond the cyl. symmetric case
- 11 parameters per slice + scale factors and registration ⇒ >225 parameters to be solved for with 2 kernels and N = 20
- 4 parameters are required for each additional kernel

A test case with a single-mode KDE shows that the stagnation conditions as well as the CM shift can be recovered accurately

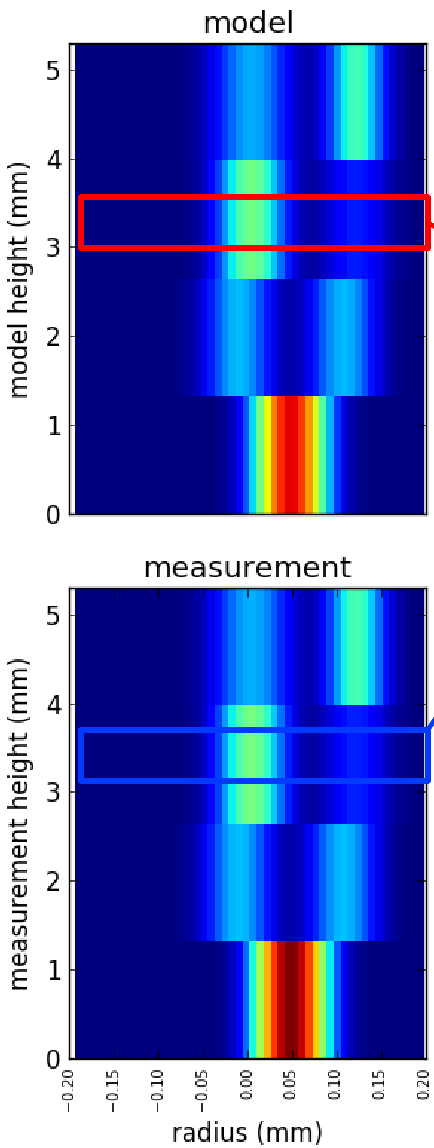


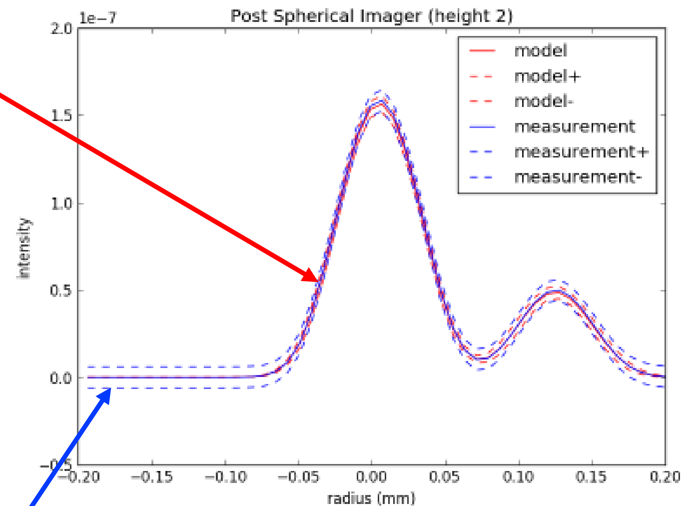


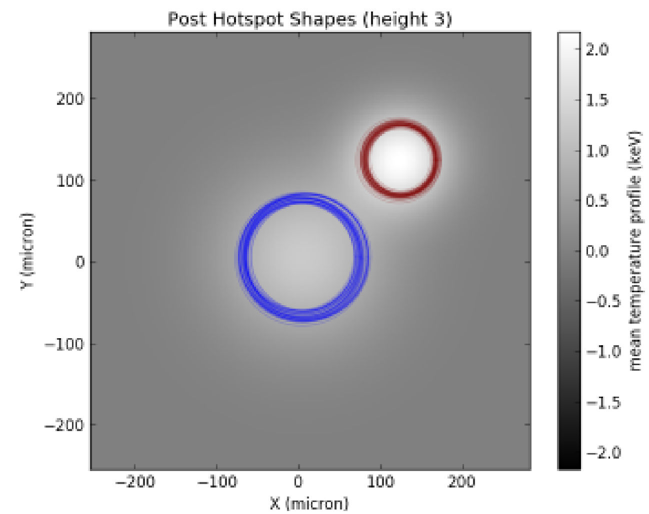
Utilizing two diagnostic views,
The CM shift of the column
proves to be easy to unfold



Preliminary Tests show that the algorithm is able to accurately unfold the shape and orientation of the plasma

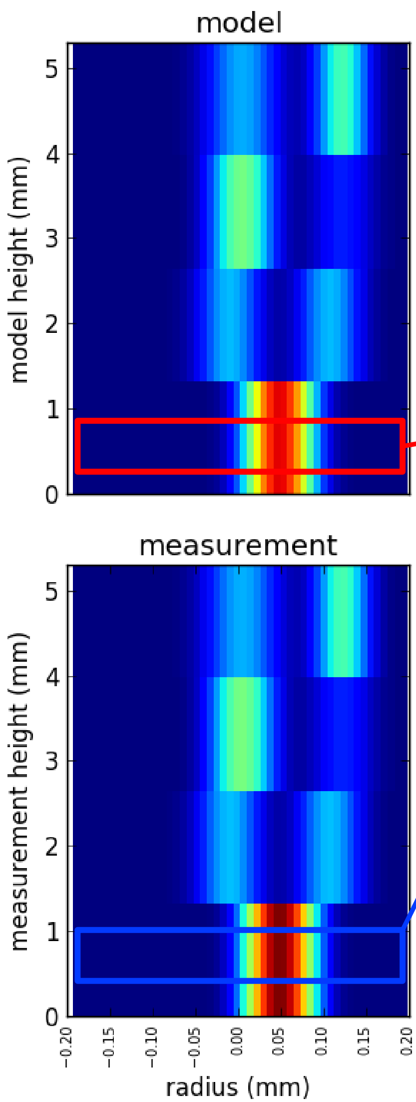


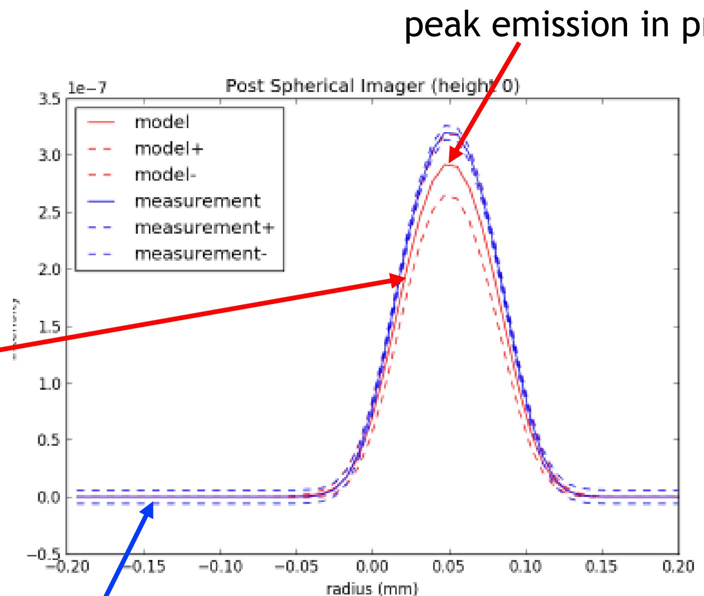


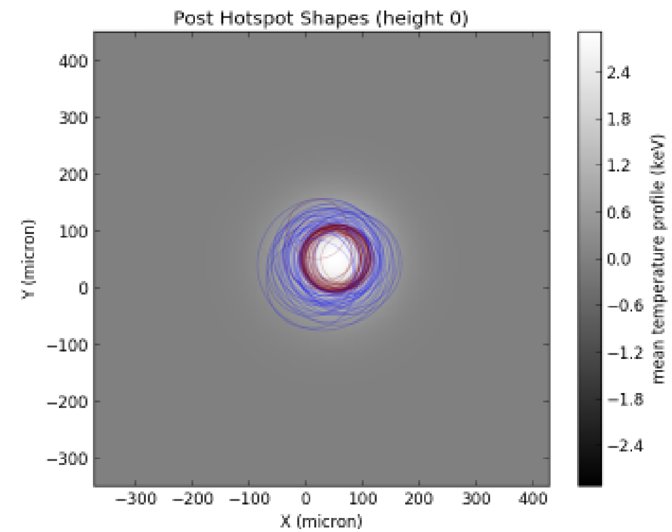


- The inversion recovers all parameter exactly for three of the four slices
- There is confusion with the case where both modes overlap
- This inversion required use of the mean-iteration to overcome bias introduced by the priors in order to obtain an acceptable solution

Preliminary Tests show that the algorithm is able to accurately unfold the shape and orientation of the plasma



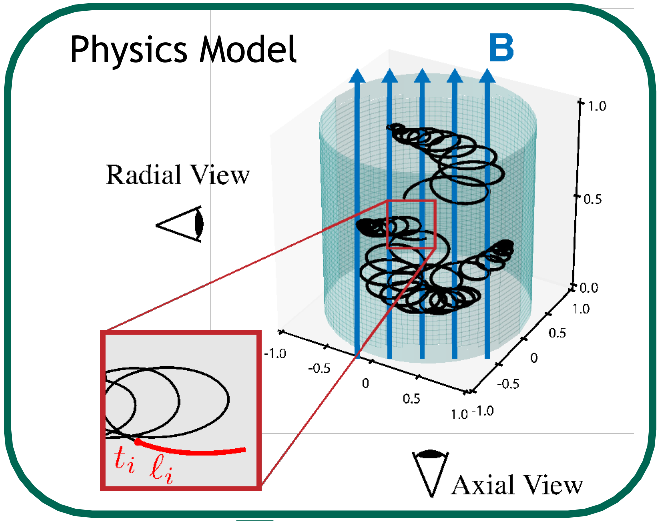


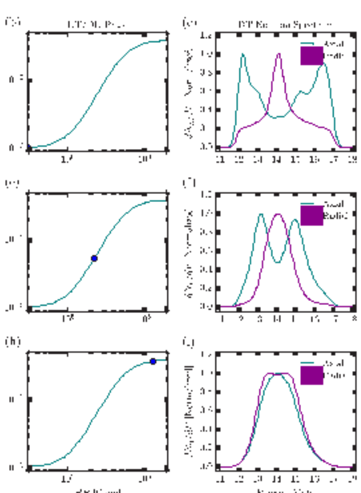


- In the case where two identical modes overlap, there is a lack of determinacy
- Due to the priors, the algorithm wants the solution to have two asymmetric modes
- This throws off the inferred temperature, radius, and peak emission in the images
- However, the pressure, areal density and mix fraction are still accurately recovered

We are developing proxy models to simplify complex calculations and incorporate more physics in the model

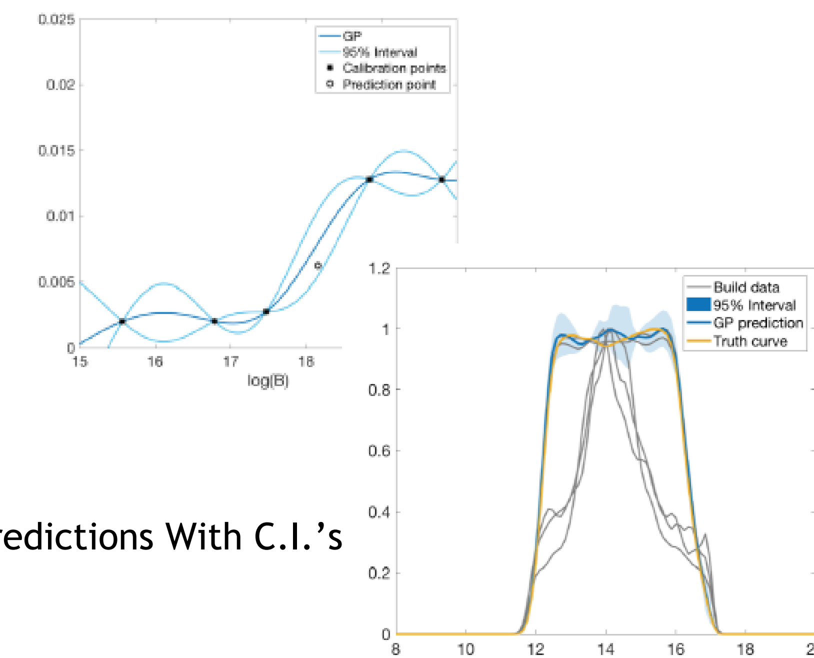
- BR (the magnetic field-radius product) is a critical burn parameter in MIF
- This can be measured via secondary DT neutron measurements, but the model is too expensive to implement inline
- We are training a Gaussian Processes model using DAKOTA to predict the DT yield and spectra based on model parameter values





G.P. Regressor

$$r(x, X) = \exp\left(-\sum_{i=1}^{M}\frac{(x - X_i)^2}{2L_i^2}\right)$$



Predictions With C.I.'s

Conclusions and future work

- The KDE expansion is extremely promising, with very encouraging early results, but is currently limited to Gaussian temperature kernels
- The Legendre expansion needs more work to perform properly, we are investigating alternative expansion methods
- This work highlights the need for a second, quasi-orthogonal high resolution imager
  - We have built in the ability to incorporate a second imager for testing
  - We will evaluate its impact on the synthetic and 3D GORGON test cases
- We are working on adding X-ray spectroscopy diagnostics to the model
  - This will likely require further surrogate modeling
- Once mature, this tool will be used to
  - Develop a deeper understanding of MagLIF through mining a large database of shots and looking for correlations and dependencies in the database
  - Guide diagnostic development
  - Guide experimental design