A Step Closer to a Validation Exercise

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Define "Validation Metric" by What You Want to Do with It

- See [O&B 2006] for CFD perspective.
- Quantitative approach to code calibration,
- Determine where model & experiment agree well & where they don't,
  - Know where to focus future effort.
- Test hypotheses,
  - E.g., does one model match experiment better than another?
- Quantitatively characterize uncertainty in model – experiment comparison,
  - Is resulting confidence interval acceptable?
  - Estimate uncertainty in predictive simulations.

Factors Desired in Validation Metrics

- Experimental measurement uncertainties,
  - Including those introduced in post-processing.
- Uncertainties in code inputs,
- Code errors.
  - E.g., inadequate spatial resolution.
- Number of experiments,
- “Primacy” of variables used for comparison.

Example Validation Metrics: [O&B 2006], [O&T 2002]

- Simulation result: $y(x)$; experimental data: $Y_n(x)$, mean $\bar{Y}(x)$, $\Rightarrow$ *estimated* error in simulation $\tilde{E}(x) = y(x) - \bar{Y}(x)$.

- Standard deviation of $Y_n(x)$ over N experiments: $s(x)$,

- 90% confidence interval for mean $\bar{Y}(x)$: $t_{0.05,N-1} s/\sqrt{N}$.

- O&B metric says: with 90% confidence, *true* error in simulation is in interval

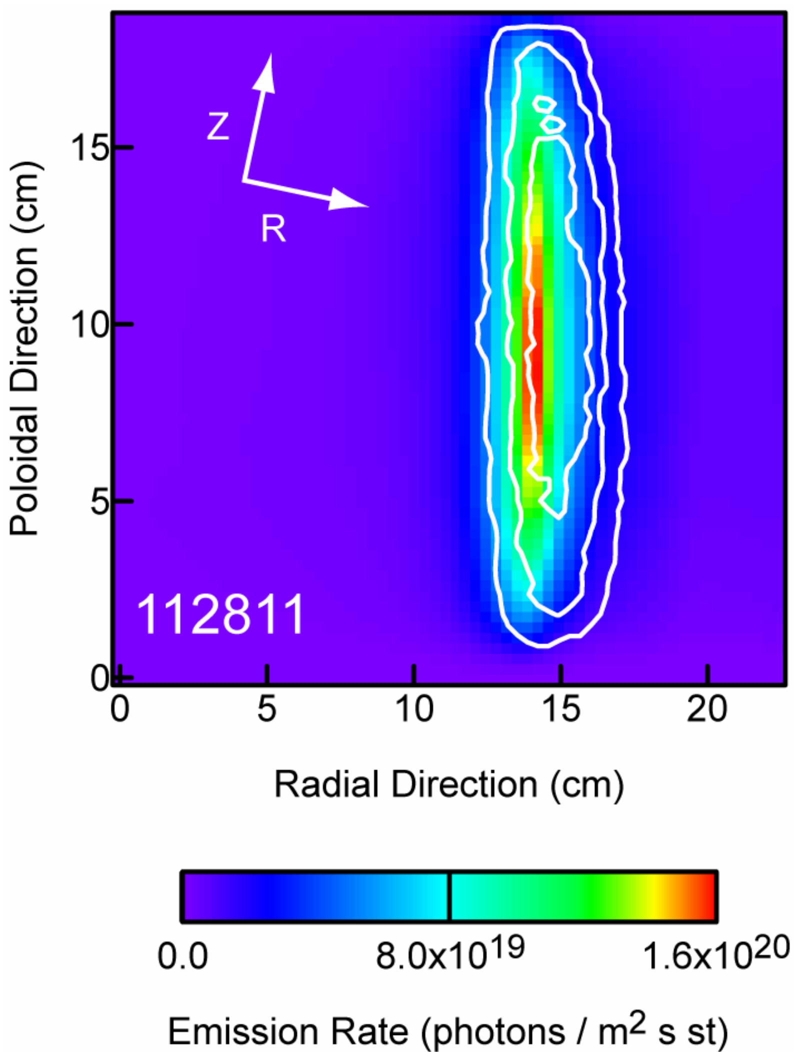
$$\left(\tilde{E}(x) - t_{0.05,N-1}\frac{s(x)}{\sqrt{N}}, \tilde{E}(x) + t_{0.05,N-1}\frac{s(x)}{\sqrt{N}}\right)$$

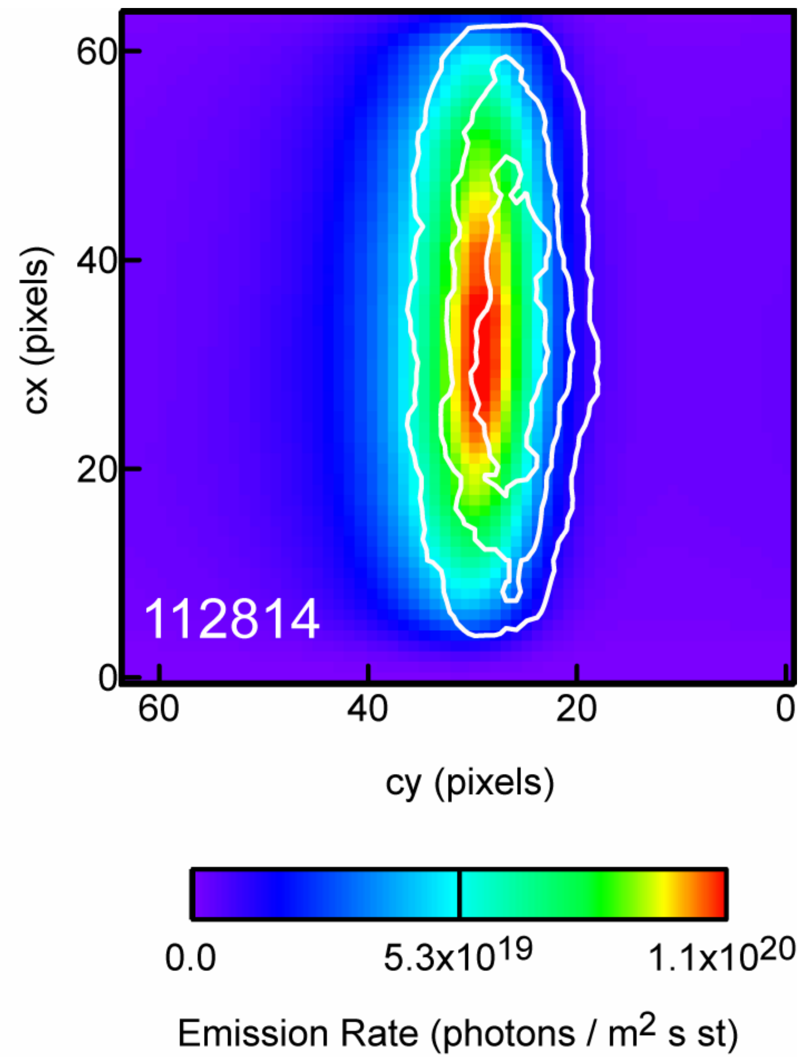
- O&T use similar analysis to get single scalar metric, $0 < V < 1$:

$$V = 1 - \frac{1}{L}\int_0^L \tanh\left[\left|\frac{y(x) - \bar{Y}(x)}{\bar{Y}(x)}\right| + \int_{-\infty}^{\infty} \frac{s(x)}{\sqrt{N}}\left|\frac{z}{\bar{Y}}\right| f(z)\, dz\right] dx.$$

  - $f(z)$ = PDF of student's t-distribution for $N-1$ degrees of freedom.

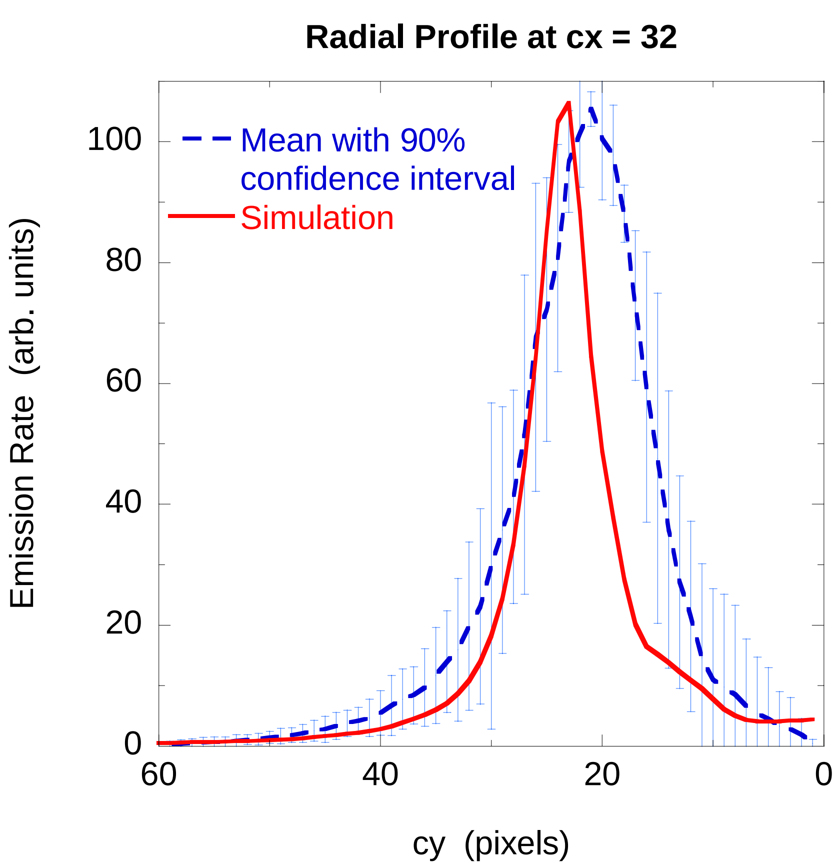
DEGAS 2 Simulations of NSTX Gas Puff Imaging Experiments Yield "Good Agreement"

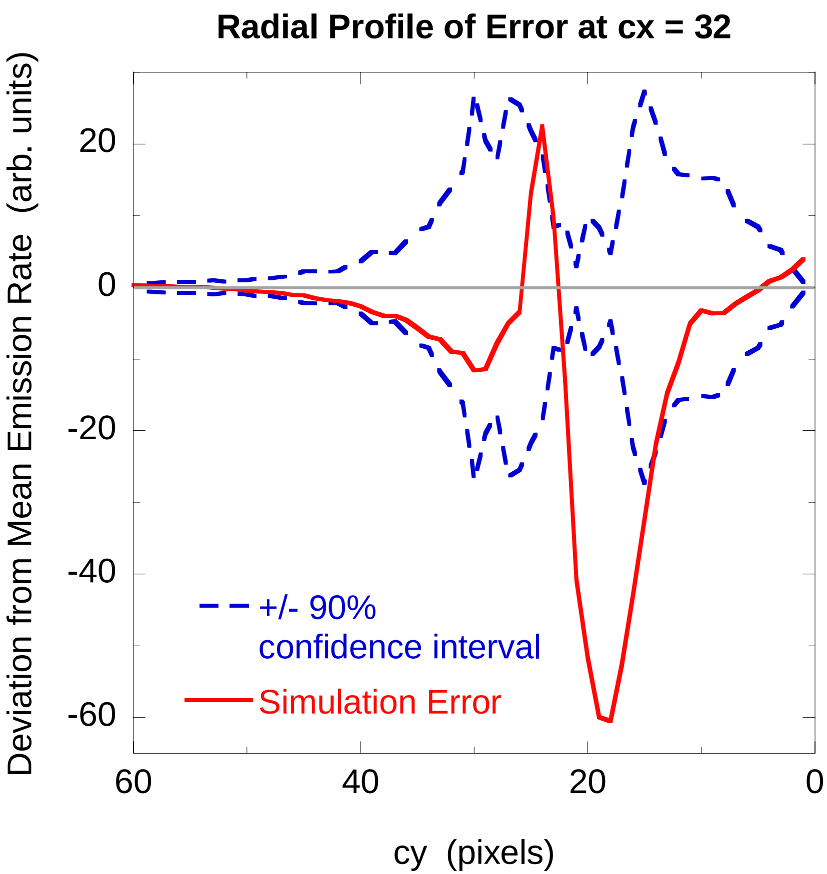




[Stotler 2007]

Evaluate O&B, O&T Metrics with GPI Data from 3 Shots - *DEMONSTRATION ONLY*!





- Global O&B “average relative error” = 62% ± 84%
- O&T metric V = 0.34

Are Other Metrics More Well Suited to Our Needs?

- [McFarland 2005] uses Bayesian Belief Networks:
  - Incorporates uncertainties in measurements & model inputs,
  - Their example utilizes a “too simple” model.
  - Hypothesis testing: does model agree with data?
  - Does not require multiple experiments.
  - Does require complex math $\Rightarrow$ enlist help of math colleagues in developing VM’s.

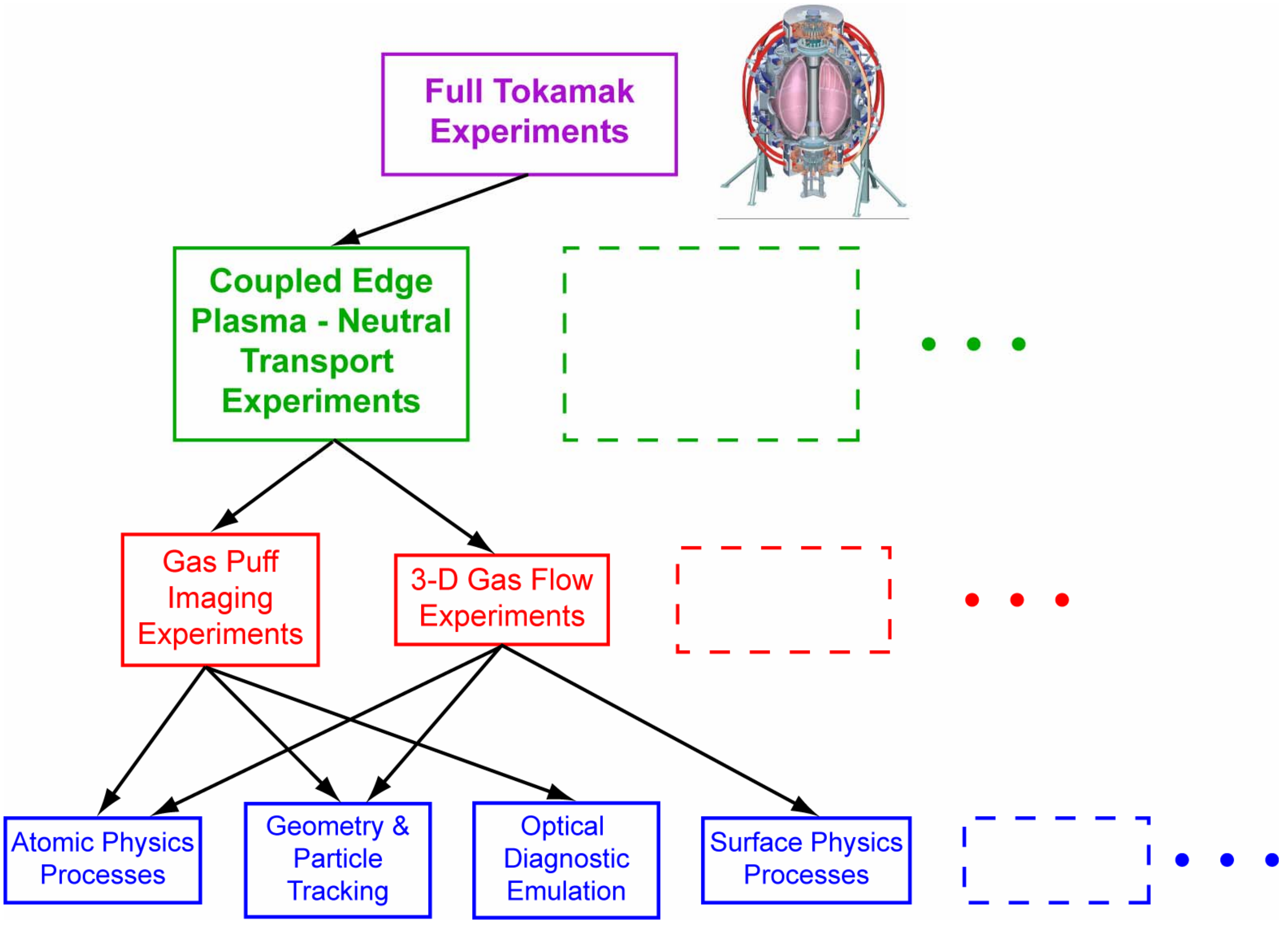
[Chen 2004] also Focuses on Uncertainty Propagation

- “Response Surface Methodologies”: metamodel used to determine impact of input uncertainty on uncertainty in results,
- Considers non-normal distributions,
  - Shows how to transform to variables with near-normal distributions $\Rightarrow$ standard methods apply.
- Techniques can be used with any VM.
- Again, mathematically involved.

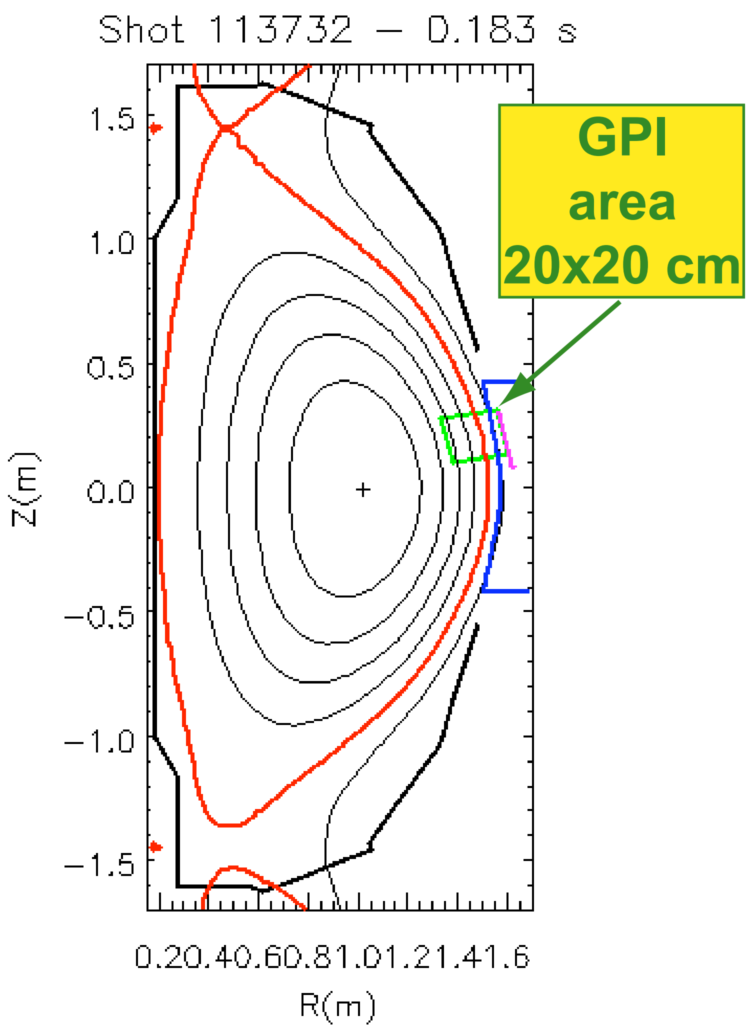
References

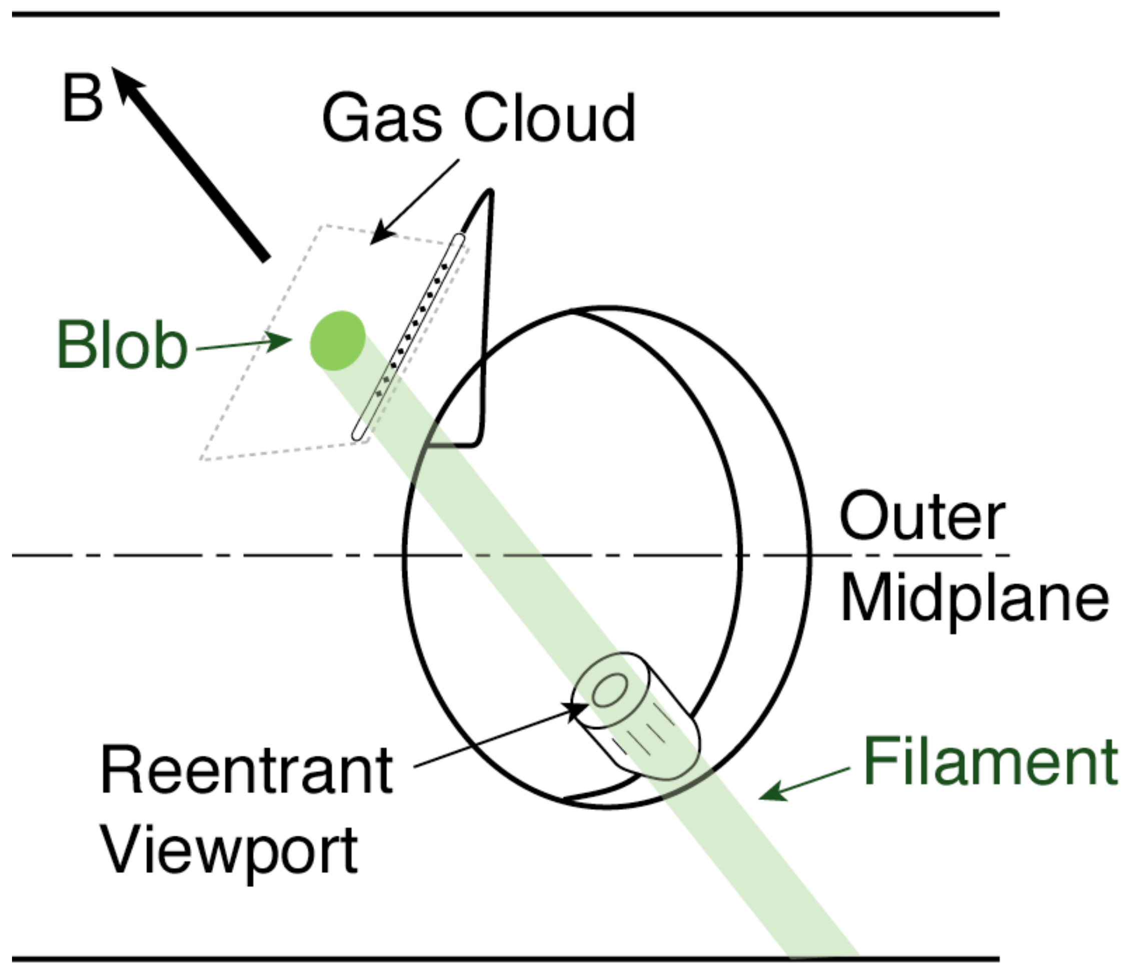
- [O&B 2006] W. L. Oberkampf and M. F. Barone, J. Comp. Phys. 217, 5 (2006).
- [O&T 2007] W. L. Oberkampf and T. G. Trucano, Prog. Aero. Sci. 38, 209 (2002).
- [McFarland 2005] J. M. McFarland and L. P. Swiler, Sandia National Laboratories Report SAND2005-5980 (Nov. 2005).
- [Chen 2004] W. Chen et al., AIAA Journal 42, 1406 (2004).
- [Stotler 2007] D. P. Stotler et al., J. Nucl. Mater. (in press) (2007).

Validation Experiments Lower on Hierarchy Have Greater Likelihood of Success

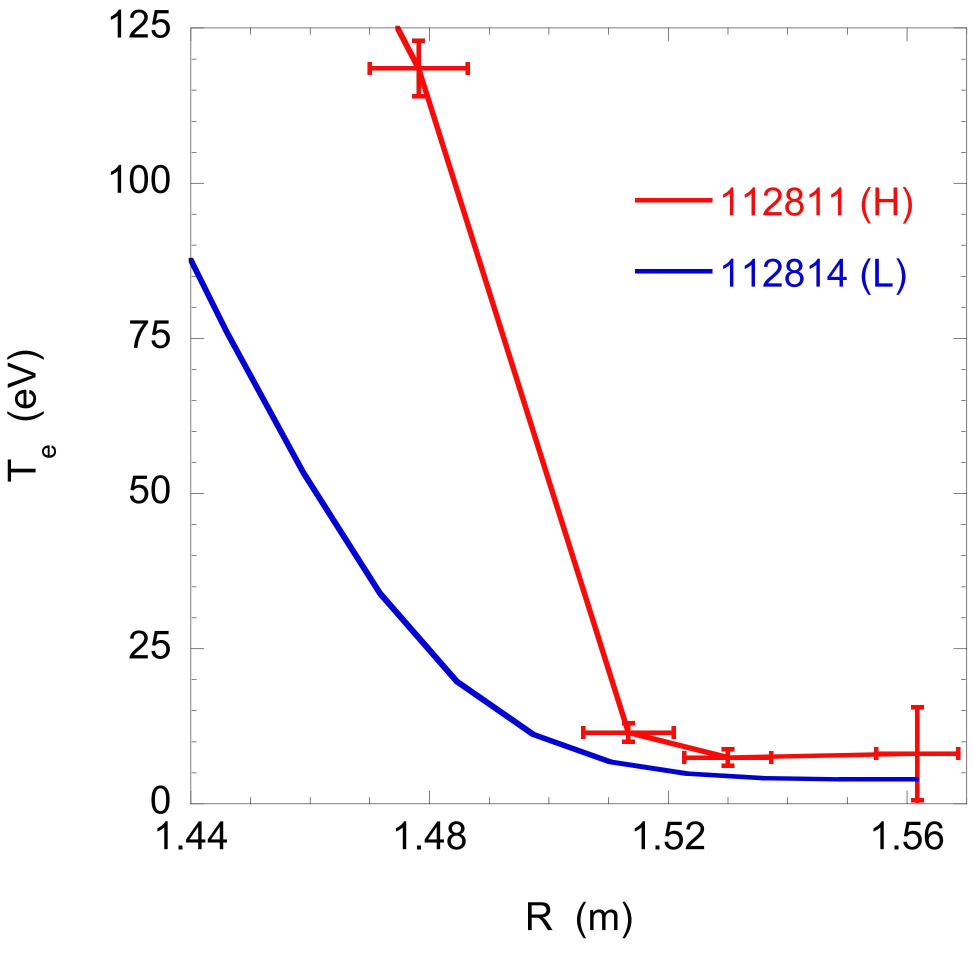


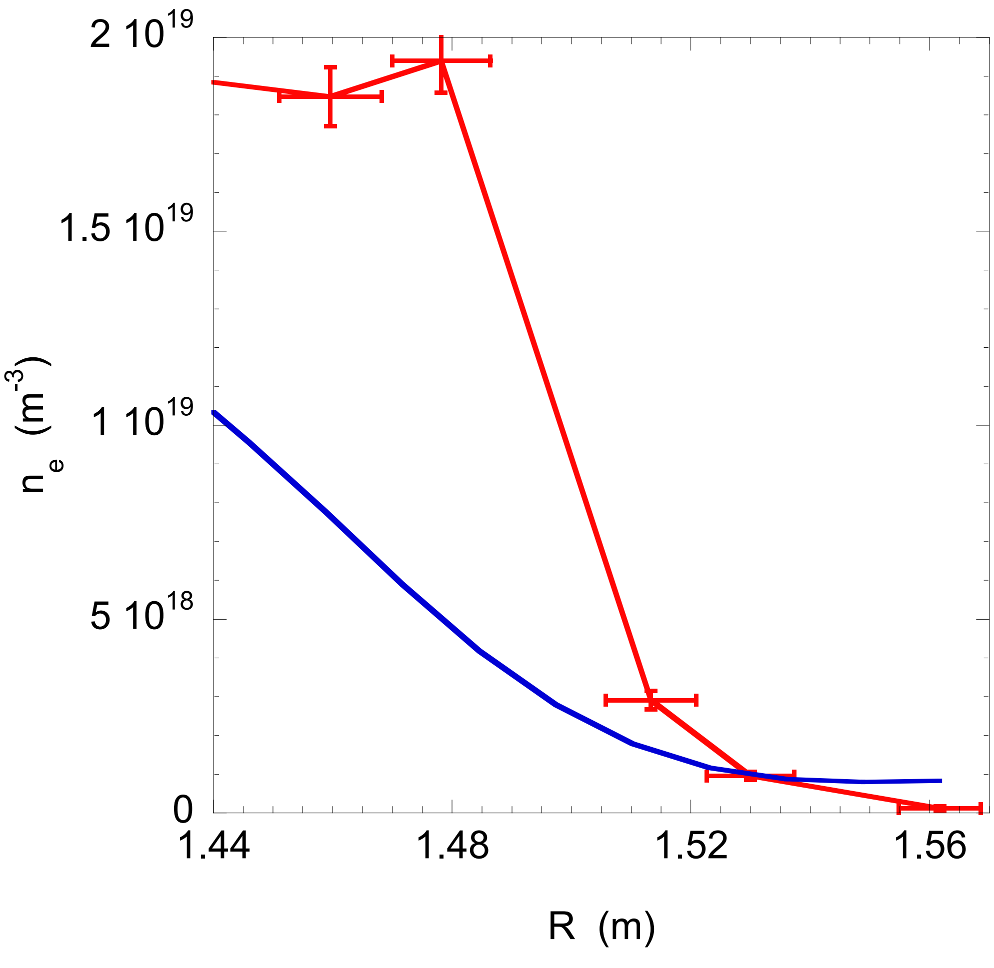
Gas Puff Imaging Hardware Configuration in NSTX





Edge Thomson Scattering Midplane Profiles for H- & L-Mode Shots

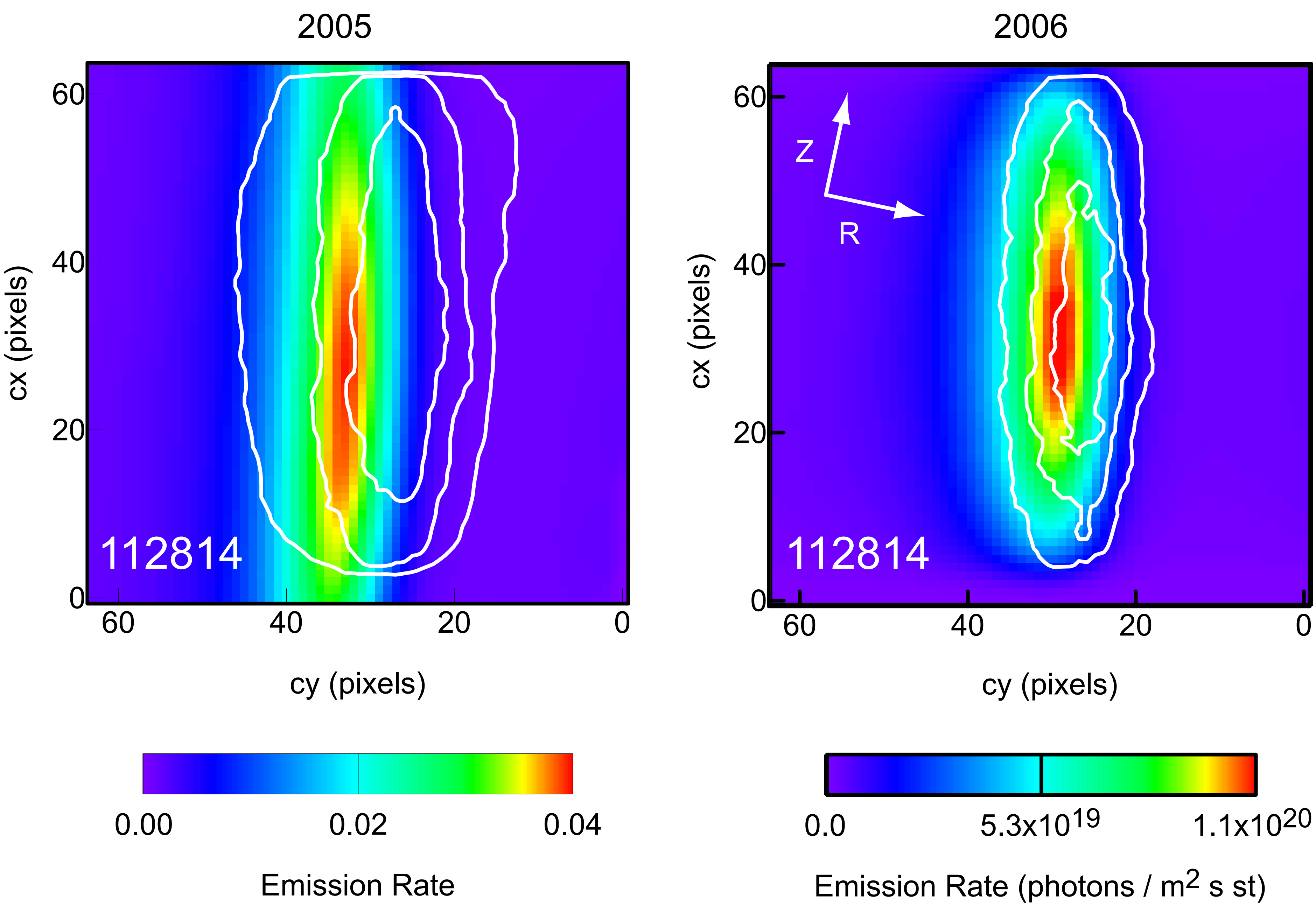




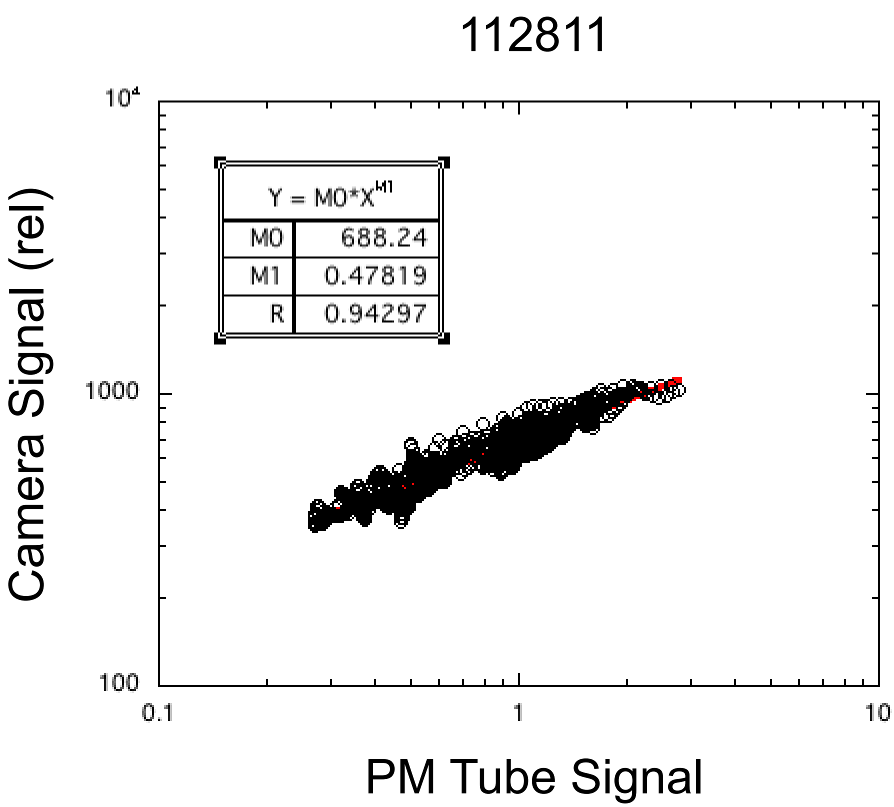
Three-Dimensional DEGAS 2 Simulations of NSTX GPI Experiments

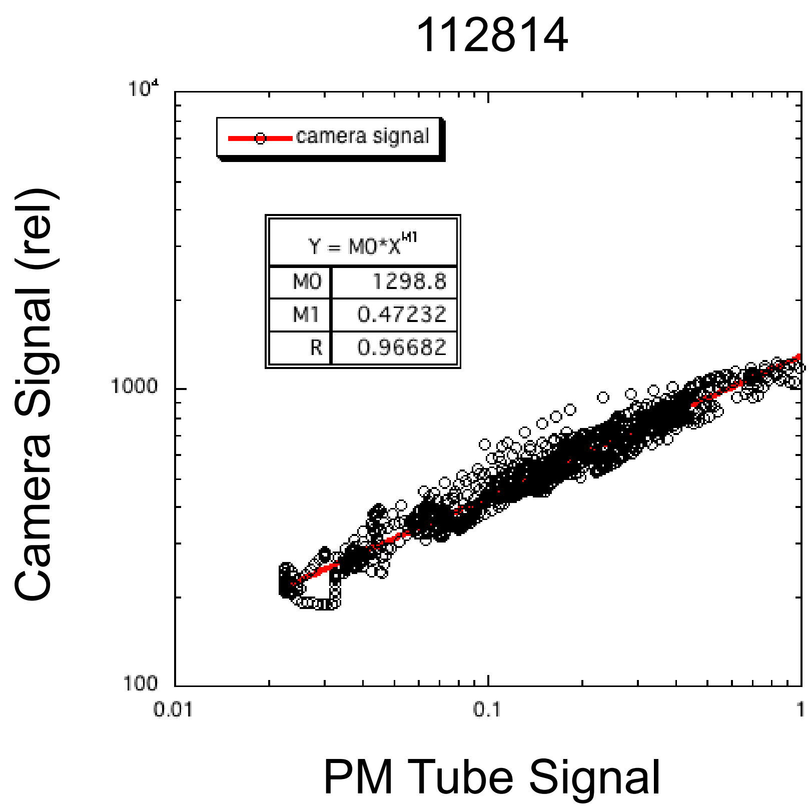
- Take from experiment:
  - EFIT equilibrium at time of interest,
  - Electron density & temperature profiles vs. R_{mid}.
- Direct simulation of 64x64 pixel view of GPI camera.
- Primary complication:
  - Steady state simulation with plasma parameters constant on flux surface,
  - But, real plasma 3-D & varying in time.
  - Justification: interested mostly in 3-D neutral density.
  - Only get Thomson scattering data at one or two time points.

Improved Agreement Result of Close Interaction Between Modeler & Experimentalist



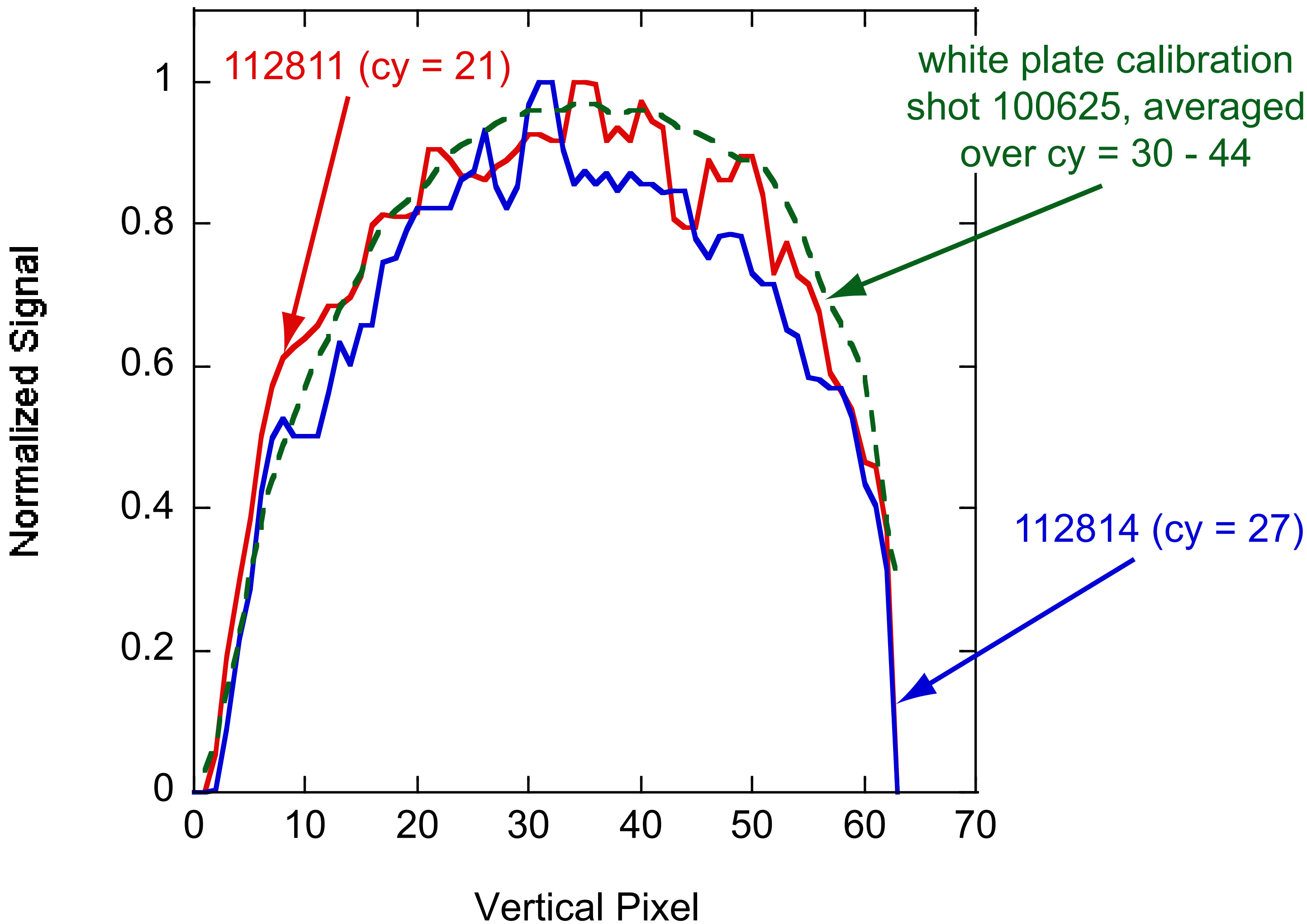
Calibrate PSI-5 Camera Nonlinear Response Against Photomultiplier Tube





- Apply *inverse* to GPI data to get something ∝ photons / (m^2 s st).

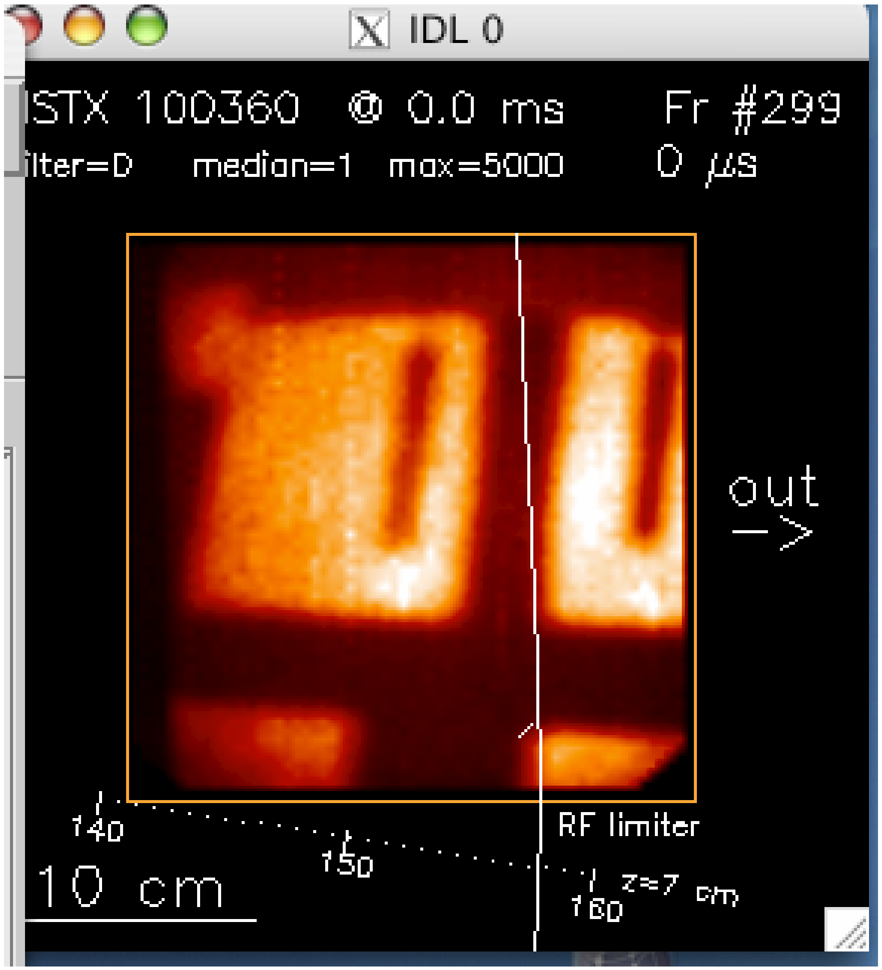
Vertical Variation Dominated by Vignetting in Optical System



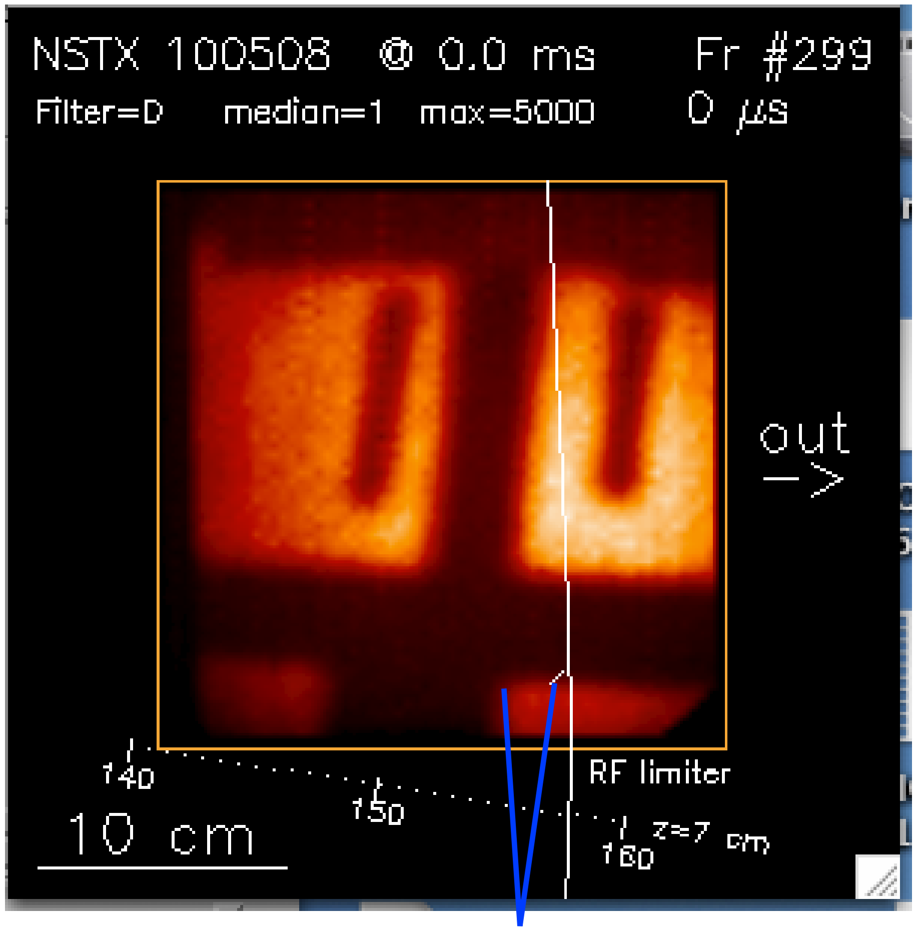
- Vertical variation of “white plate” calibration similar to that of GPI experiments,
- Use to define filter function & apply to simulated camera image.

Relative Calibration of GPI Camera Geometry

Before



After



6 pixel shift