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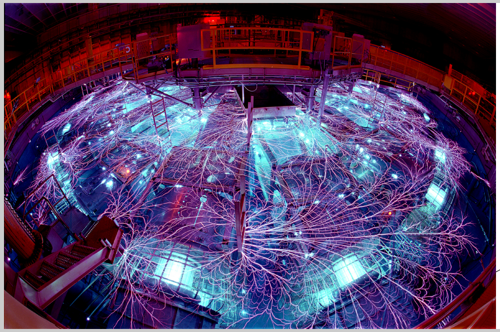

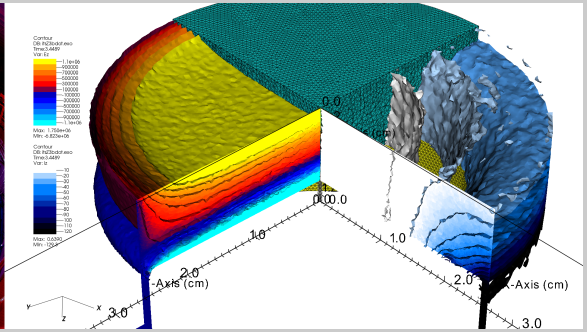

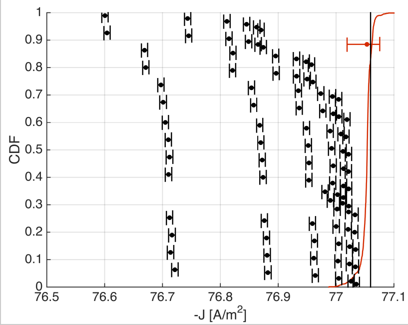

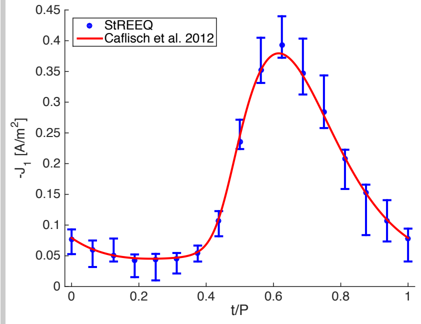

Numerical Uncertainty Estimation for Stochastic Particle-in-Cell Simulations Applied to Verification and Validation

Keith Cartwright and Gregg Radtke, *Sandia National Laboratories, New Mexico*

Gaseous Electronics Conference (GEC) 68, October 14, 2015

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

SANDIA NATIONAL LABORATORIES ADVANCED ELECTROMAGNETICS

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Background: Importance of V&V

ALWAYS/NEVER: the quest for safety, security, and survivability

https://www.youtube.com/watch?v=DQEB3LJ5psk

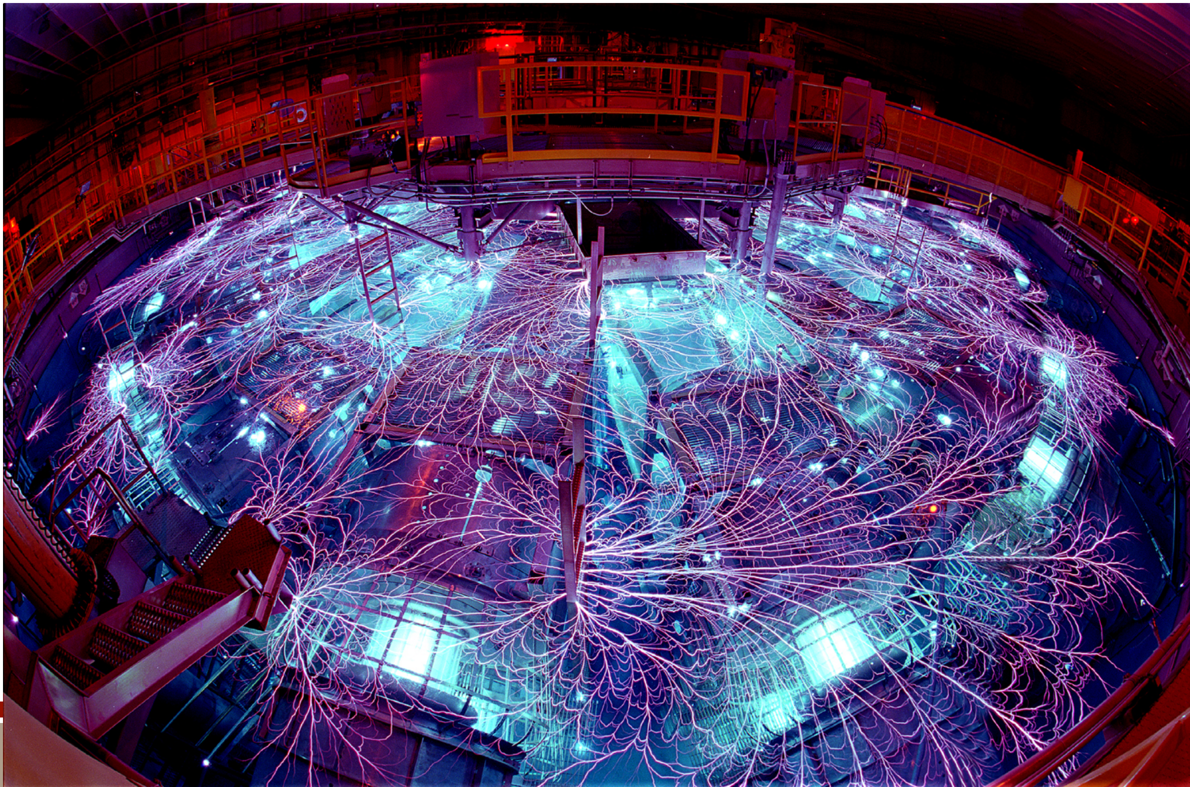
- That the weapons in America's stockpile would always work if called upon
- That the weapons would never, could never, detonate unintentionally; either as a result of accident, equipment failure, or even human malfeasance.

Since the US has signed the Comprehensive Test Ban Treaty (but not ratified it) there have been no US nuclear test detonations.

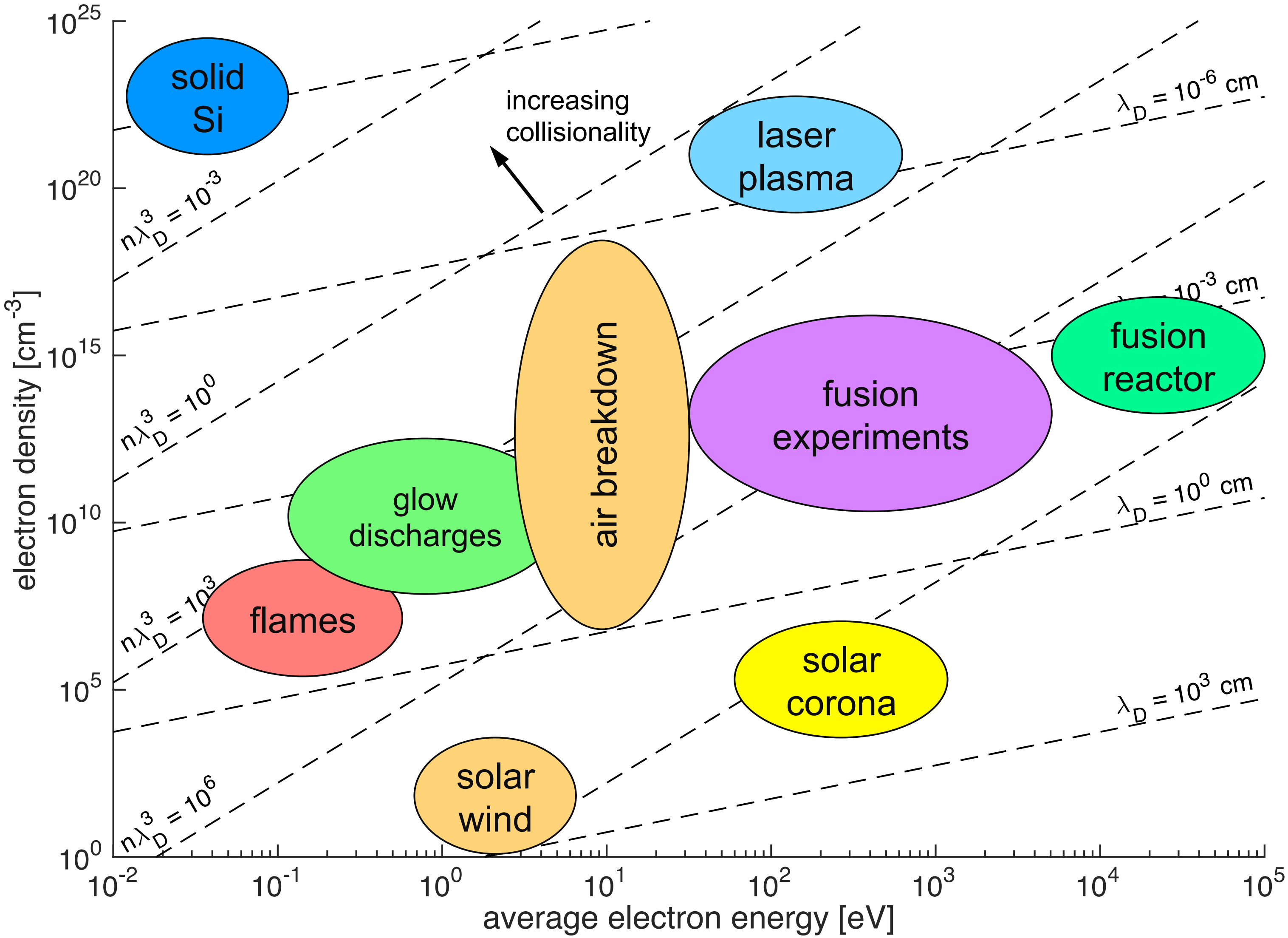
Instead, there is the Science Based Stockpile Stewardship Program

- Experimental programs
- Computational simulation programs

These experiments are part of the validation for cavity System Generated Electromagnetic Pulse (SGEMP) and Source Region EMP (SREMP) simulations.

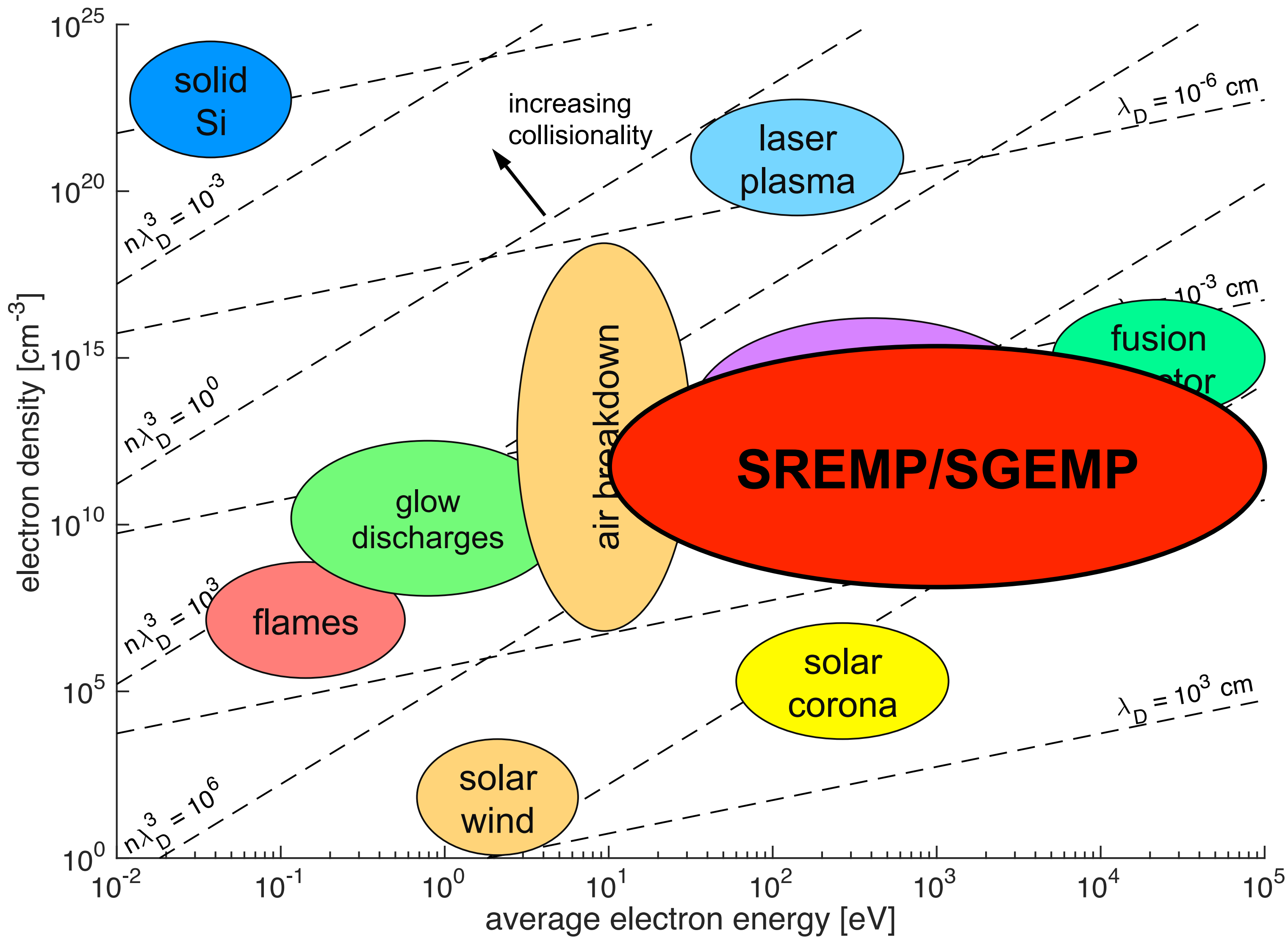


SGEMP/SREMP Plasma Regime

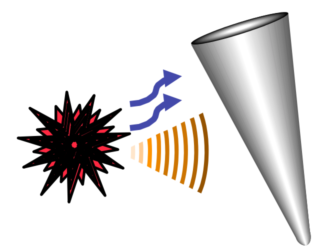


See, for example, Lieberman and Lichenberg (2005)

SGEMP/SREMP Plasma Regime



SGEMP/ SREMP



See, for example, Lieberman and Lichenberg (2005)

Balance of V&V and Importance

Increasing completeness and rigor…and cost →

PREDICTIVIE ATTRIBUTE	Level 0 Low-Consequence M&S-Informed, e.g., Scoping or Res Activities Score=0	Level 1 Low-Consequence M&S-Informed, e.g., Design Support Score=2	Level 2 High-Consequence M&S-Informed, e.g., Qualification Support, Score=4	Level 3 High-Consequence M&S-Based, e.g., Qualification Score=6
Representation or Geometry Fidelity Are you overlooking important effects because of defeaturing or stylization	• Grossly defeatured or stylized representation based on judgment or practical considerations	• Significant defeaturing or stylization based on judgment or practical considerations • or lower fidelity representation justified w a significantly defeatured or stylized representation	• Limited defeaturing or stylization judged to retain the essential elements of "as built" • or appropriate lower fidelity representation justified w a slightly defeatured or stylized representation	• Highest fidelity representation "as is" w/o sig defeaturing or stylization • or appropriate lower fidelity representation justified w highest fidelity representation
Physics and Material Model Fidelity How science-based are the models?	• Unknown model form represented with ad hoc knob non-uniquely calibrated to IET • Empirical model applied w significant extrapolation, non-uniquely calibrated with IET	• Empirical model applied w/o significant extrapolation, uniquely calibrated with SET • Physics informed model applied w significant or unknown extrapolation, unique calibrations with SET • Physics-informed model applied w/o significant extrapolation, non-unique calibrations with IET	• Physics informed models applied w/o significant extrapolation, unique calibrations with SET • Physics-based model applied w significant or unknown extrapolation	• Well accepted physics-based model applied w/o significant extrapolation
Code Verification Are software errors or algorithm deficiencies corrupting simulation results?	• Judgment only	• Code managed to SQE standards • Sustained unit/regression testing w significant coverage of required Features and Capabilities (F&Cs)	• Code managed and assessed (internally) against SQE standards • Sustained verification test suite w significant coverage of required F&Cs	• Code managed and assessed (externally) against SQE standards • Sustained verification test suite w significant coverage of required F&Cs and their interactions
Solution Verification Are numerical errors corrupting simulation results?	• Judgment only • Sensitivity to discretization and algorithm parameters explored in SRQs not directly related to the decision context	• Sensitivity to discretization and algorithm parameters explored in SRQs directly related to the decision context • Numerical errors estimated in SRQs not directly related to decision context	• Numerical errors estimated in SRQs directly related to the decision context • Rigorous numerical error bounds quantified in SRQs not directly related to the decision context	• Rigorous numerical error bounds quantified in SRQs directly related to the decision context
Validation How accurate are the models?	• Judgment only • Qualitative accuracy w/o significant SET coverage	• Qualitative accuracy w significant SET coverage • Quantitative accuracy w/o assessment of unc and w/o significant SET coverage	• Quantitative accuracy w/o assessment of unc • w significant SET coverage and IETs	• Quantitative accuracy w assessment of unc • w significant SET coverage, IETs, and full system test
UQ and Sensitivities What is the impact of variabilities and uncertainties on performance and margins?	• Judgment only • Deterministic assessment of margins (e.g., bounding analyses) • Informal "what if" assessments of unc, margins, and sensitivity	• Aleatory and epistemic uncertainties represented and propagated w/o distinction • Sensitivity to uncertainties explored	• Aleatory and/or epistemic uncertainties represented separately and propagated w significant strong assumptions • Quantitative sensitivity analysis w significant strong assumptions • Sensitivity to numerical errors explored	• Aleatory and/or epistemic uncertainties represented separately and propagated w/o significant strong assumptions • Quantitative sensitivity analysis w/o significant strong assumptions • Numerical errors quantified

V&V Informal Definitions

- **Code Verification:** assuring correct model implementation
- **Solution Verification:** assuring simulation converges according to parameters (Δx, Δt, etc.)
  - Considerably harder for multi-physics problems
  - Monotonic convergence is only type well understood mathematically
- **Benchmarking:** comparison between two or more simulation codes (not verification, but can be very useful)
- **Validation:** comparing simulation to experiment to ensure correct model was implemented
- **Uncertainty Quantification:** estimation of uncertainties to allow for a true comparison between the simulation and experiment
  - Experimental uncertainties
  - Simulation uncertainties: numerical error, input parameters, geometric tolerances, etc.

Outline

Focus: V&V for SGEMP and SREMP simulations

- Radiation Induced Plasma Experimental Validation
  - 10 mm “B-dot” cassette on Z-machine
  - Simulation using combined PIC (plasma) and Monte Carlo (photon)
    - Residuals-based numerical uncertainty estimates
    - Latin hypercube input parameter uncertainties

- Advanced Numerical Error Estimation for PIC Code Output
  - Stochastic Richardson extrapolation based method
  - Error estimates based on multiple fitting strategies and bootstrapping
  - Preliminary results applied to B-dot simulation

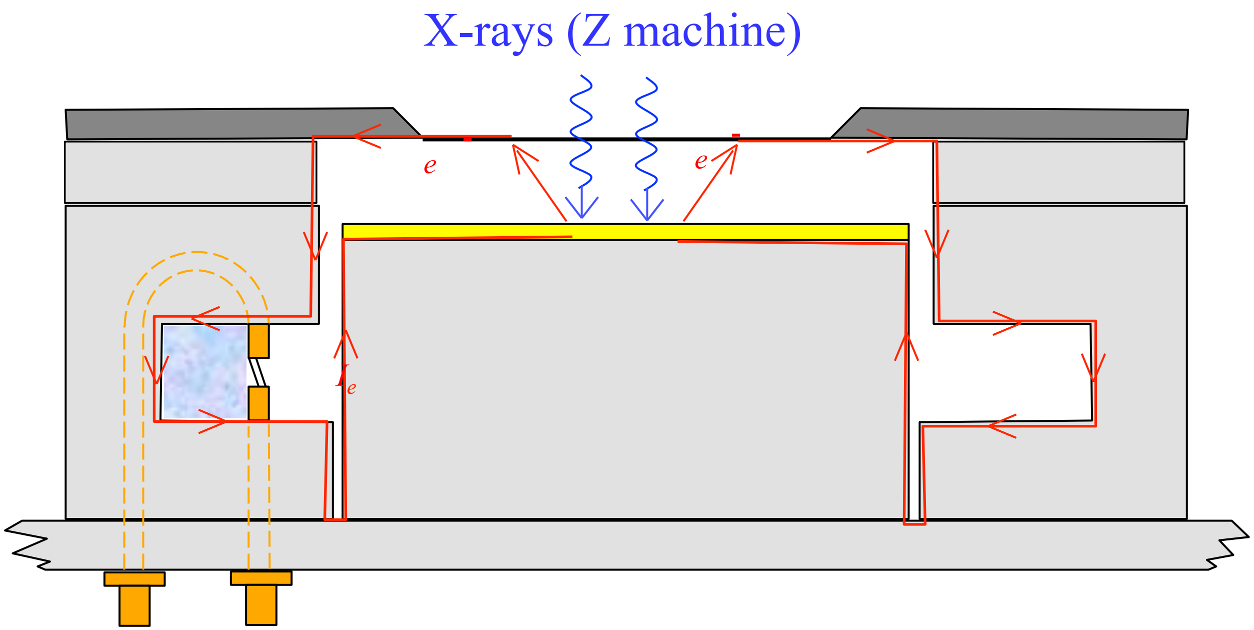
Radiation Induced Plasma Validation Experiment

Epistemic uncertainties:

- Gas pressure
- X-ray spectrum
- Geometry
- Gas cross-section
- Secondary electrons
- Backscatter electrons

Aleatory (normally distributed) uncertainties:

- Yield



- Simulated using:
  - EMPHASIS (EM PIC, plasma)
  - ITS (Monte Carlo photon transport)

Source Uncertainties (SS Wire Array)

- Yield:

High Yield Cases

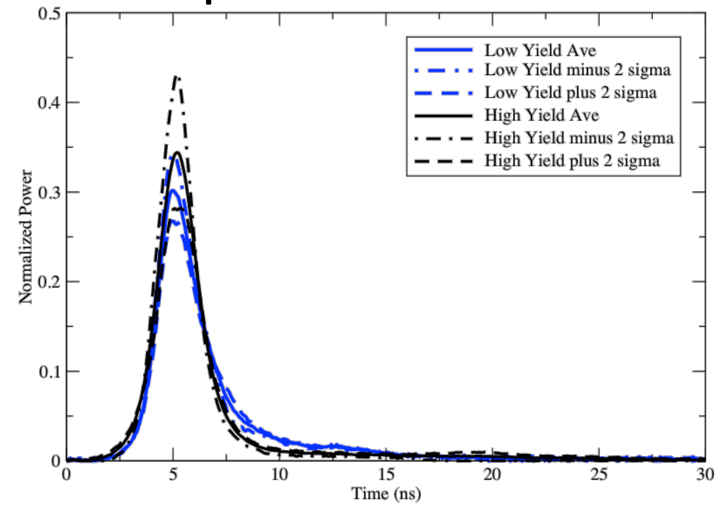
Shot Number	Yield, >5 keV (kJ)
Z2234	79 ± 12
Z2235	73 ± 11
Z2236	71 ± 11
Z2237	89 ± 16
Z2328	80 ± 11
Z2329	78 ± 8.3
Average	78 ± 12

Low Yield Cases

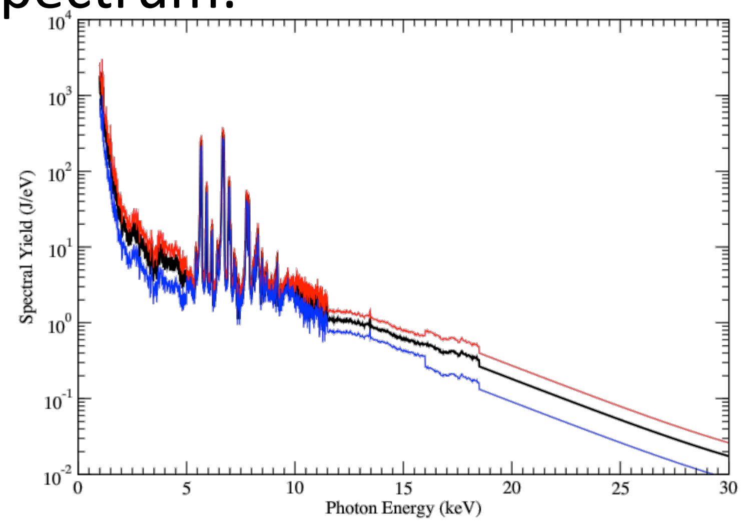
Shot Number	Yield, >5 keV (kJ)
Z2326	60 ± 17
Z2327	52 ± 10
Average	56 ± 14

plus/minus one sigma (68% Confidence Interval)

- Pulse shape:



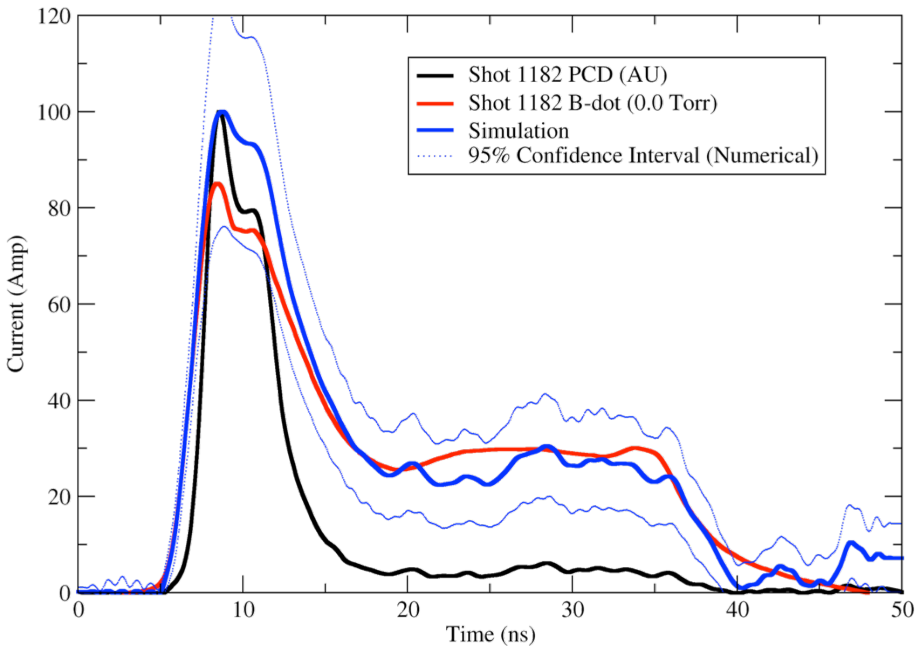
- Spectrum:



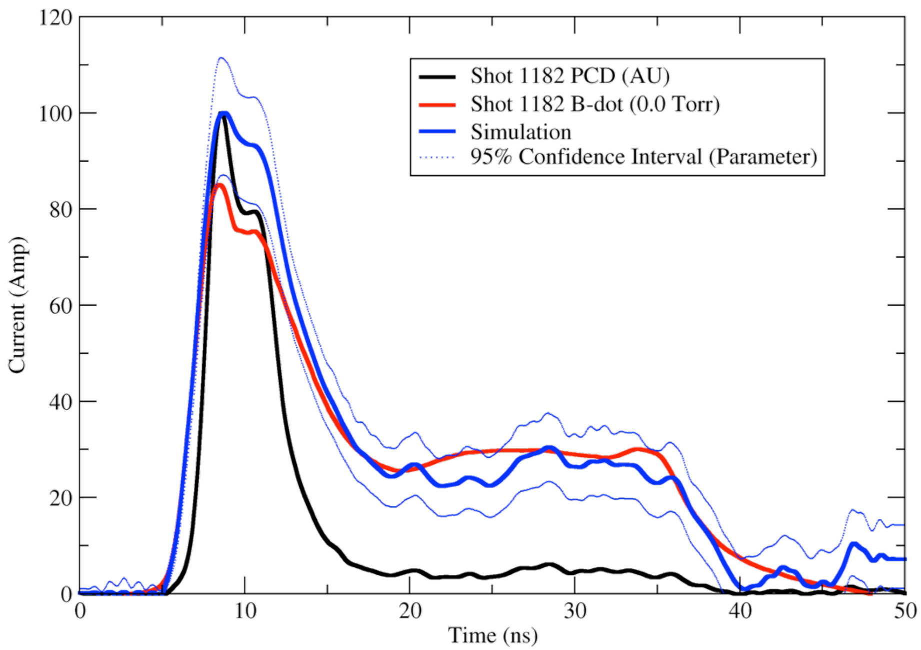
B-dot Vacuum Physics

- Space charge limited emission dominates the whole radiation pulse
  - Stiff numerical solution
- Uncertainty dominated by radiation transport (spectrum and pulse)

Numerical Uncertainty

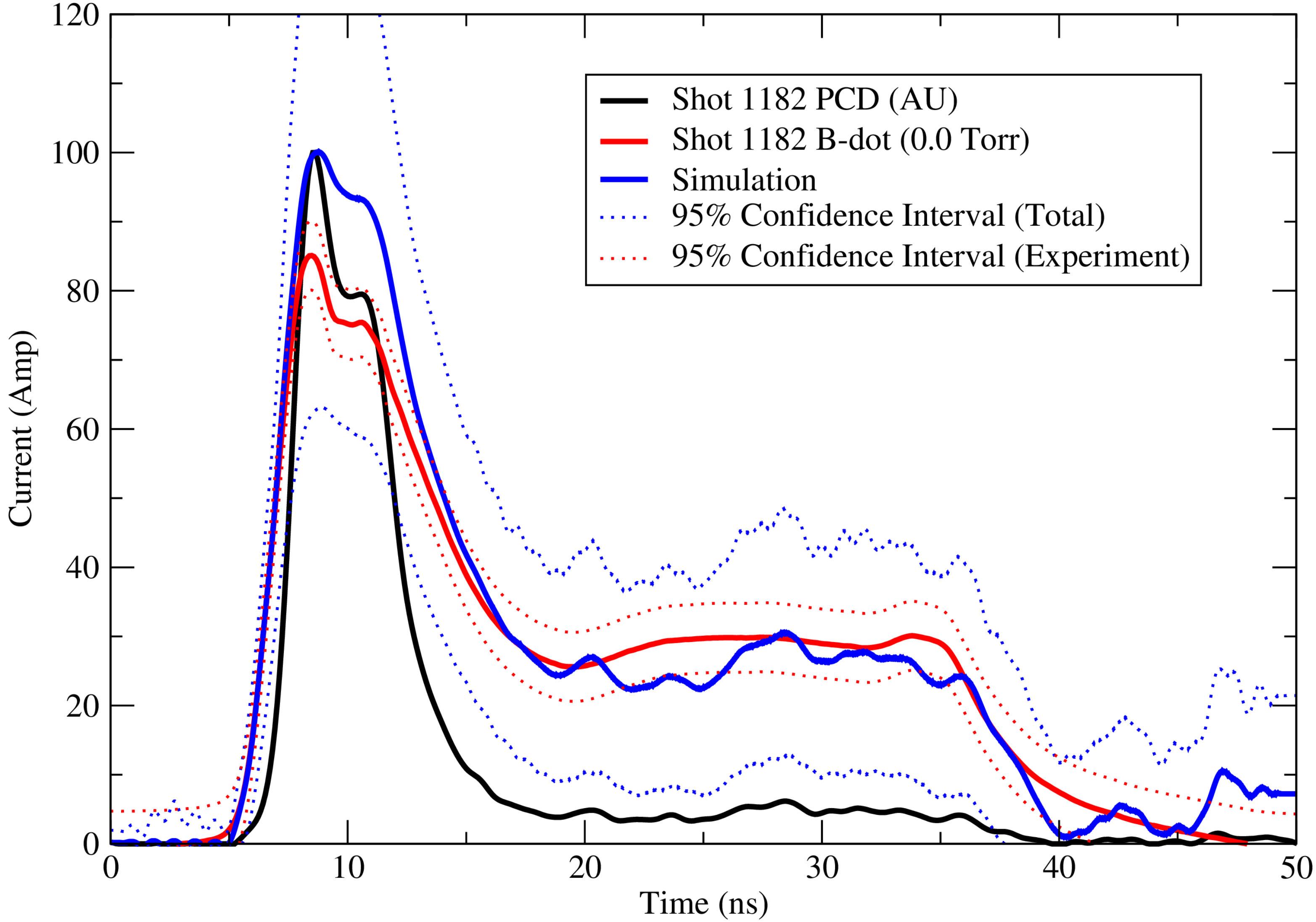


Epistemic and Aleatory Uncertainty



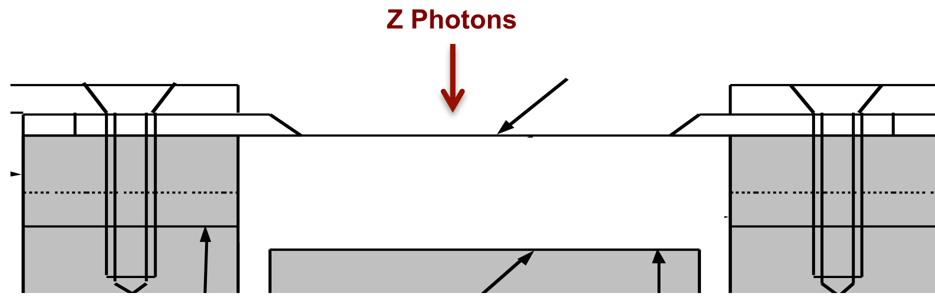
B-dot error is ±5 Amps

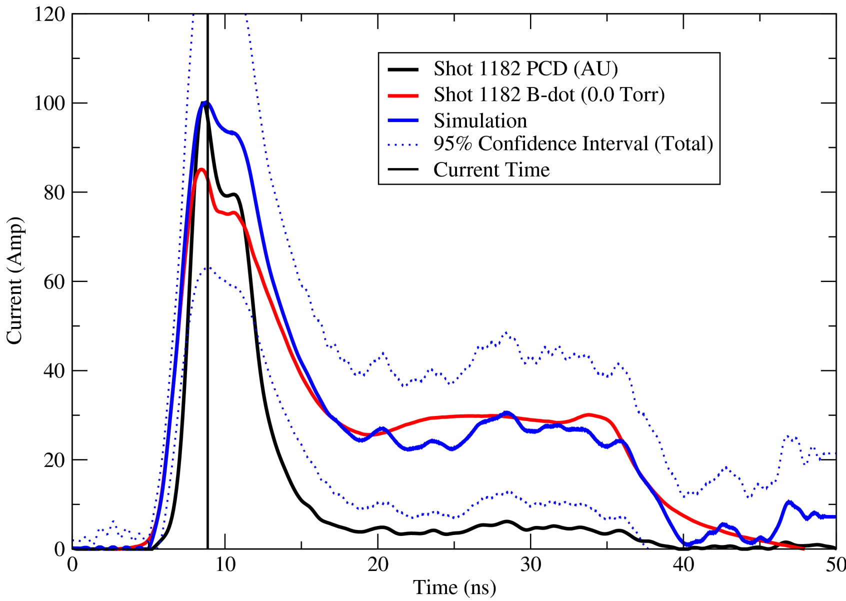
Vacuum Shot Simulation / Experiment Agreement

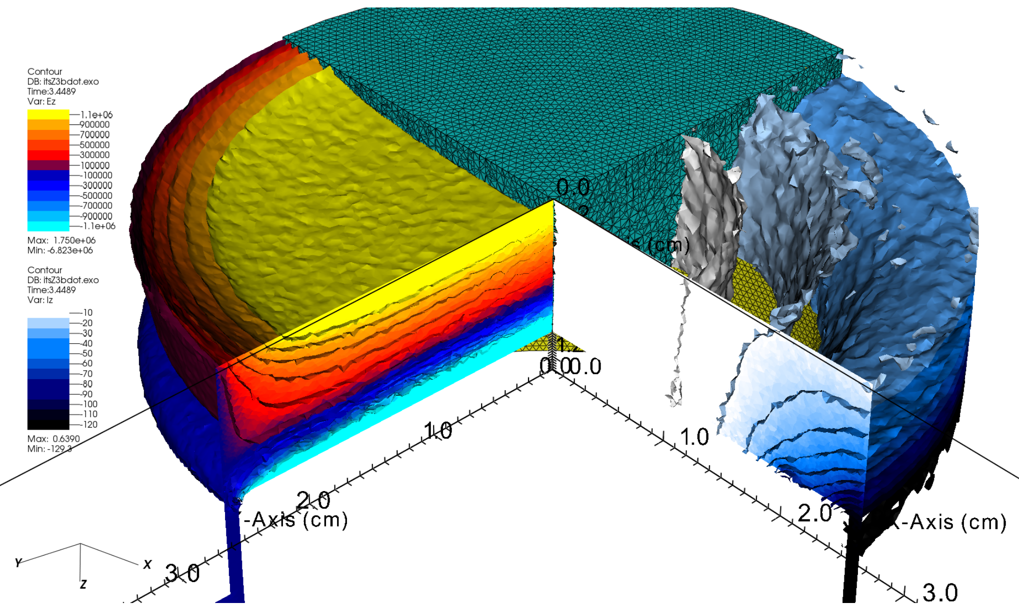


Maximum Surface Electric Fields

- Shot 1182 B-dot 0.0 Torr-8.8ns





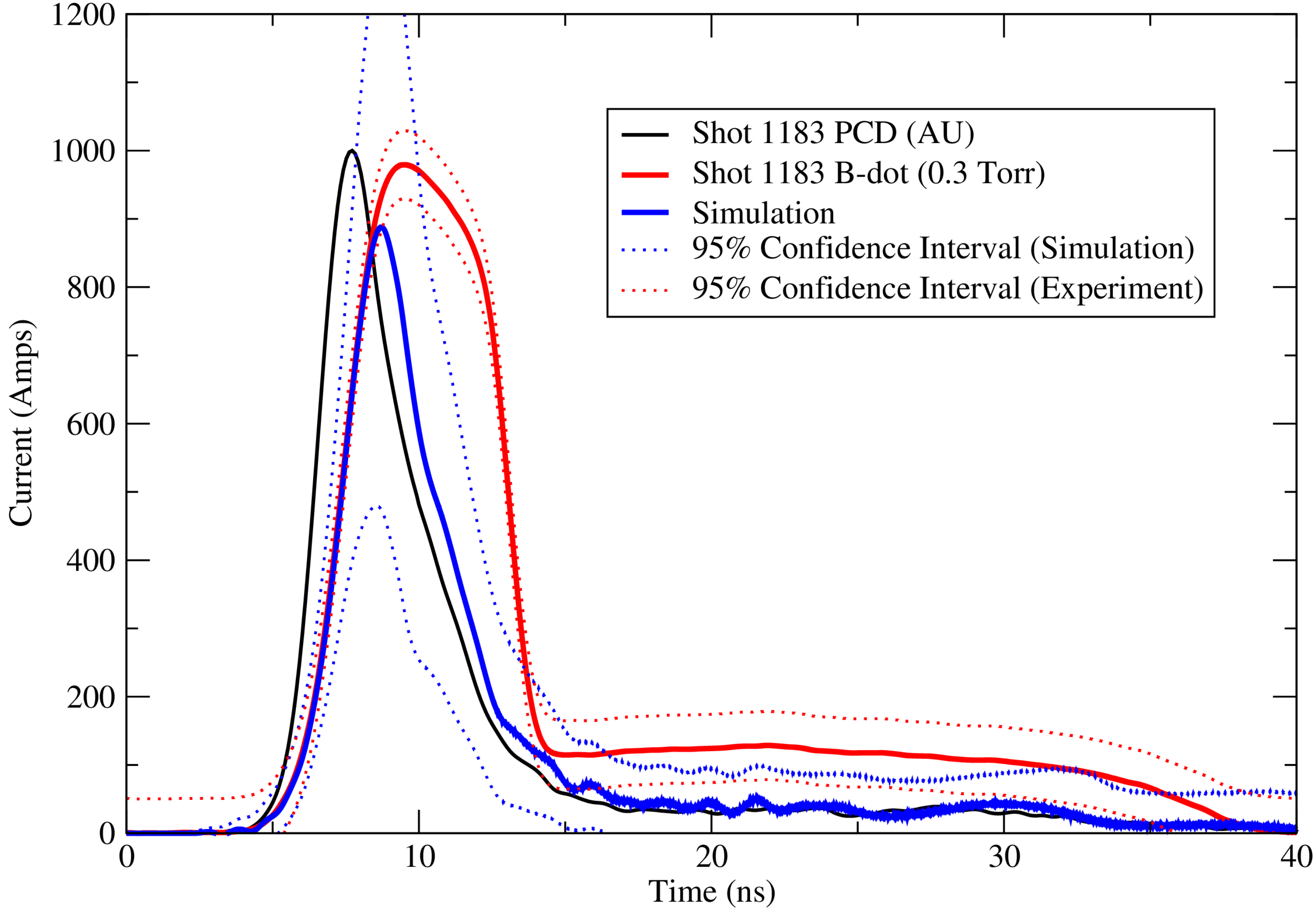


B-dot Gas physics

N_2 pressures 0.3 Torr

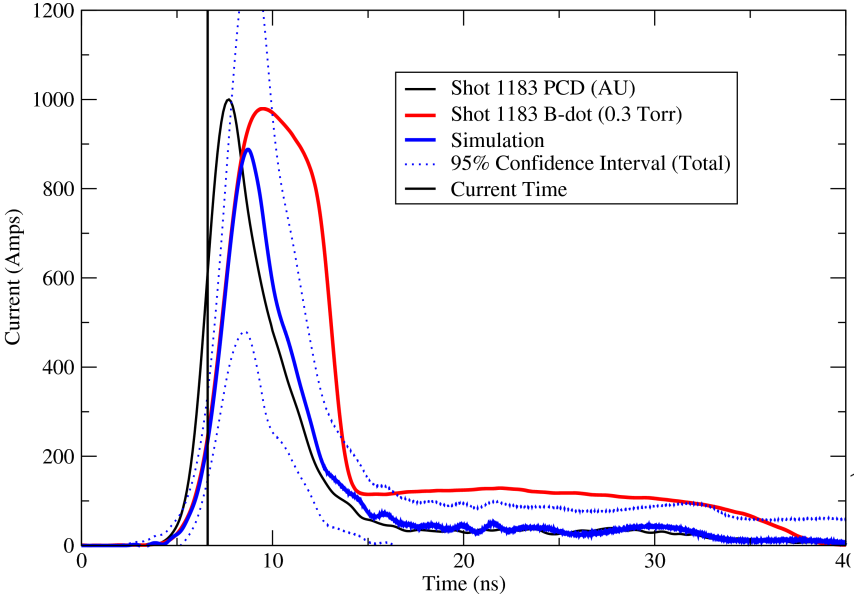
- During the rise of the radiation pulse the electrons are space charge limited
  - Ion accumulation allows for more current than the vacuum case
  - Uncertainty due to knowledge of cross sections
- Electric field reversal occurs on the wall around the time of the radiation maximum
  - The field reversal allows for additional effects to influence the simulation
- Uncertainty due to radiation transport (spectrum and pulse)

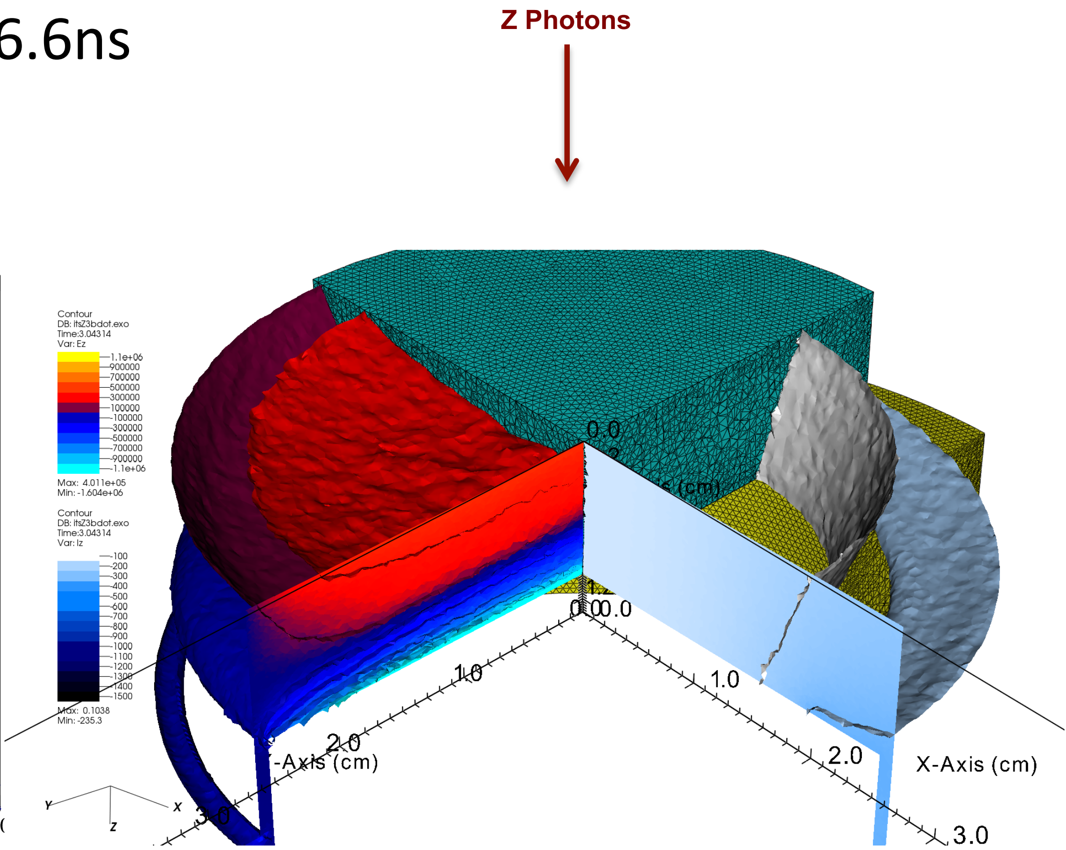
Gas Shot Simulation / Experiment Disagreement



Maximum Surface Electric Fields

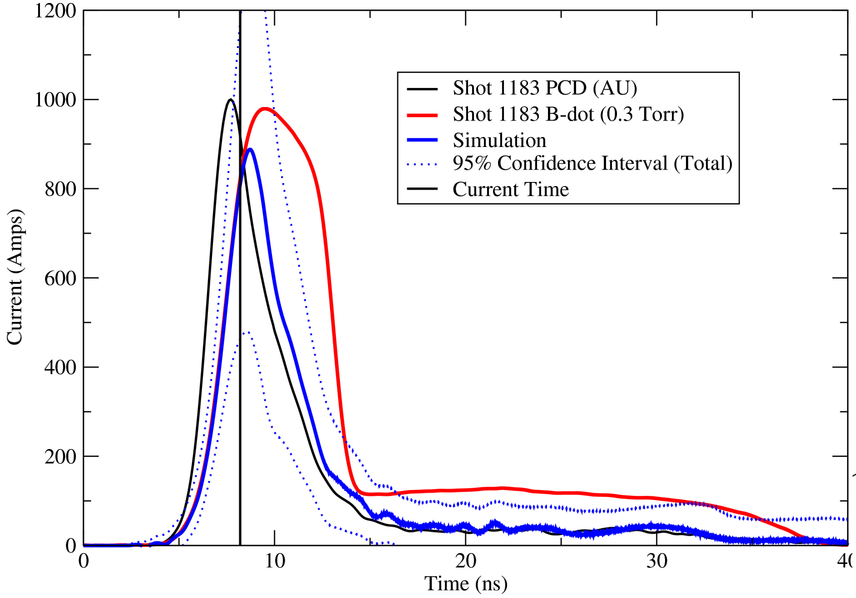
- Shot 1183 B-dot 0.3 Torr-6.6ns

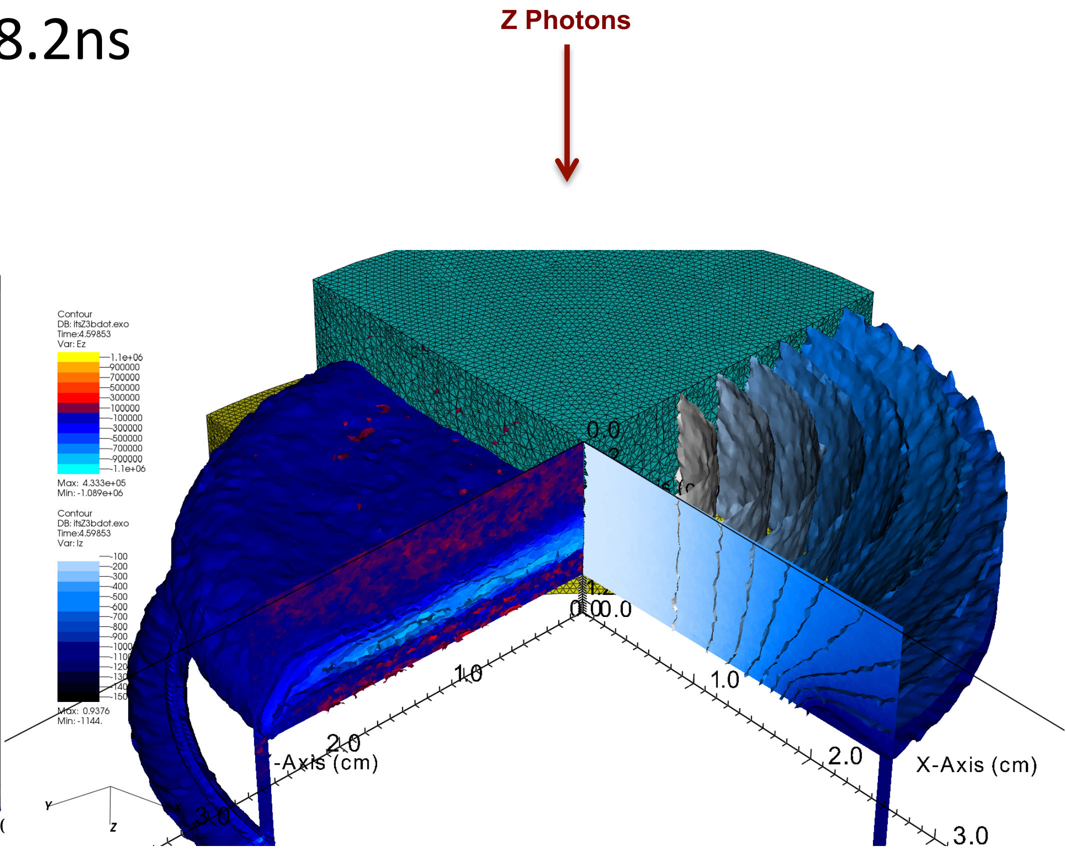




Electric Field Reversal on the Graphite Surface

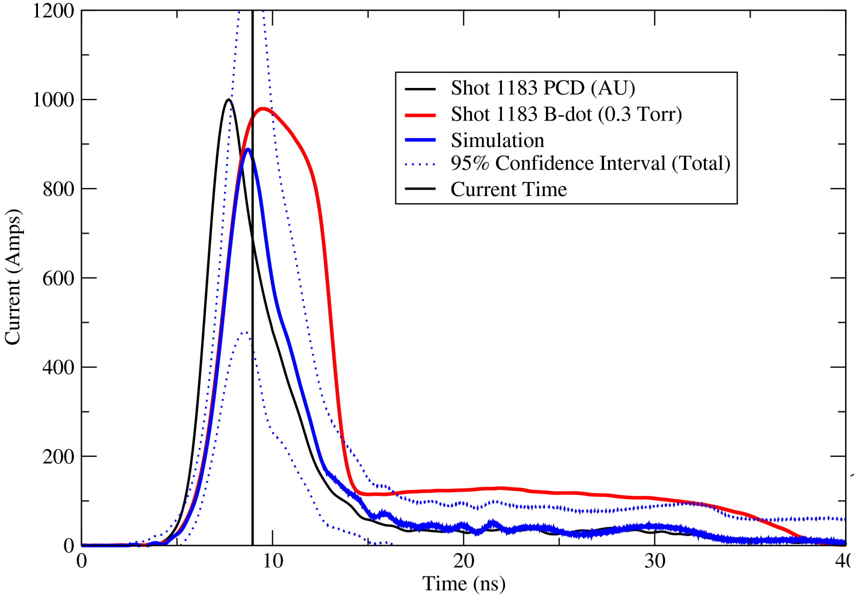
- Shot 1183 B-dot 0.3 Torr-8.2ns

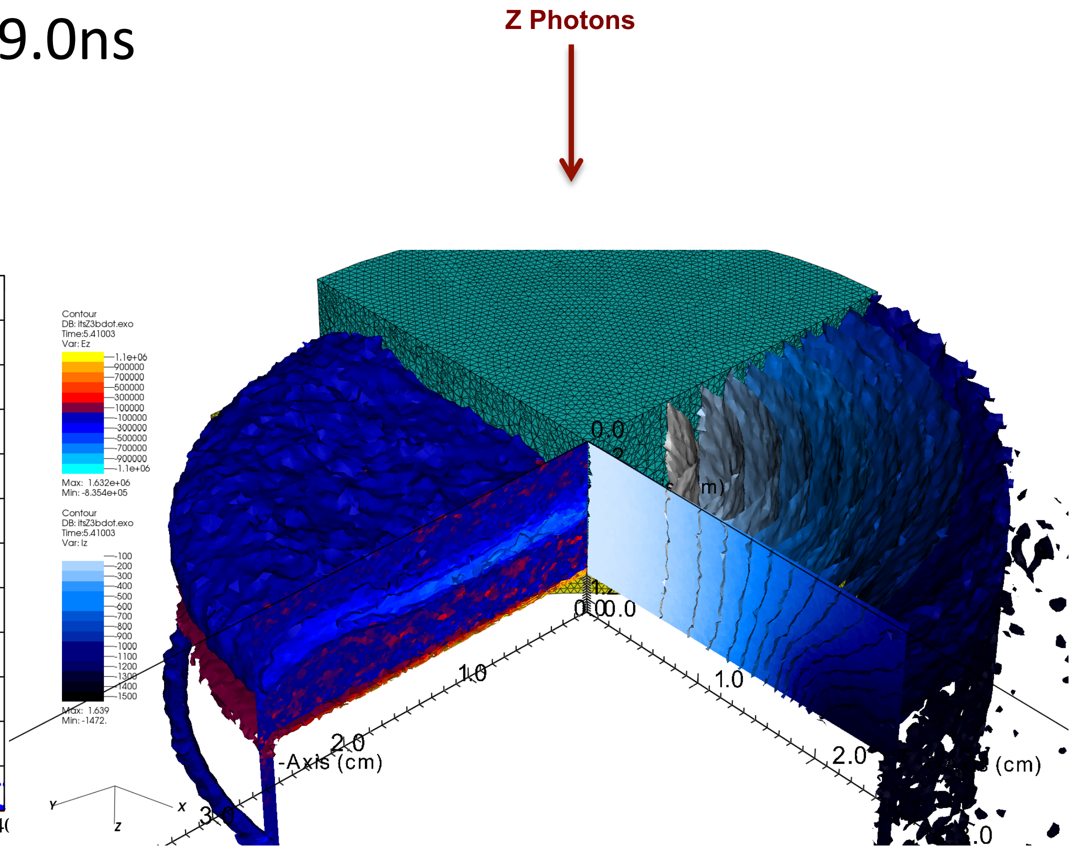




Electric Field Reversal on the Gold Surface

- Shot 1183 B-dot 0.3 Torr-9.0ns

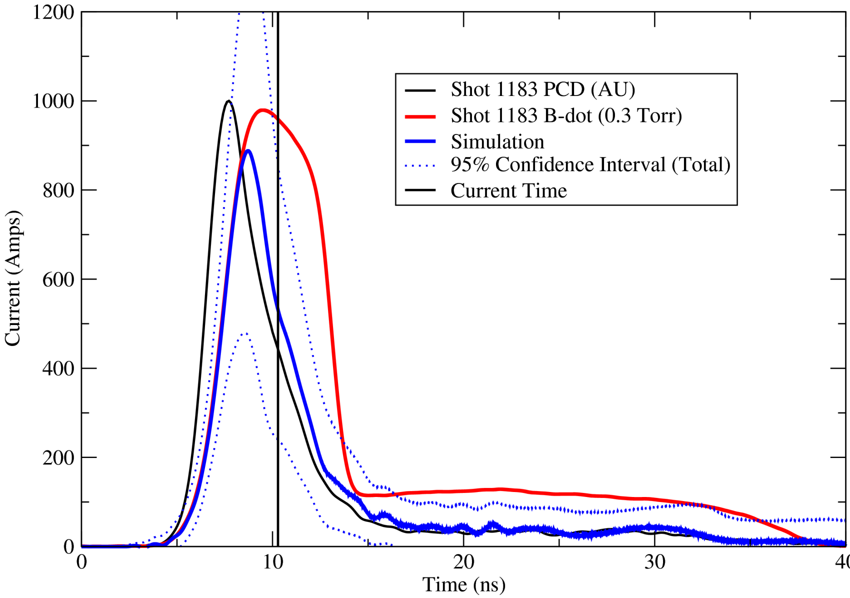


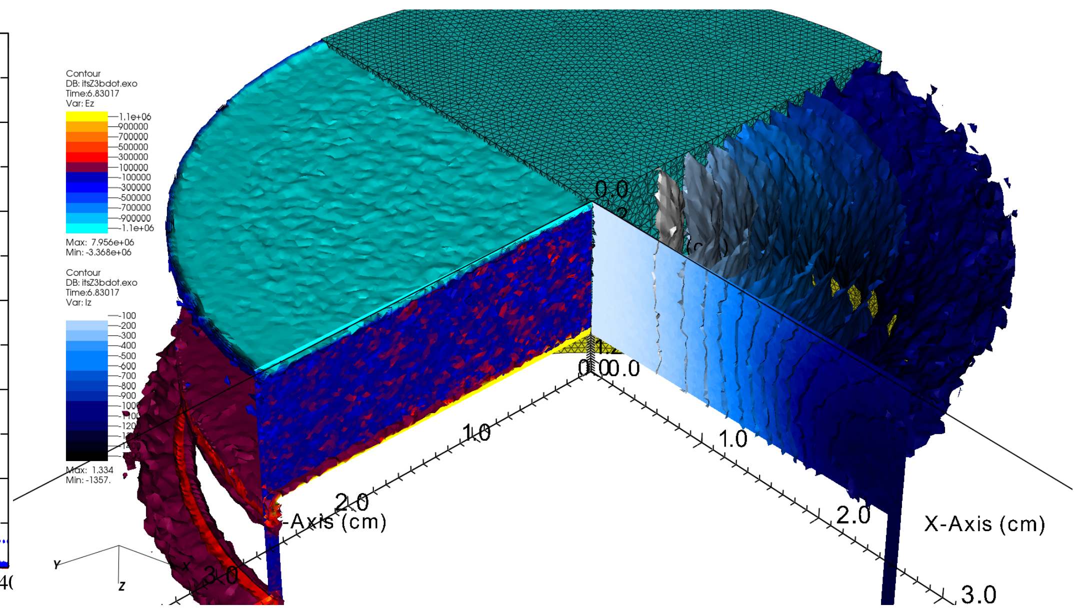


Plasma Diffusion to the Walls

- Shot 1183 B-dot 0.3 Torr-10.3ns

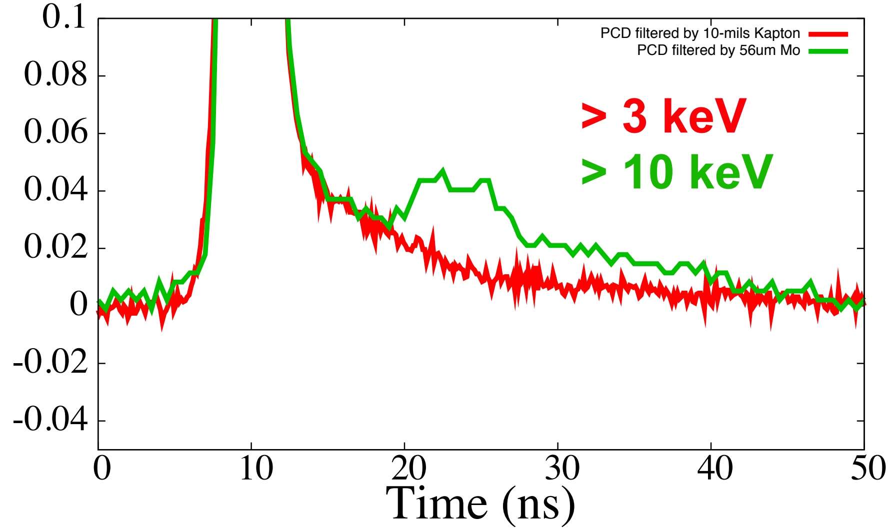
Z Photons



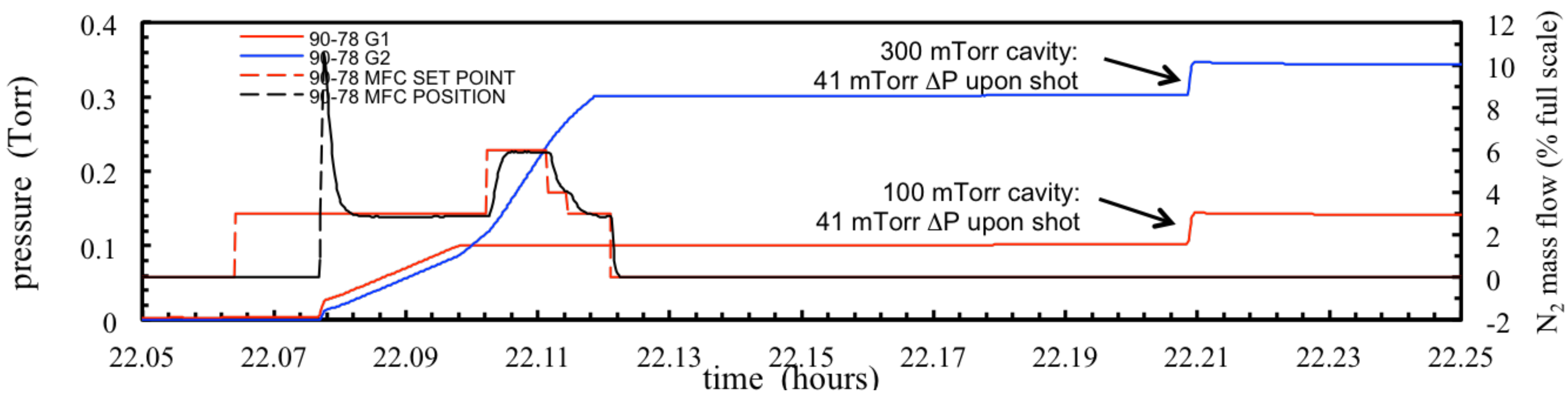


What Was Left Out

- Currently we know that
  - Photon spectrum is a function of time
  - Blow-off/out-gassing is more of an issue than was previously expected



NIF facility (LLNL) cassette pressure history



Numerical Error Estimation

- Inherent difficulties:
  - Computationally expensive, large scale simulations
  - Multiple length scales, time scales, regimes
  - Multiple numerical discretization parameters (grid, time, MPW)
  - PIC plasma: stochastic noise $\sim 1/\sqrt{N}$ (Monte Carlo sampling)
- Methods for deterministic code output
  - Grid convergence index (GCI) (Initial version Pat Roache, 1998)
    - GCI = $F_s \, |Y_1 - Y_2| \, / \, (r^\gamma - 1)$; empirical "safety factor": $1.25 < F_s < 3$
  - Robust verification analysis (Bill Rider, et. al. 2012-)
    - Multi-fitting scheme (using nonlinear optimization) with various error norms, weighting schemes and regularizations
    - Eliminates F_s by using a diversity of estimates
- Stochastic Richardson Extrapolation Based Error Quantification (StREEQ)
  - Inspired by Rider's work, but tailored to stochastic response data
  - Bootstrapping to propagate the stochastic noise

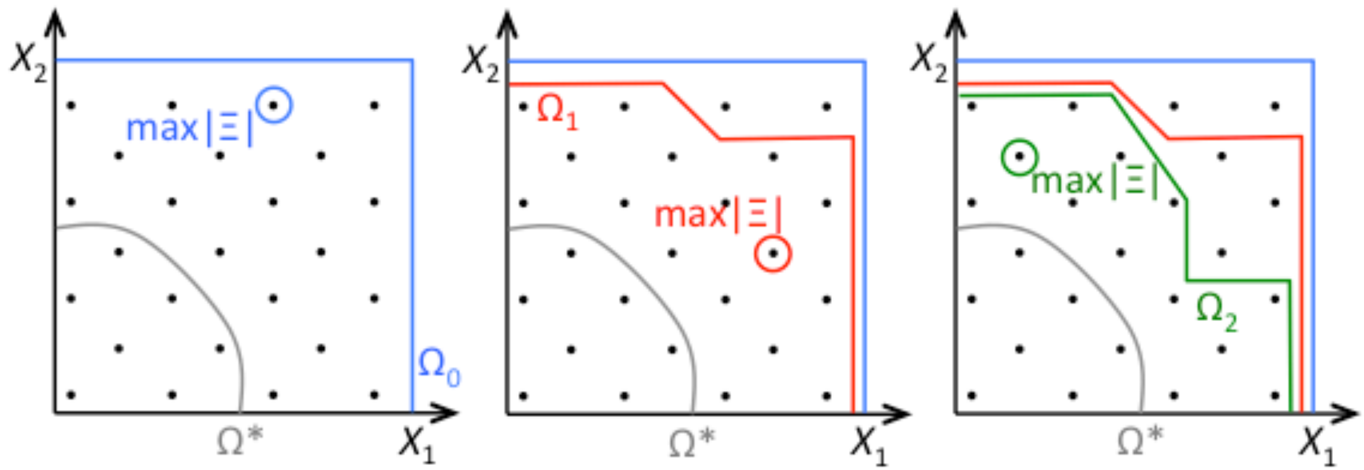
StREEQ: Stochastic Richardson Extrapolation based Error Quantification

- Discretization error model: $$\mu_j^b = \beta_0 + \sum_q \beta_q X_{qj}^{\gamma_q} + \sum_q \sum_{r>q} \beta_{qr} X_{qj}^{\gamma_q} X_{rj}^{\gamma_r} + \varepsilon_j$$
  - Discretization parameters, i.e. $X_{1j} = \Delta x/\Delta x_0$, $X_{2j} = v_0 \Delta t/\Delta x_0$, etc.
  - Bootstrap sample means μ_j^b, convergence rates γ_q, and residual ε_j
  - Other forms are possible, may be code dependent
- Objective function $$G(\beta,\gamma) = \left\| w \cdot \left(\beta_0 + \sum_q \beta_q X_q^{\gamma_q} + \sum_q \sum_{r>q} \beta_{qr} X_q^{\gamma_q} X_r^{\gamma_r} - \mu \right) \right\|_p$$
- Error norms:
  - L_1 minimally sensitive to outliers
  - L_2 is standard least-squares approach
  - L_∞ is maximally sensitive to outliers
- Residual weights: to favor less refined or more refined data
- In total, nine fitting models for each bootstrap sample
- Fits performed using multi-start nonlinear optimization

see Radtke, Cartwright, and Musson, SAND2015-8620

StREEQ Error Estimation

- Estimated converged result distribution $$\tilde{\beta}_{0,j}^{bm} = \beta_0^{bm} + \frac{M-1}{M-N_{\text{fit}}}\varepsilon_j^{bm}$$
  - β_0^{bm} from multiple bootstrap (*b*) and fitting model (*m*) fits
  - Residuals ε_j^{bm} correct for lack-of-fit error
- Distributions in β_0 and γ used to estimate converged results and convergence rates with uncertainties (confidence intervals)
- Credibility established from residual distributions and F-test (L_2)
- Successive discretization-domain refinement to find optimal (minimum variance) numerical error estimate

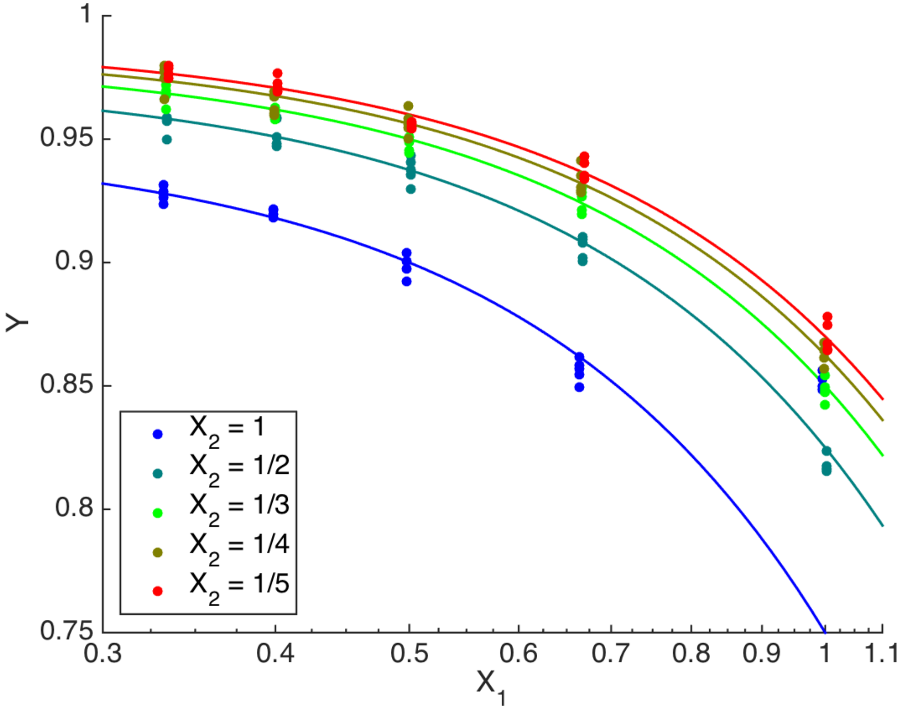


Results for Engineered Data Set

- Data set with built in bias

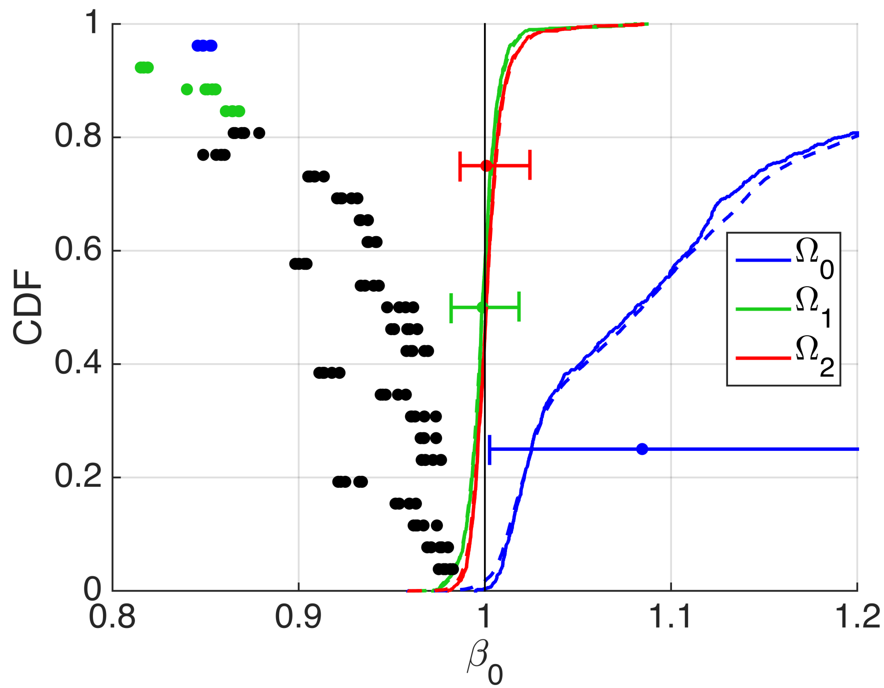
$$Y = 1 - 0.1X_1^2 - 0.05X_2 - 0.1X_1^2X_2 + \varepsilon + 0.1X_1^7X_2^{7/2}\sin\left(2\pi\left[\log\left(X_1\sqrt{X_2}\right) + 0.25\right]\right)$$

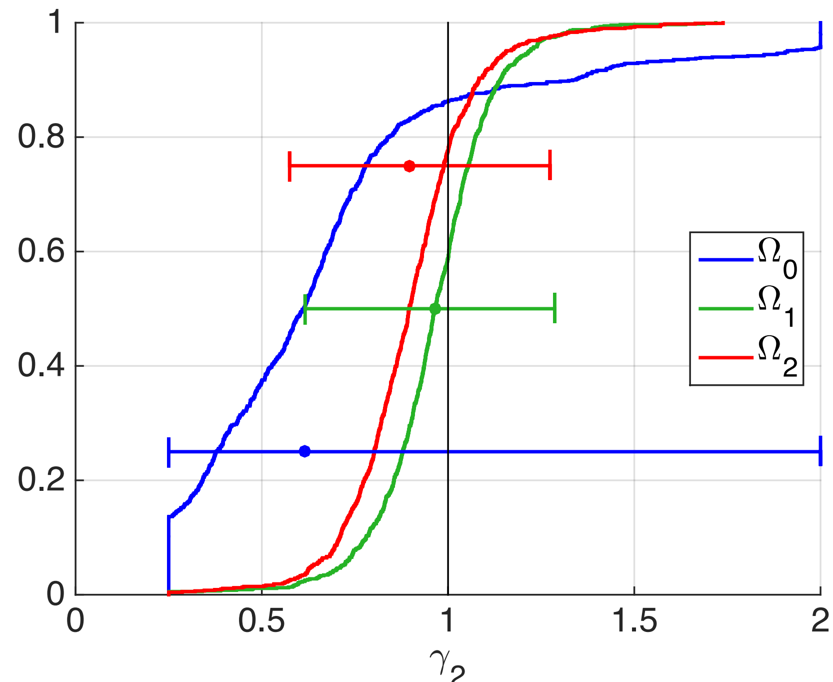
  - Random noise ε with zero mean
  - Bias is oscillatory with fast decay for *X* -> 0



Results for Engineered Data Set (II)

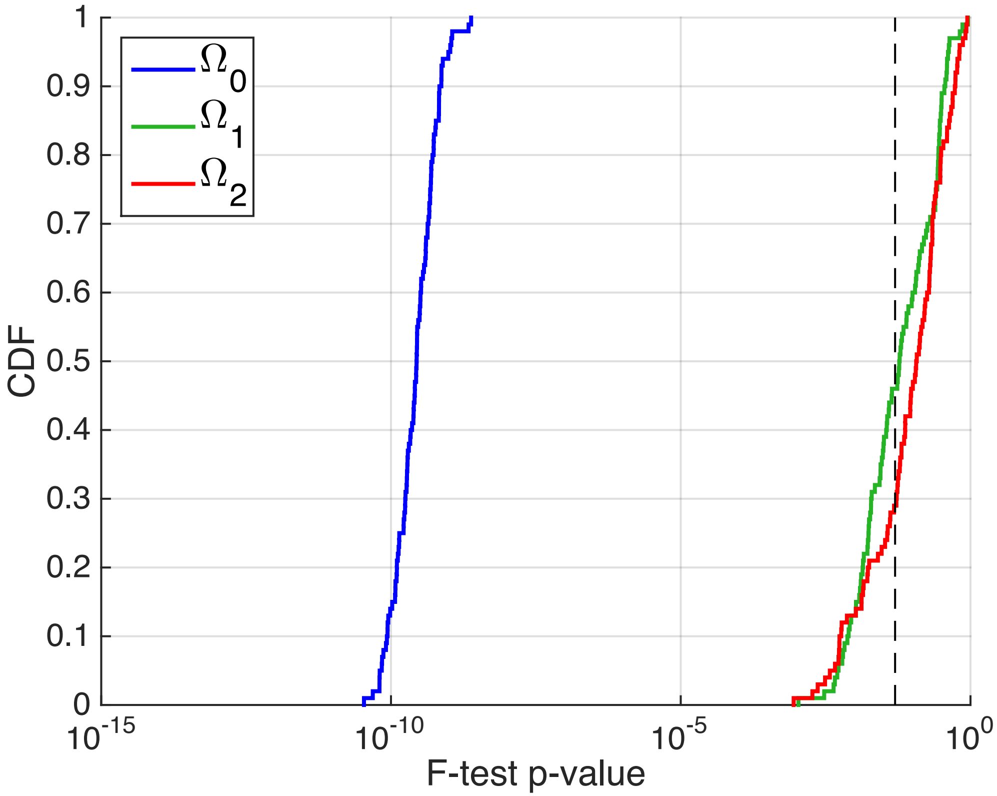
- Normally distributed, 5 samples per discretization level
  - Bias in data leads to increased uncertainty due to multiple fit models and lack-of-fit corrections
  - Minimum variance in β_0 prediction for reduced domain Ω_1

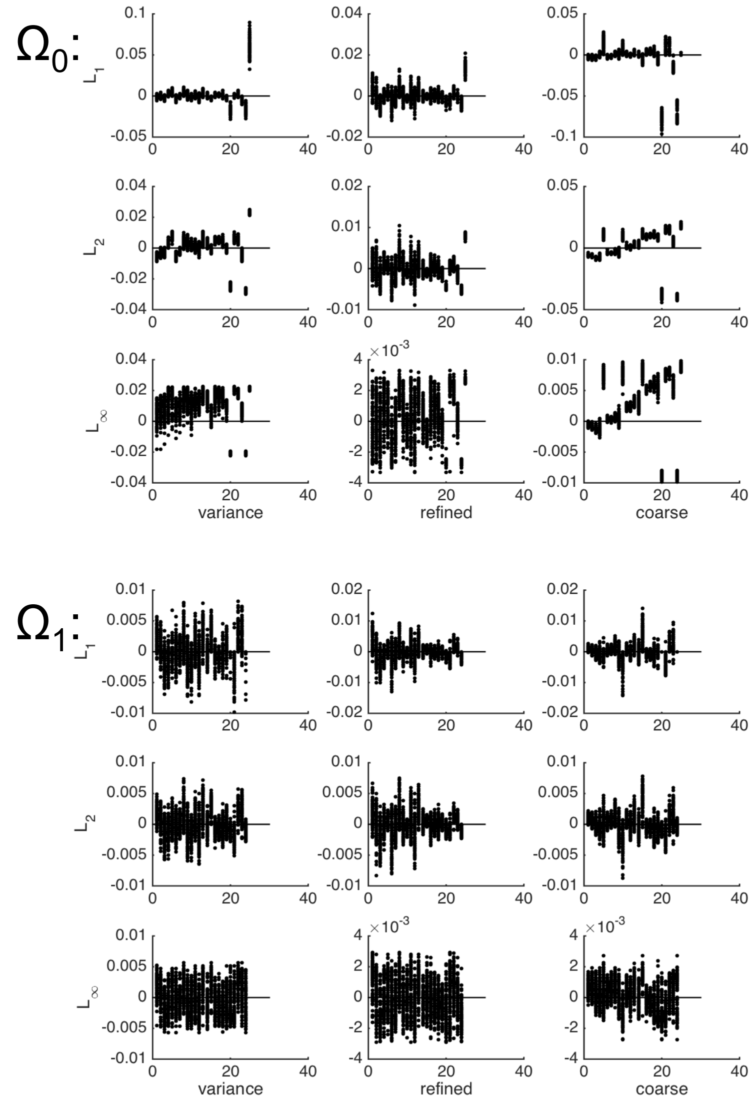




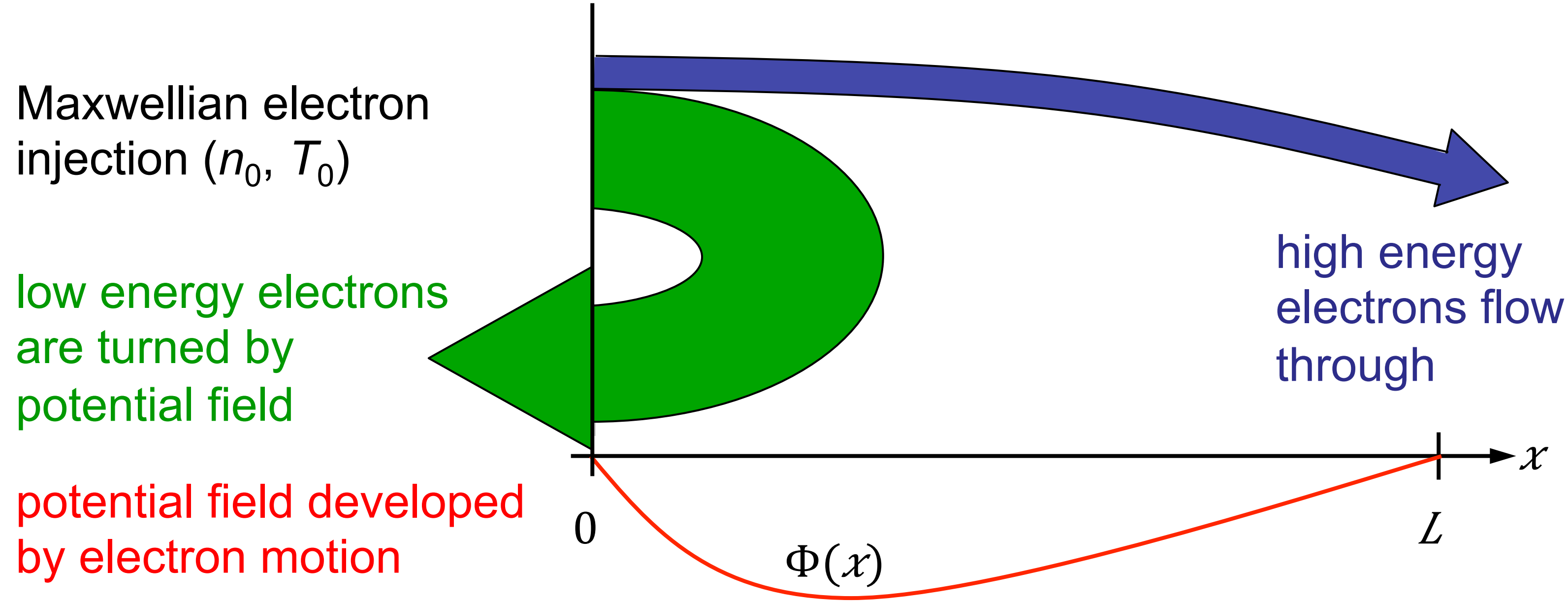
Results for Engineered Data Set (III)

- Credibility assessment





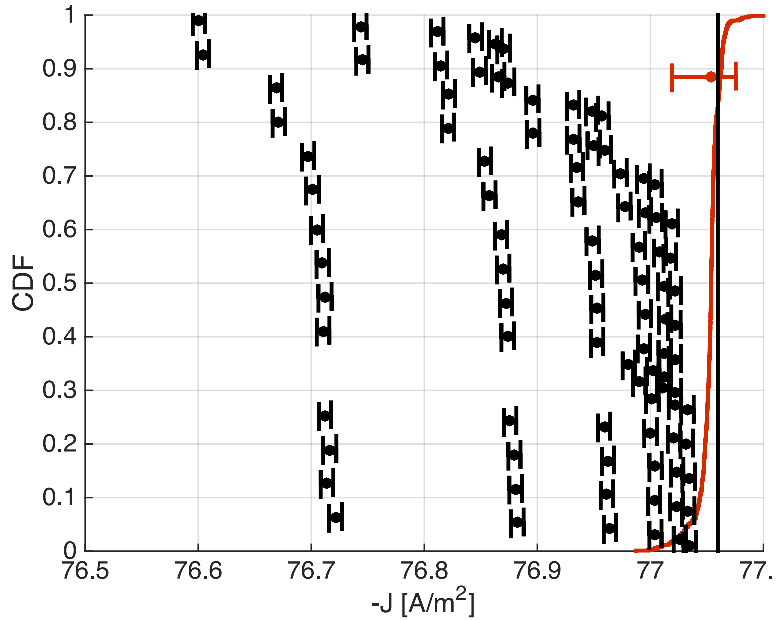
Steady Electron Diode Verification

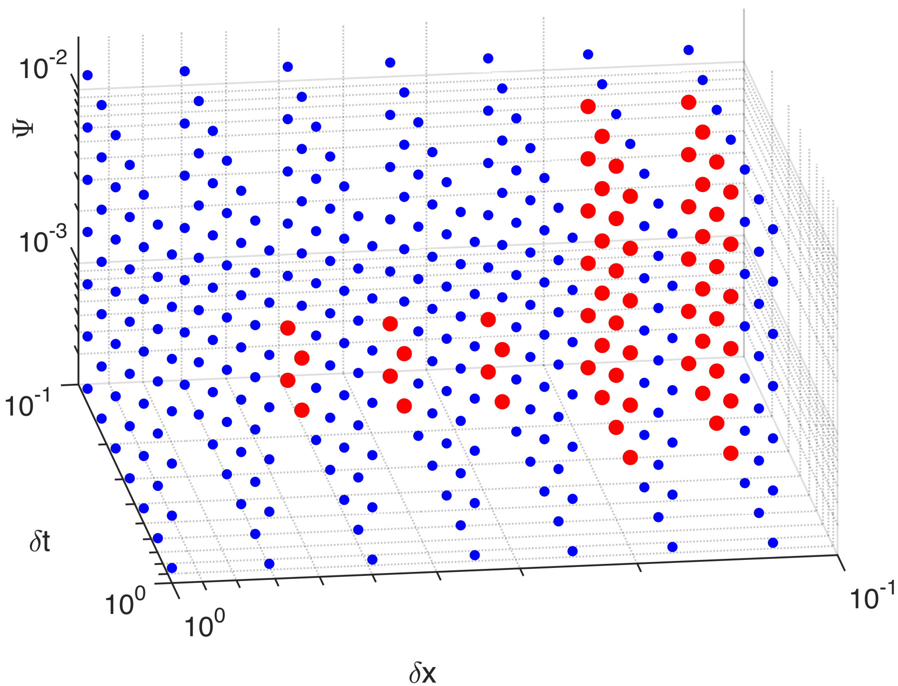


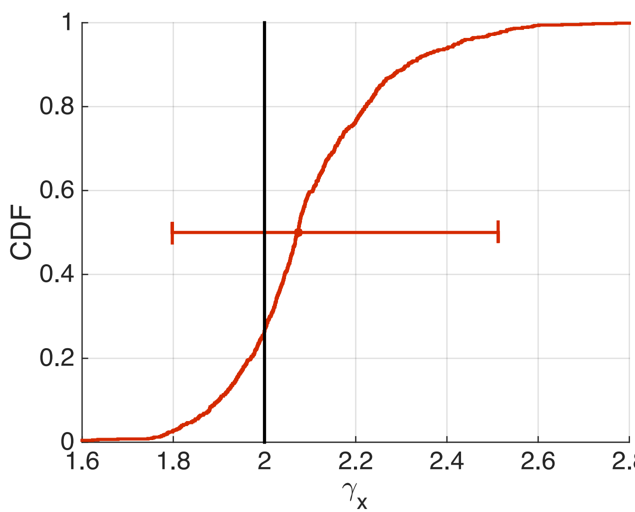
- Simulated using Sandia's Aleph electrostatic PIC plasma code
  - Quantity of interest: total current through diode (-J)
  - Input parameters: n_0 = 10^{16} m^{-3}, T_0 = 10 V, L = $20\lambda_D$
  - Exact result: -J = 77.0596 A/m^2 (numerical quadrature)
- Dimensionless convergence parameters:
  - Grid size $\delta x = \Delta x/\lambda_D$, time step $\delta t = \lambda_D \omega_p \Delta t/\Delta x$, and macroparticle weight Ψ = MPW/($n_0 A \lambda_D$)

Steady Electron Diode Verification (II)

- Code verification problem
  - Enormous data set (700 replications for 343 discretization levels)
  - Precise verification of exact solution and convergence rates

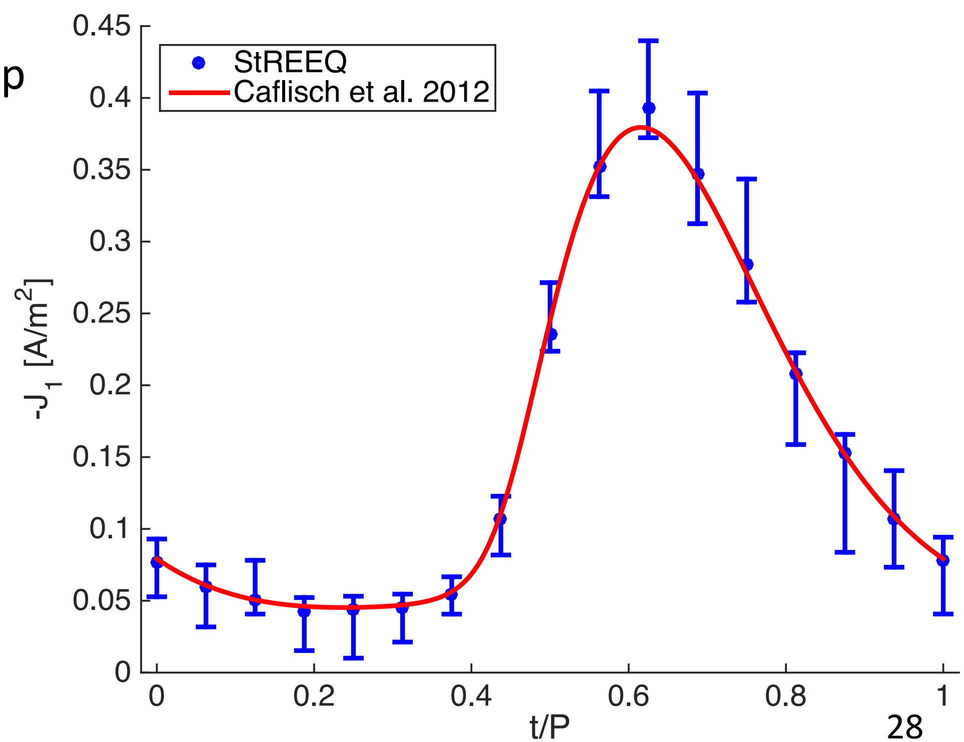






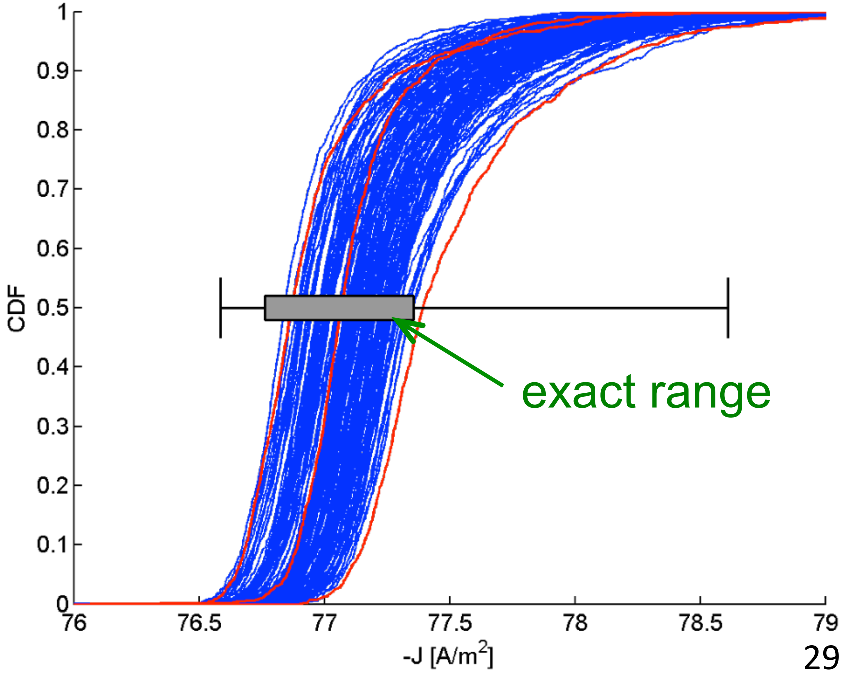
Time-Periodic Electron Diode

- One-dimensional time-periodic diode exact solution: Caflish, et al. 2012.
  - Cold electron injection with sinusoidal density variation
  - Periodic cathode electrical potential
  - Results in current which exceeds the space charge limit on average
- Time-dependent verification problem
  - Automated selection of optimal discretization domain for each step
  - Captures known solution as a function of time



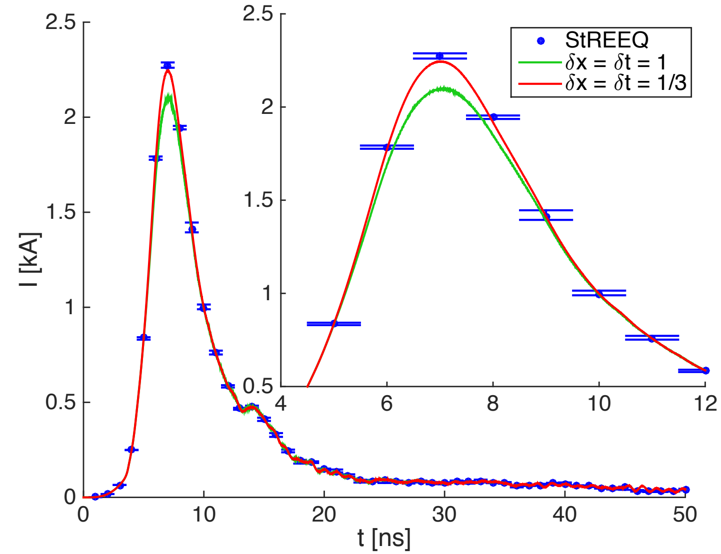
Combined Uncertainty Estimation

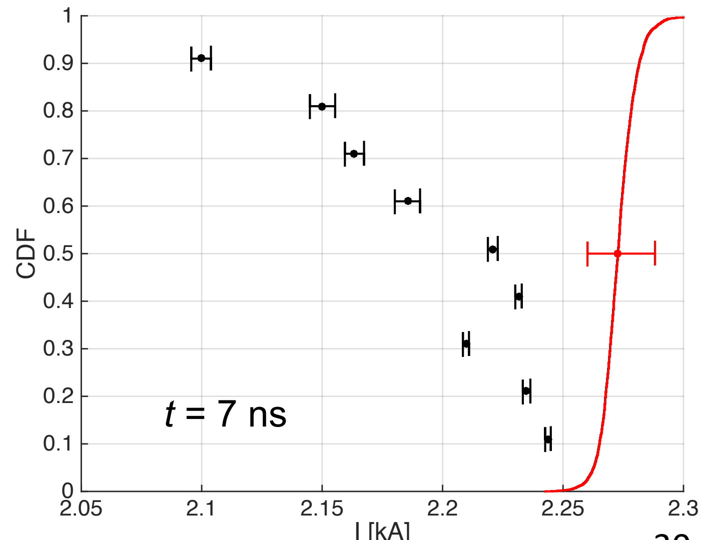
- StREEQ numerical error estimation can be combined with input parameter uncertainty estimates
  - Input parameter uncertainty samples at coarse resolution
  - StREEQ analyses at a few points in input parameter space
  - Combined approach incorporates both sources of uncertainty and is centered about the fully-converged value
- Example is electron diode example using mixed aleatory-epistemic uncertainty approach
- Complicated when numerical error is strong function of input parameters (work in progress)



Application to B-dot (preliminary)

- 1 mm vacuum B-dot simulation (EMPHASIS)
- StREEQ results used to diagnose simulation inefficiencies:
  - Simulations were over-resolved in MPW
  - First-order time convergence was observed (expected second-order)
  - Ongoing code modifications to improve simulation algorithms
- Future work:
  - Use StREEQ in code verification problems for EMPHASIS (and other Sandia codes)
  - Incorporate StREEQ into future validation experiments





Conclusion

- Systematic V&V is critical for establishing simulation credibility in high consequence work
  - Complete physics generally required
- V&V for plasma simulation has numerous challenges
- Radiation induced plasma validation experiment
  - Careful validation can uncover missing physics from experiments
  - Future work: improve numerical error estimation
- Numerical error estimation for PIC plasma simulations
  - StREEQ method accounts for discretization and stochastic noise using multi-fitting approach
  - Achieved excellent results for electron diode code verification problems
  - Currently being used to improve simulations B-dot experiments

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