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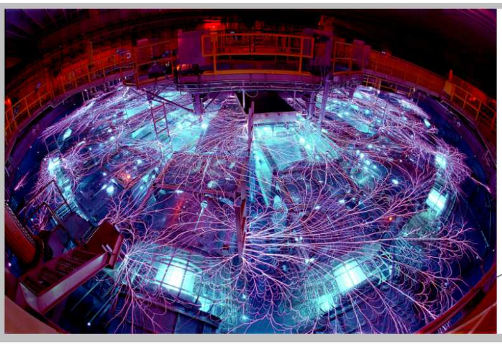

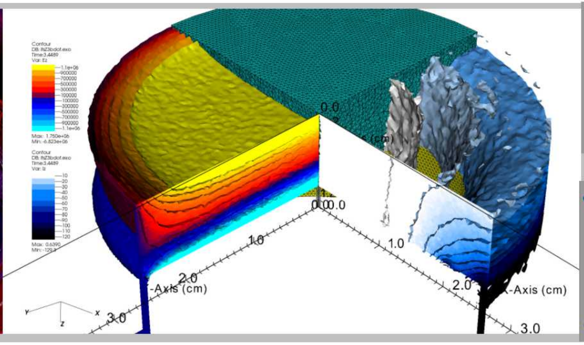

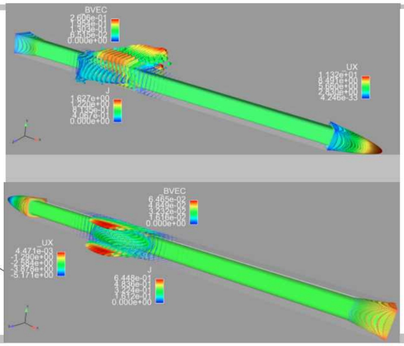

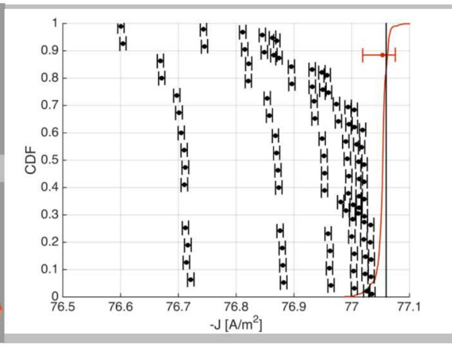

Uncertainty Estimation Applied to Verification and Validation (V&V): SAND2015-321293

Keith Cartwright, Gregg Radtke, and Eric Cyr

Sandia National Laboratories, New Mexico

Sandia National Laboratories Advanced Electromagnetics

CCR Center for Computing Research

U.S. Department of Energy

NNSA National Nuclear Security Administration

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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

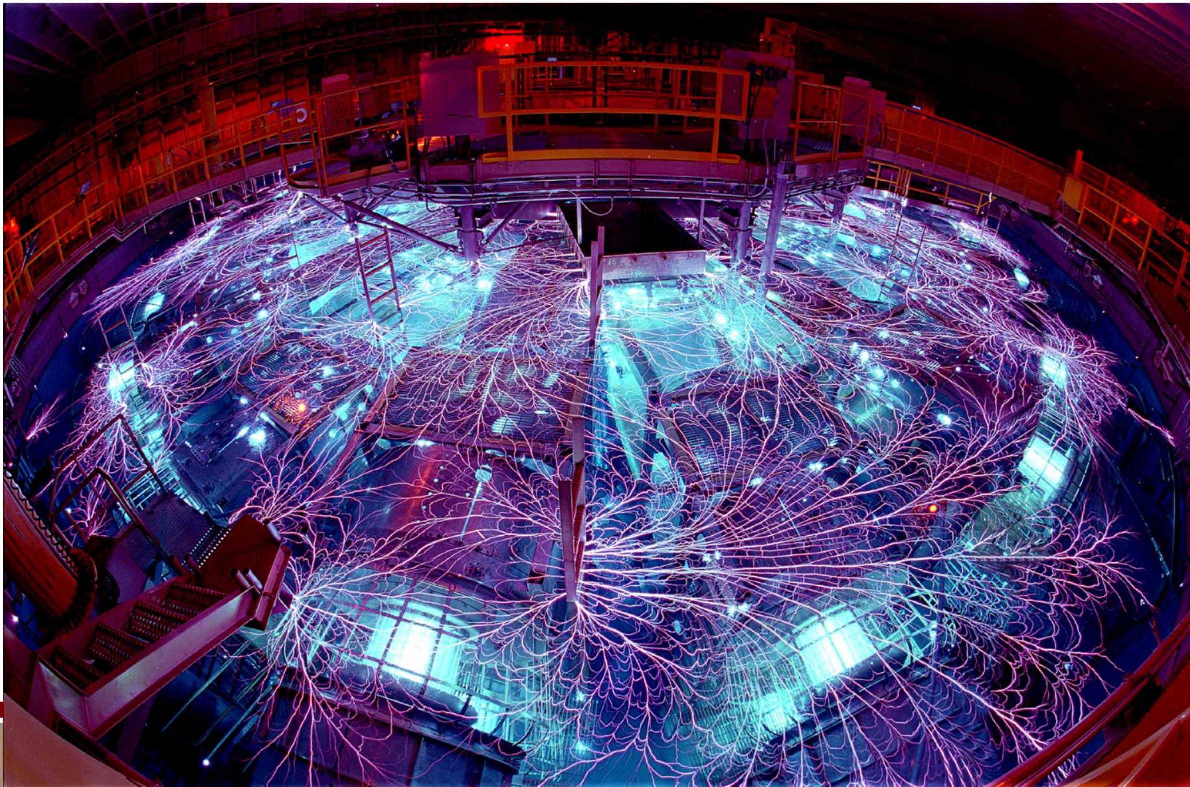
- That the weapons in America's stockpile would always work if called upon
- That the weapons would never, could never, detonate unintentionally; either as a result of accident, equipment failure, or even human malfeasance.

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.



Outline

- Verification and Validation
- Computer Simulation of Plasmas
- Radiation Induced Plasma Experimental Validation
- Advanced Uncertainty Quantification Methods
  - Embedded Forward and Adjoint Sensitivity Analysis
  - Numerical Error Estimation for Stochastic Code Output
- Conclusion

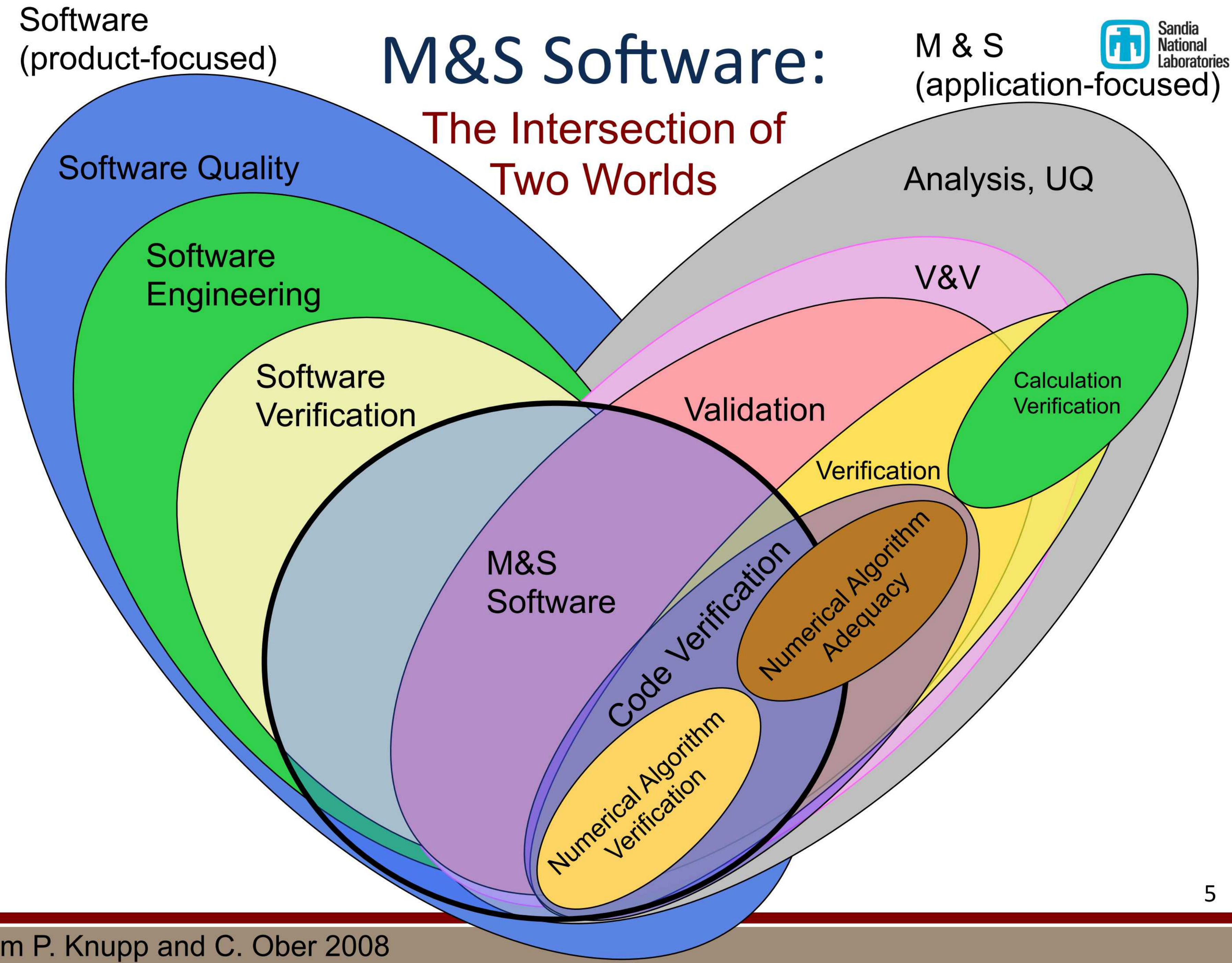
Balance of V&V and Importance

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

M&S Software:

The Intersection of Two Worlds



From P. Knupp and C. Ober 2008

Informal Definitions

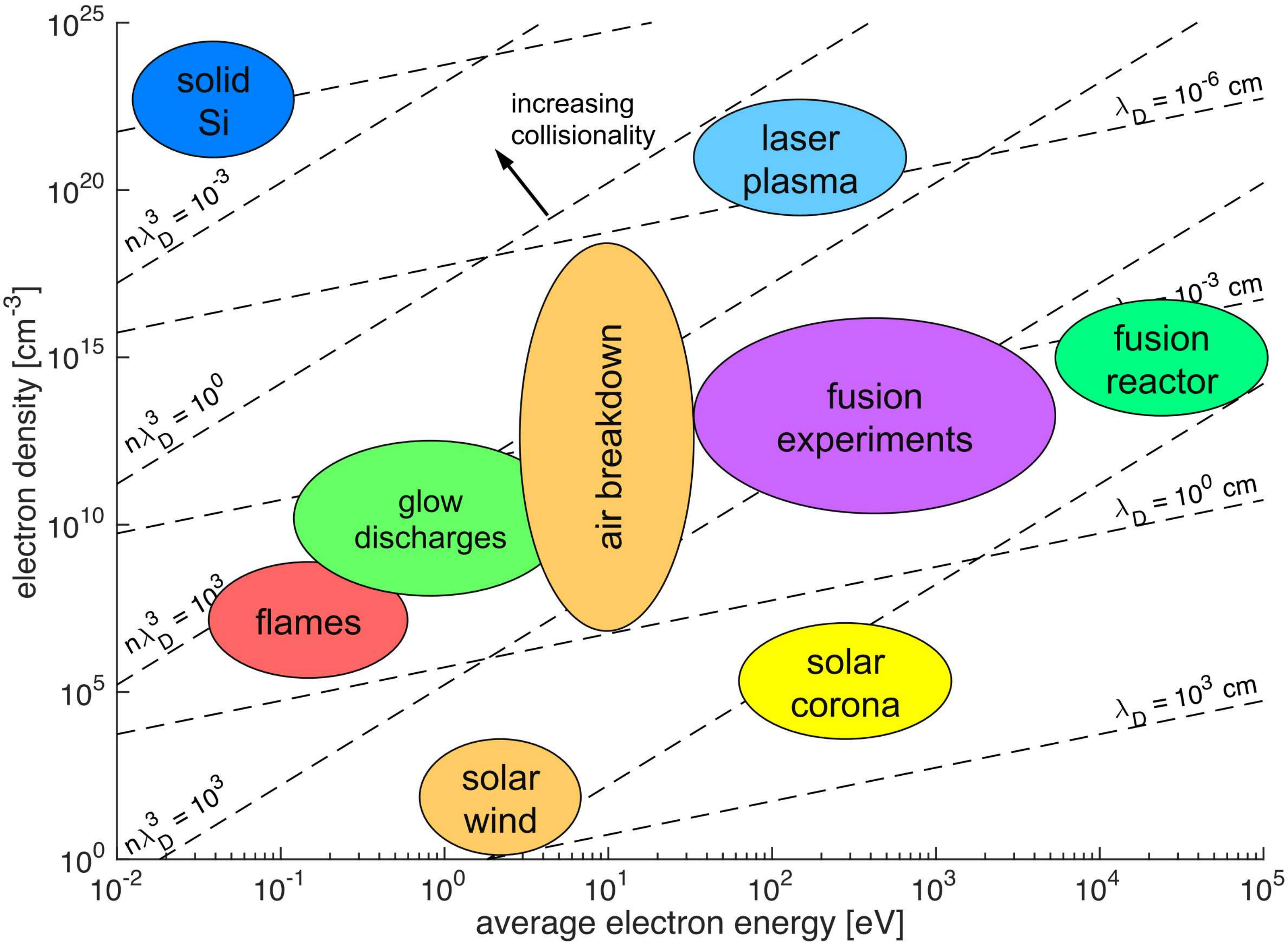
- **Verification:** assuring correct model implementation
  - Related to Software Quality Assurance (SQA)
- **Solution Verification:** assuring that the simulation converges as expected with numerical parameters
  - Easy for single physics, but hard for multi-physics problems
  - Monotonic convergence (near the converged solution) is the only type which is well understood mathematically
- **Benchmarking:** comparison of output from two or more simulation codes
  - Neither Validation nor Verification, but very useful

Informal Definitions (Cont.)

- **Validation:** comparing simulation to experiment
  - Tests that the correct model was implemented
- **Uncertainty Quantification:** estimation of uncertainties to allow for a true comparison between the simulation and experiment
  - Simulation uncertainties: numerical error, input parameter uncertainty, geometric tolerances, etc.
  - Experimental uncertainties

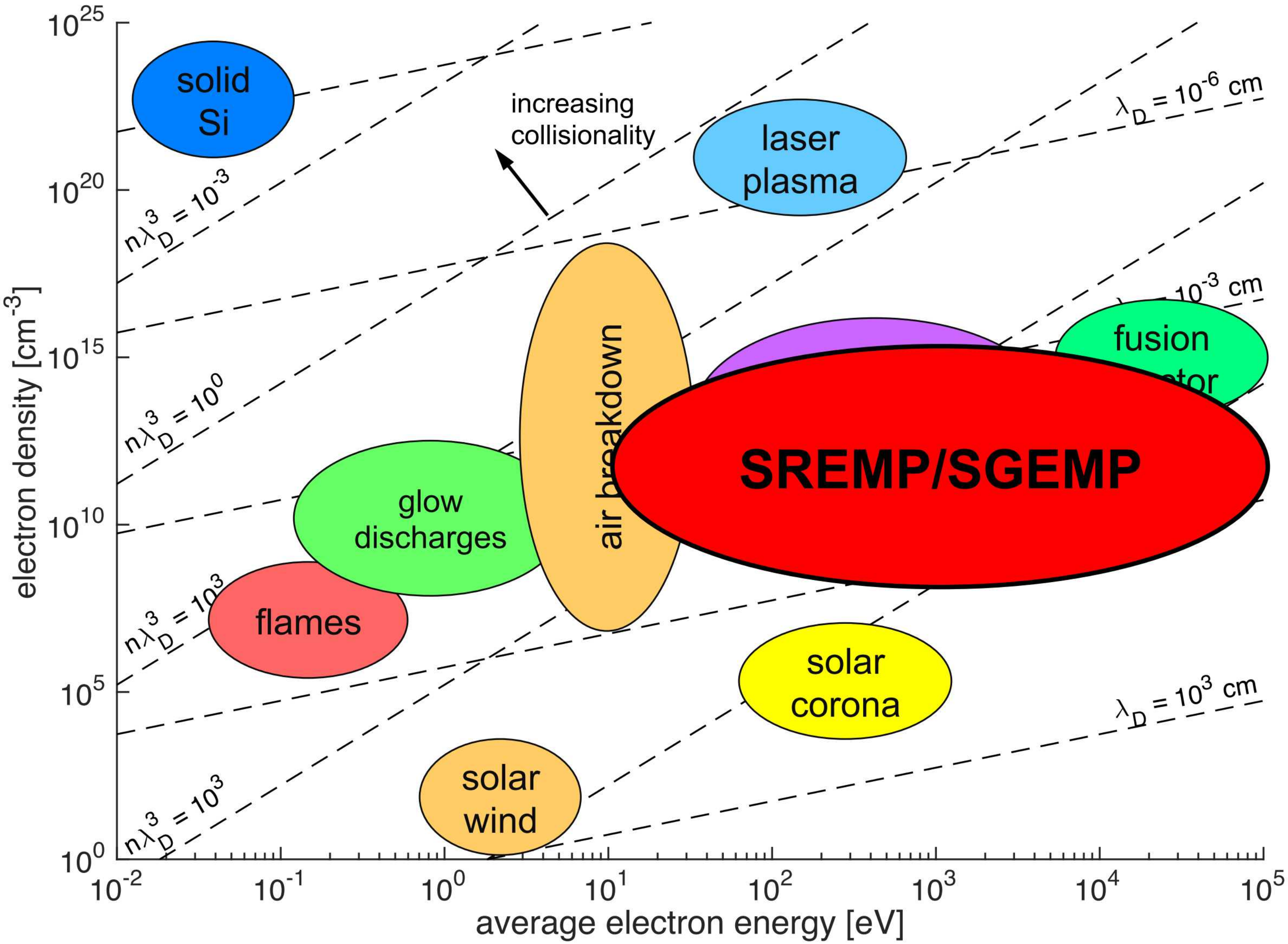
For more formal and exact definitions see "ASME V&V 20-2009" or "Verification and Validation in Scientific Computing" by Oberkampf and Roy

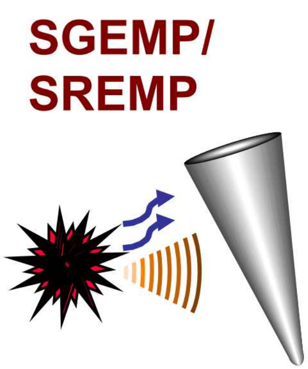
SGEMP/SREMP Plasma Regime



See, for example, Lieberman and Lichenberg (2005)

SGEMP/SREMP Plasma Regime





See, for example, Lieberman and Lichenberg (2005)

Plasma Equations

- Maxwell's equations

$$\underbrace{\nabla\times\mathbf{E}=-\frac{\partial\mathbf{B}}{\partial t}\qquad\nabla\times\mathbf{H}=\mathbf{J}+\frac{\partial\mathbf{E}}{\partial t}}_{\text{dynamical equations}}\qquad\underbrace{\begin{matrix}\nabla\cdot\mathbf{B}=0\\ \nabla\cdot\mathbf{D}=\rho\end{matrix}}_{\text{initial condition constraints}}\qquad\underbrace{\begin{matrix}\mathbf{D}=\varepsilon\mathbf{E}\quad\mathbf{J}=\sigma\mathbf{E}\\ \mathbf{B}=\mu\mathbf{H}\end{matrix}}_{\text{constitutive relations}}$$

- Relativistic Klimontovich equation
  - For each species *s* (electrons, ions, neutrals, photons, etc.)

$$N_s(\mathbf{x},\mathbf{u},t)=\sum_p\delta\left[\mathbf{x}-\mathbf{x}_{s,p}(t)\right]\delta\left[\mathbf{u}-\mathbf{u}_{s,p}(t)\right],\ \mathbf{u}=\mathbf{v}\Big/\sqrt{1-v^2/c^2}$$

$$\frac{\partial N_s(\mathbf{x},\mathbf{u},t)}{\partial t}+\mathbf{v}\cdot\nabla_{\mathbf{x}}N_s(\mathbf{x},\mathbf{u},t)+\underbrace{\frac{q_s}{m_s}(\mathbf{E}+\mathbf{v}\times\mathbf{B})\cdot\nabla_{\mathbf{v}}N_s(\mathbf{x},\mathbf{u},t)}_{\text{Lorentz force}}=\underbrace{\left[\frac{\partial N_s(\mathbf{x},\mathbf{u},t)}{\partial t}\right]_C}_{\text{collisions}}$$

$$\left.\begin{matrix}\rho(\mathbf{x},t)=\sum_s q_s\int d\mathbf{v}\ N_s(\mathbf{x},\mathbf{v},t)\\ \mathbf{J}(\mathbf{x},t)=\sum_s q_s\int d\mathbf{v}\ \mathbf{v}N_s(\mathbf{x},\mathbf{v},t)\end{matrix}\right\}\text{charge and currents in Maxwell's equations}$$

See, for example, Nicholson, Introduction to Plasma Theory (1983)

Boltzmann Equation

- Boltzmann equation
  - Distribution function: $N_s(\mathbf{x},\mathbf{u},t) = f_s(\mathbf{x},\mathbf{u},t) + \delta N_s(\mathbf{x},\mathbf{u},t)$
  - Fields: $\mathbf{E}(\mathbf{x},t) = \langle \mathbf{E}(\mathbf{x},t) \rangle + \delta\mathbf{E}(\mathbf{x},t)$, $\mathbf{B}(\mathbf{x},t) = \langle \mathbf{B}(\mathbf{x},t) \rangle + \delta\mathbf{B}(\mathbf{x},t)$

$$\underbrace{\frac{\partial f_s(\mathbf{x},\mathbf{u},t)}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} f_s(\mathbf{x},\mathbf{u},t) + \frac{q_s}{m_s}\left(\langle\mathbf{E}\rangle + \mathbf{v}\times\langle\mathbf{B}\rangle\right)\cdot\nabla_{\mathbf{v}} f_s(\mathbf{x},\mathbf{u},t)}_{\text{Vlasov equation}}$$

$$= \underbrace{-\frac{q_s}{m_s}\left\langle\left(\delta\mathbf{E} + \mathbf{v}\times\delta\mathbf{B}\right)\cdot\nabla_{\mathbf{v}} N_s(\mathbf{x},\mathbf{u},t)\right\rangle}_{\text{Coulomb collisions}} + \underbrace{\left\langle\frac{\partial N_s(\mathbf{x},\mathbf{u},t)}{\partial t}\right\rangle_C}_{\text{molecular/atomic collisions}}$$

See, for example, Nicholson, Introduction to Plasma Theory (1983)

Computer Simulation of Plasmas

Particle-In-Cell (PIC) Method

- Monte Carlo sampling of the Boltzmann Equation
  - Particle mover solves: for fixed **E**, **B** $\frac{\partial N_s}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} N_s + \frac{q_s}{m_s}\left(\mathbf{E}+\mathbf{v}\times\mathbf{B}\right)\cdot\nabla_{\mathbf{v}} N_s = 0$
  - Collisions sampled probabilistically: $\frac{\partial N_s}{\partial t} = \left[\frac{\partial N_s}{\partial t}\right]_C$
  - Self-consistent FEM solution of Maxwell's Equations based on interpolated ρ, **J**
- Features:
  - Simulates plasma kinetically
  - Computationally expensive:
    - Must resolve Debye length: $\Delta x \le \lambda_D = \sqrt{\varepsilon_0 k T_e / n_e e^2}$
    - Must resolve plasma frequency and cyclotron frequency
    - Electromagnetic PIC must resolve light speed CFL: $\Delta t \le \Delta x / c$

Computer Simulation of Plasmas

Multi-fluid approximation

- Moments of Boltzmann equation: $\int d\mathbf{v},\ \int d\mathbf{v}\ \mathbf{v}, \ldots,$ etc.

$$\frac{\partial n_s}{\partial t} + \nabla\cdot(n\mathbf{u}) = \left[\frac{\partial n_s}{\partial t}\right]_C$$

$$m_s n_s\left(\frac{\partial \mathbf{u}_s}{\partial t} + \mathbf{u}_s\cdot\nabla\mathbf{u}_s\right) = -\nabla p_s + q_s n_s\left(\mathbf{E} + \mathbf{u}_s\times\mathbf{B}\right) + m_s n_s\left[\frac{\partial \mathbf{u}_s}{\partial t}\right]_C$$

$$\frac{\partial \varepsilon_s}{\partial t} + \mathbf{u}_s\cdot\nabla p_s = q_s n_s \mathbf{u}_s\cdot\mathbf{E} + \left[\frac{\partial \varepsilon_s}{\partial t}\right]_C,\quad \varepsilon_s = \frac{p_s}{\gamma_s - 1} + \frac{m_s n_s u_s^2}{2}$$

- Higher-order closures are possible
  - See e.g. WARPX code, Uri Shumlak, U. Washington
- Solution methods: FEM, FD, etc.
- Hybrid (kinetic-fluid) methods are possible

Radiation Induced Plasma Validation Experiment

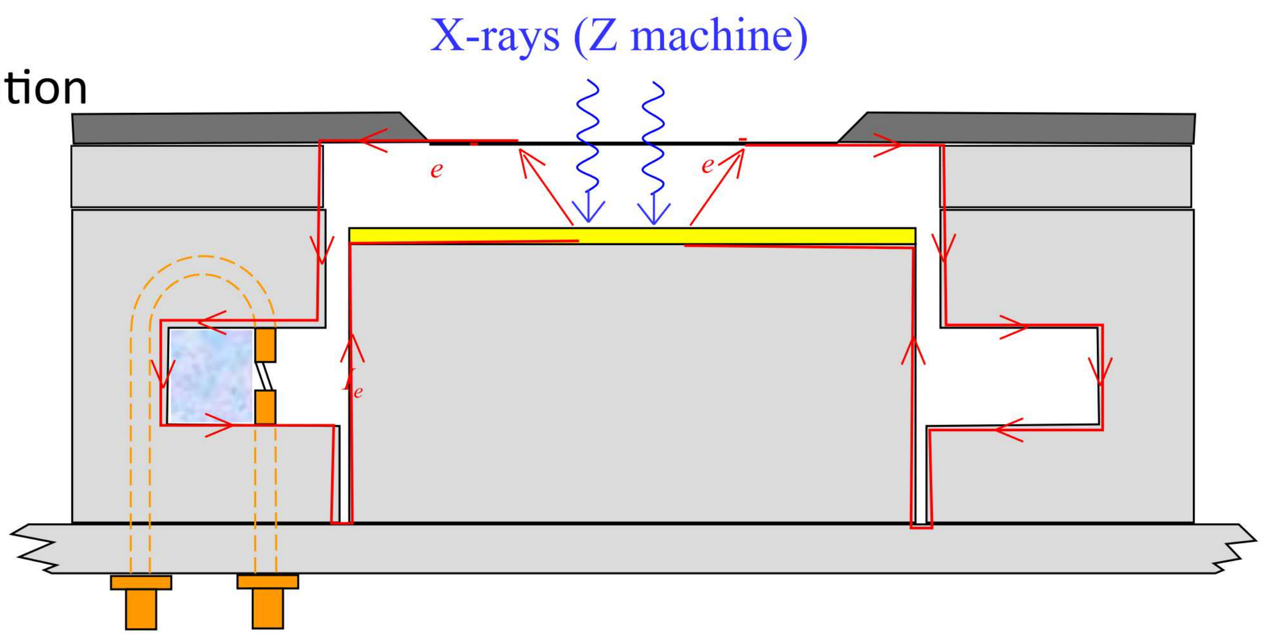
Keith Cartwright, *Electromagnetic Theory Group*

Epistemic uncertainties:

- Gas pressure
- Geometry
- Low-energy extrapolation photo-electrons
- X-ray spectrum
- Gas cross-section
- Secondary electrons
- Backscatter electrons

Aleatory (normally distributed) uncertainties:

- Yield



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

Yield and Pulse Shape Uncertainty

High Yield Cases

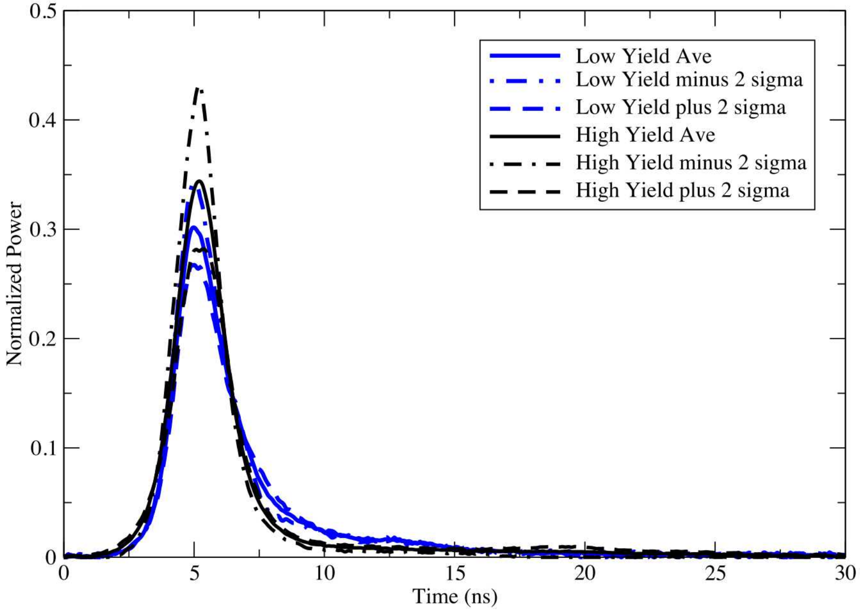
Shot Number	Yield, >5 keV (kJ)
Z2234	79 ± 12
Z2235	73 ± 11
Z2236	71 ± 11
Z2237	89 ± 16
Z2328	80 ± 11
Z2329	78 ± 8.3
Average	78 ± 12

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)

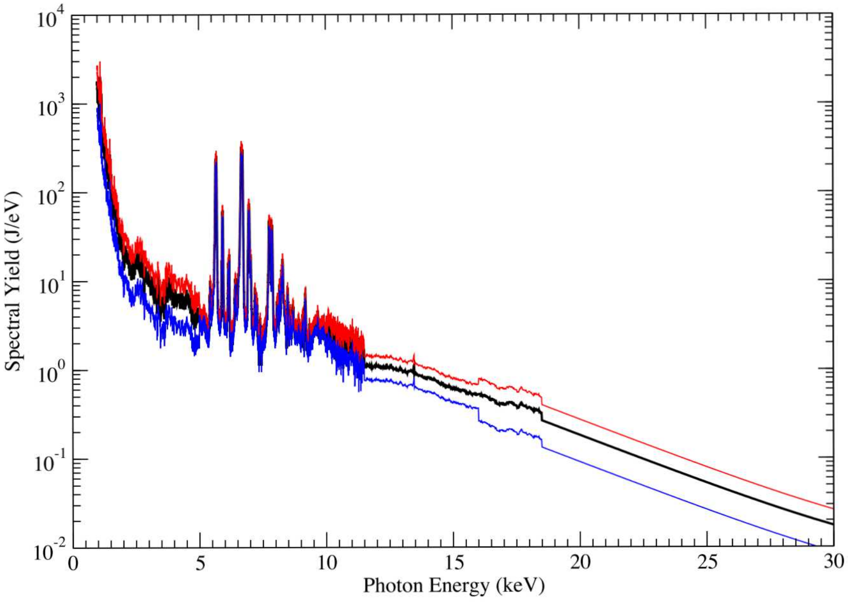
Pulse Shape

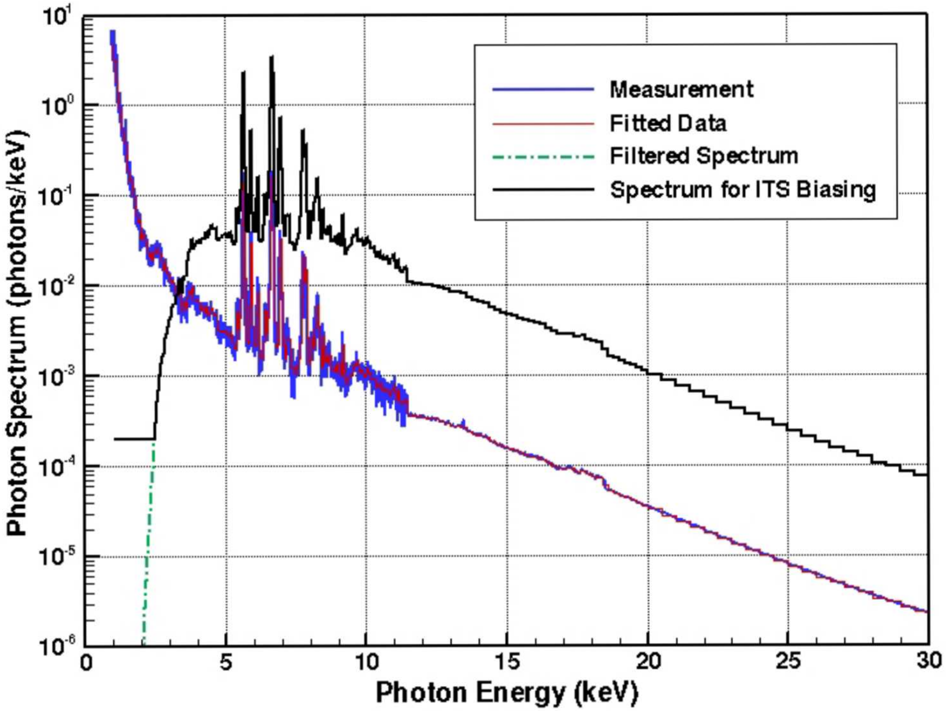


Most important source of uncertainty in simulations shown on following slides

Z-Spectrum

- Efficient source sampling with a biased spectrum
- Filtered spectrum has average energy of 7.1 keV rather than 1.5 keV
- Set floor for photon energy < 2.5 keV to avoid over-biasing

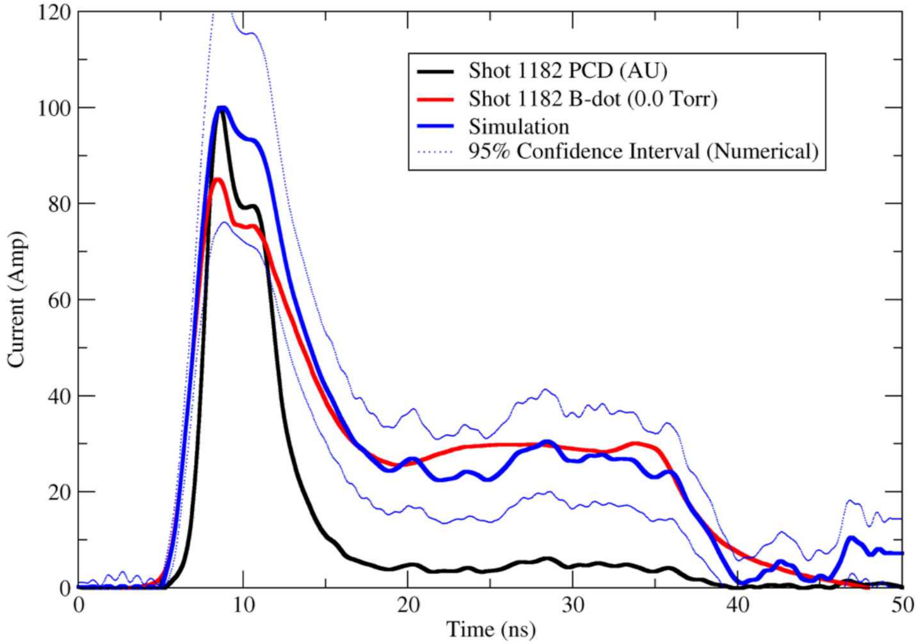




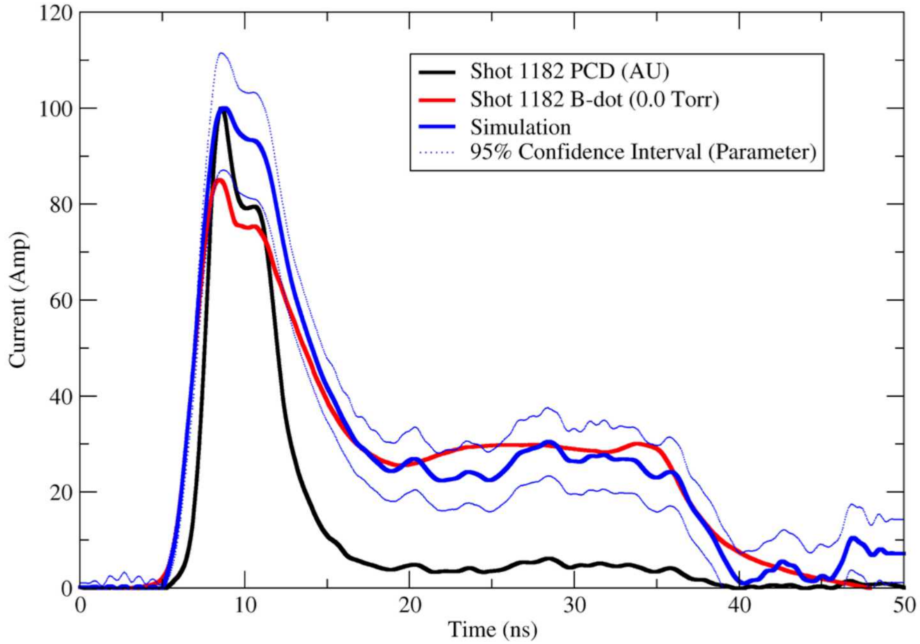
B-dot Vacuum Physics

- Space charge limited emission dominates the whole radiation pulse
  - Stiff numerical solution
- Uncertainty dominated by radiation transport
  - Distribution and flux of emitted electrons

Numerical Uncertainty

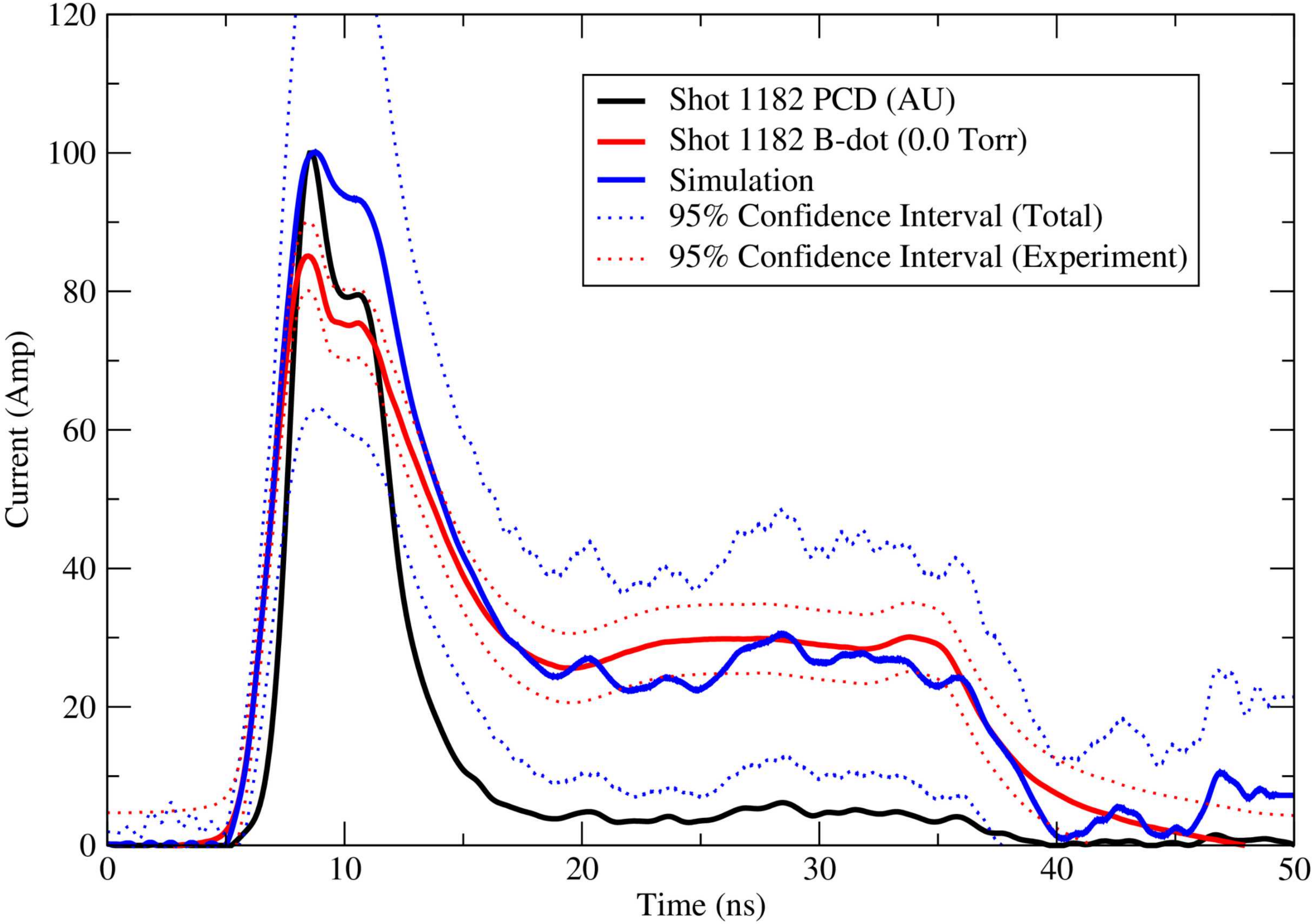


Epistemic and Aleatory Uncertainty



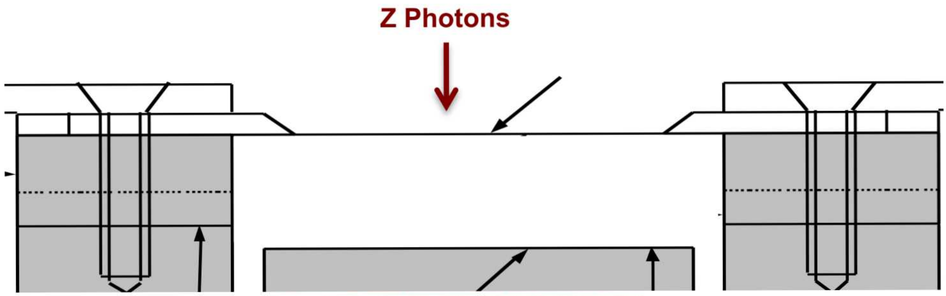
B-dot error is ±5 Amps

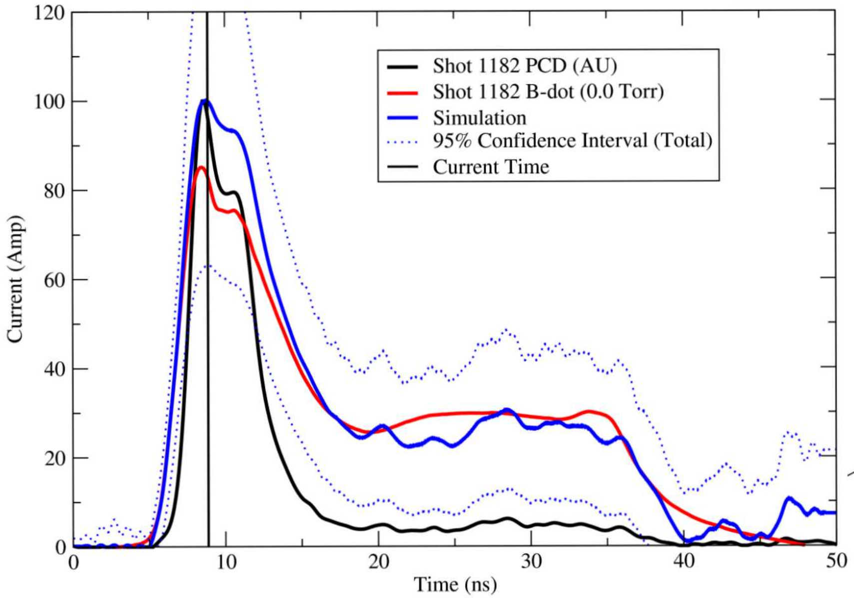
Vacuum Shot Simulation / Experiment Agreement

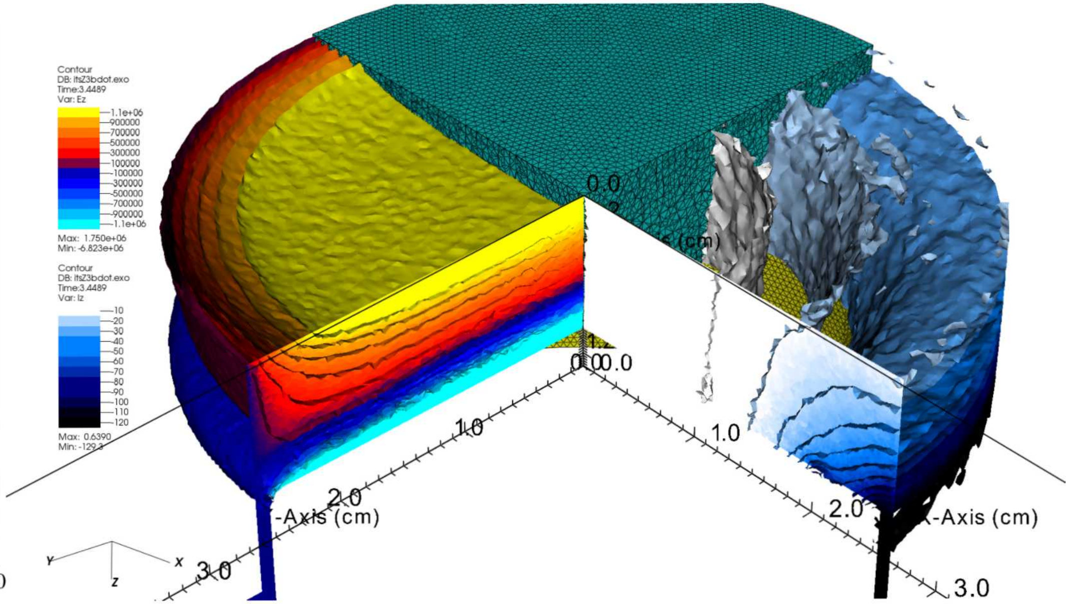


Maximum Surface Electric Fields

- Shot 1182 B-dot 0.0 Torr-8.8ns





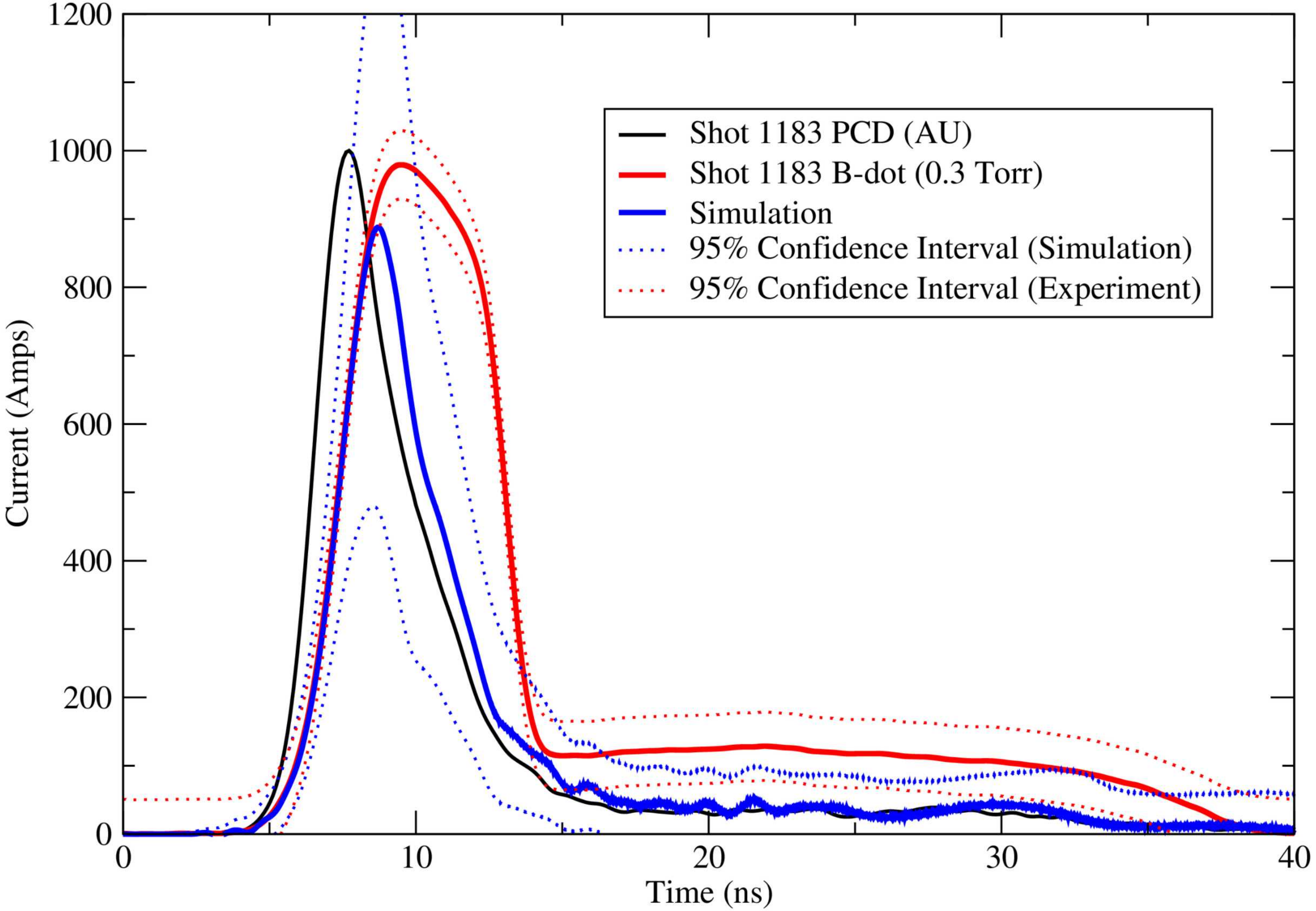


B-dot Gas physics

N_2 pressures 0.3 Torr

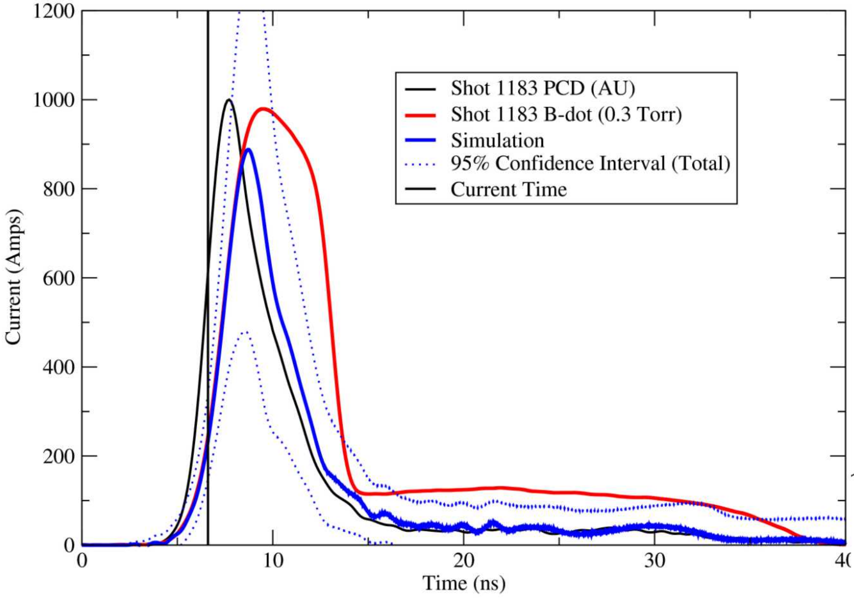
- During the rise of the radiation pulse the electrons are space charge limited
  - Ion neutralization allows for more current than the vacuum case
  - Uncertainty due to knowledge of cross sections
- Electric field reversal occurs on the wall around the time of the radiation maximum
  - The field reversal allows for additional effects to influence the simulation
    - Lower energy photo-electrons
      - Uncertainty is larger for lower energy radiation transport
    - True (thermal) secondary electron
      - Uncertainty of true secondaries yield
- Uncertainty of initial radiation
  - Distribution and flux of emitted electrons

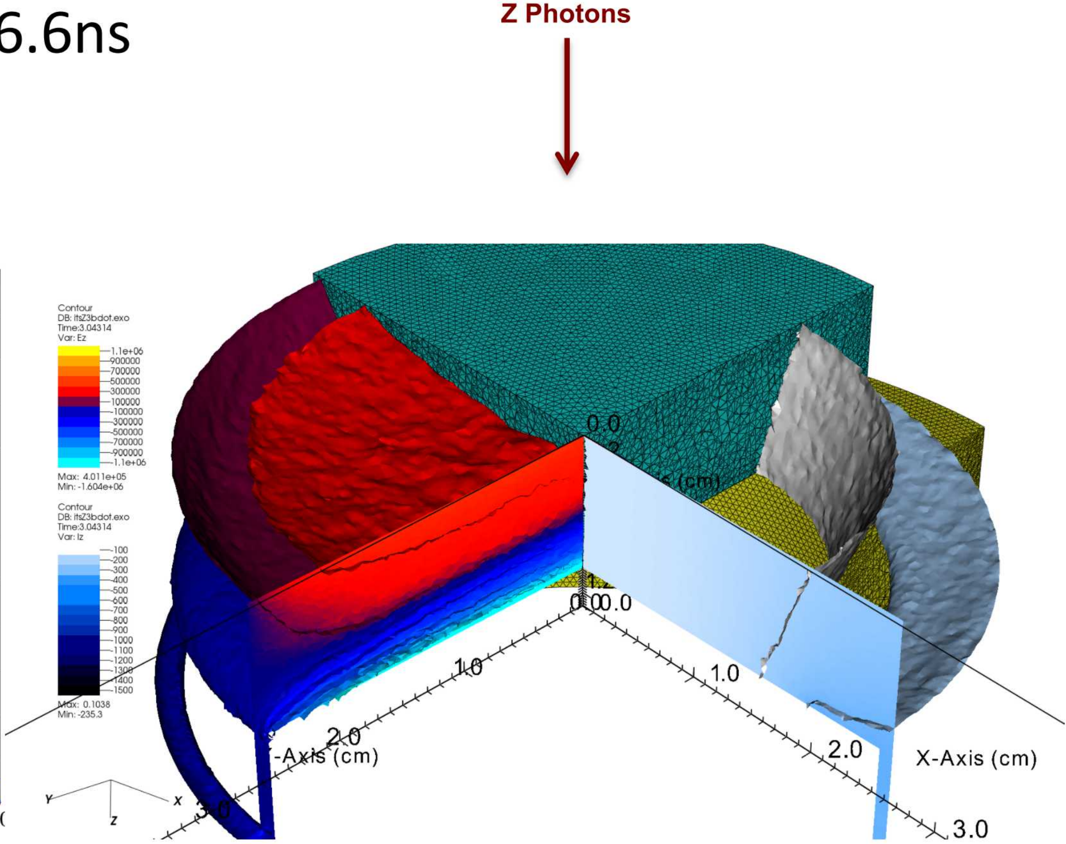
Gas Shot Simulation / Experiment Disagreement



Maximum Surface Electric Fields

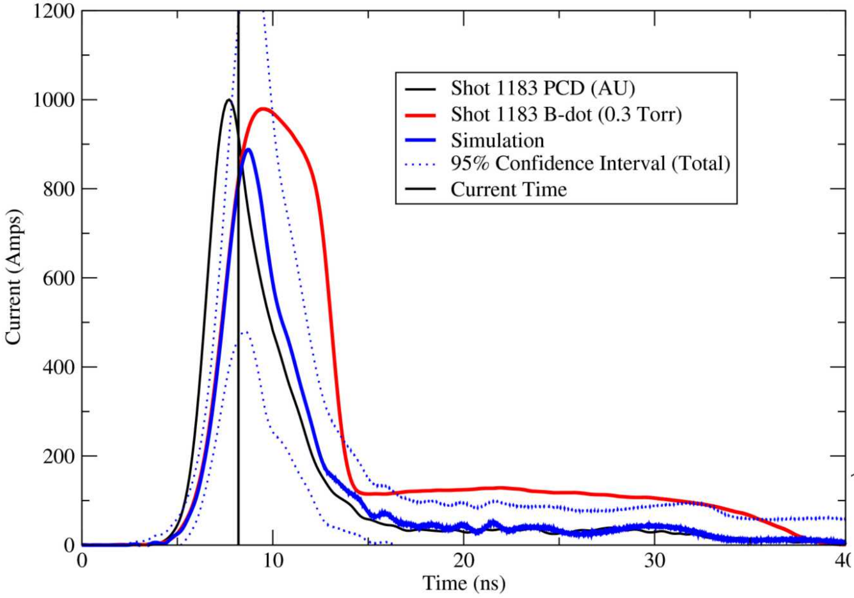
- Shot 1183 B-dot 0.3 Torr-6.6ns

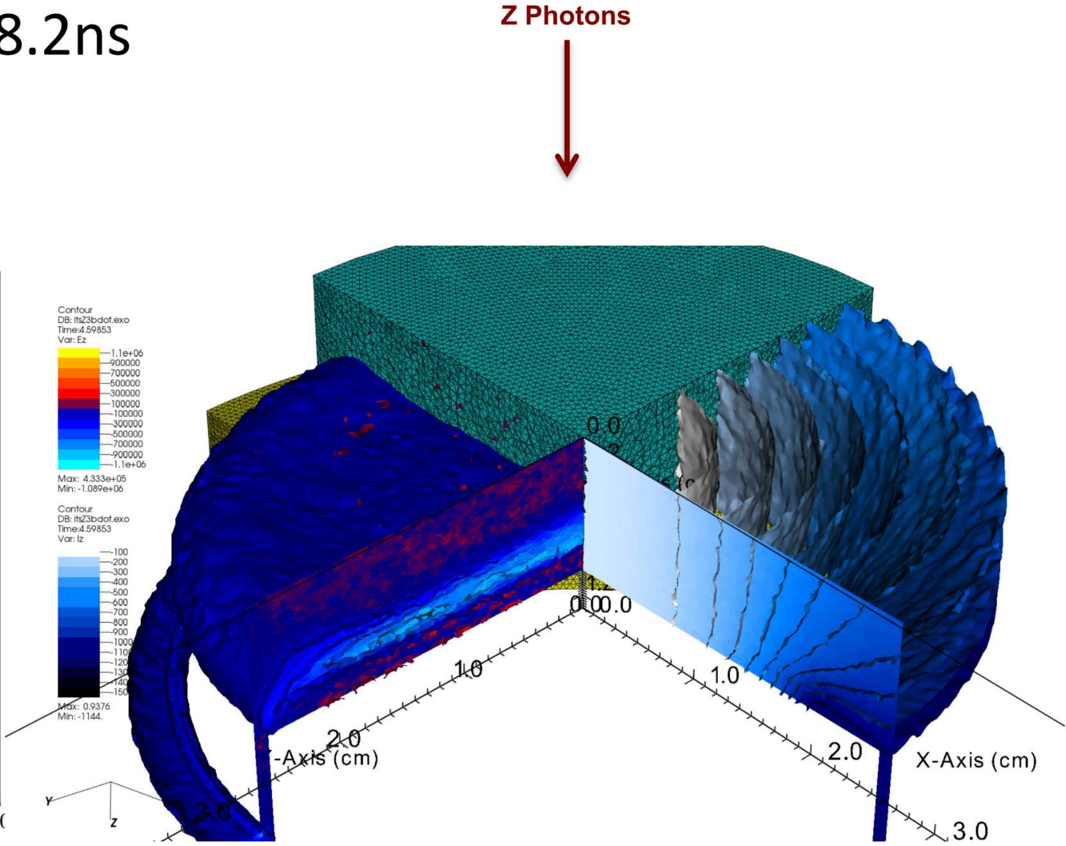




Electric Field Reversal on the Graphite Surface

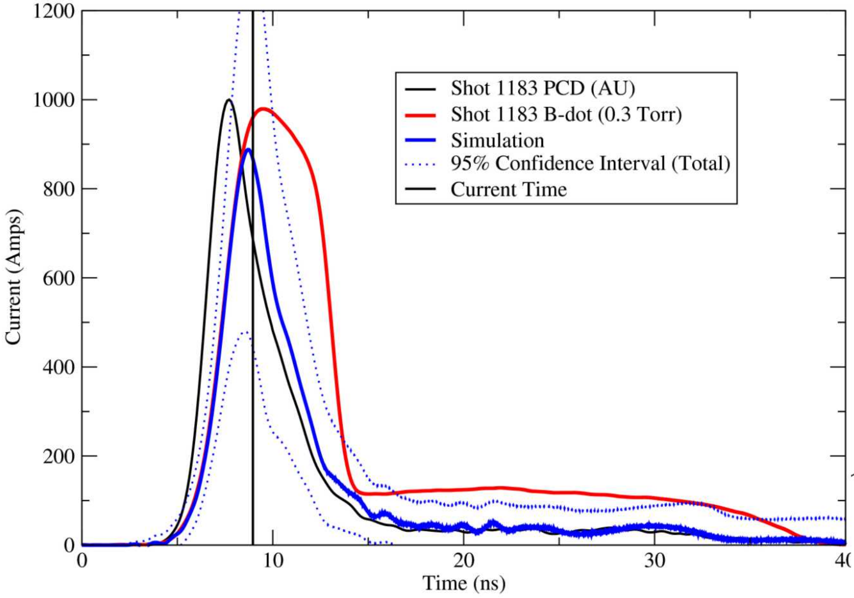
- Shot 1183 B-dot 0.3 Torr-8.2ns

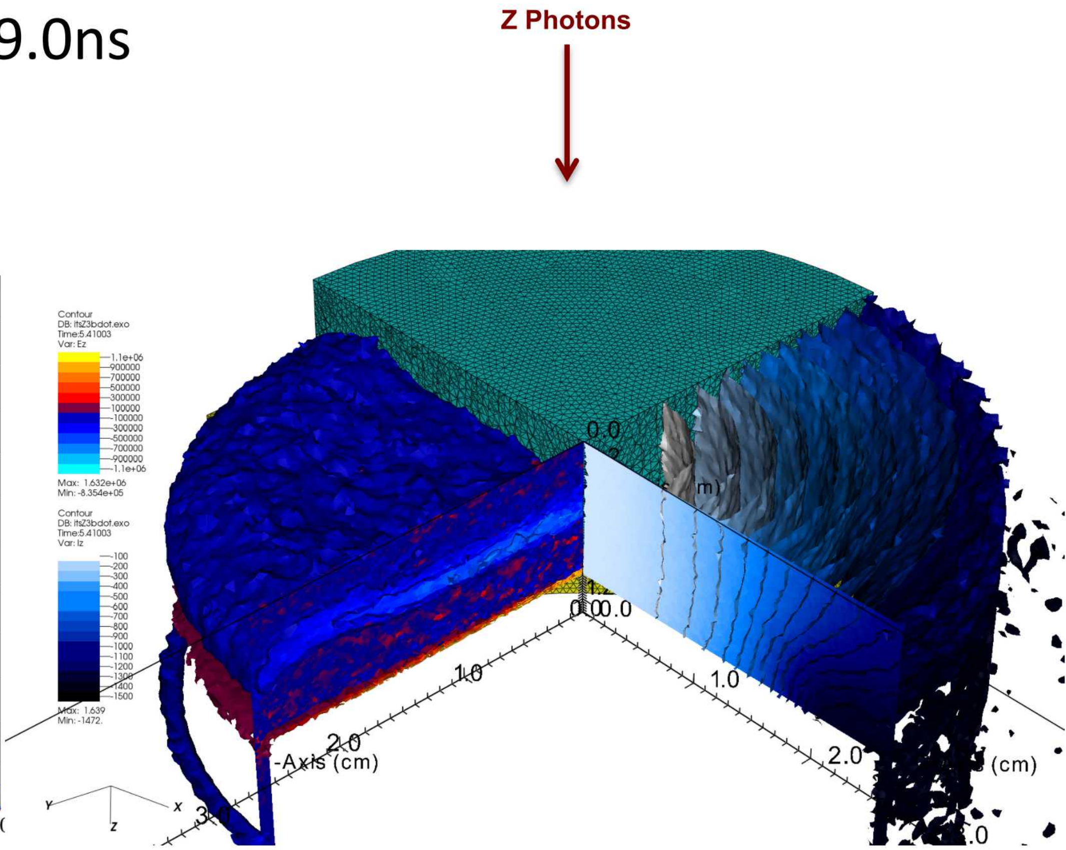




Electric Field Reversal on the Gold Surface

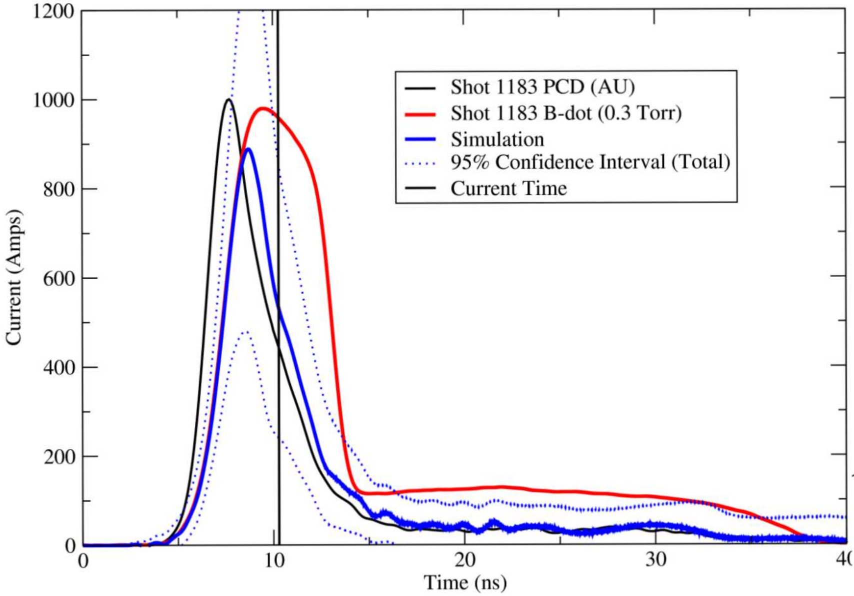
- Shot 1183 B-dot 0.3 Torr-9.0ns



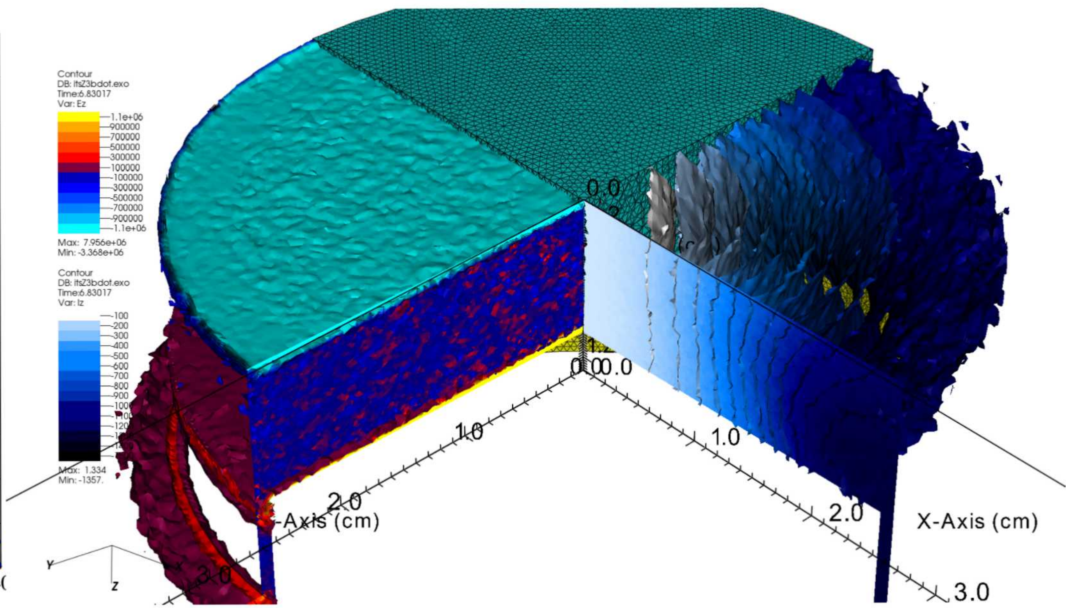


Plasma Diffusion to the Walls

- Shot 1183 B-dot 0.3 Torr-10.3ns



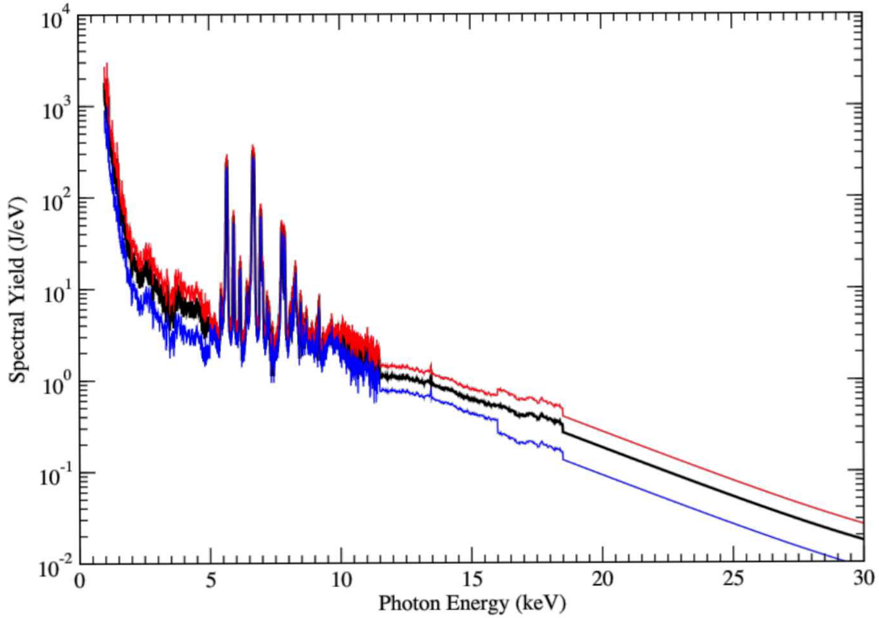
Z Photons



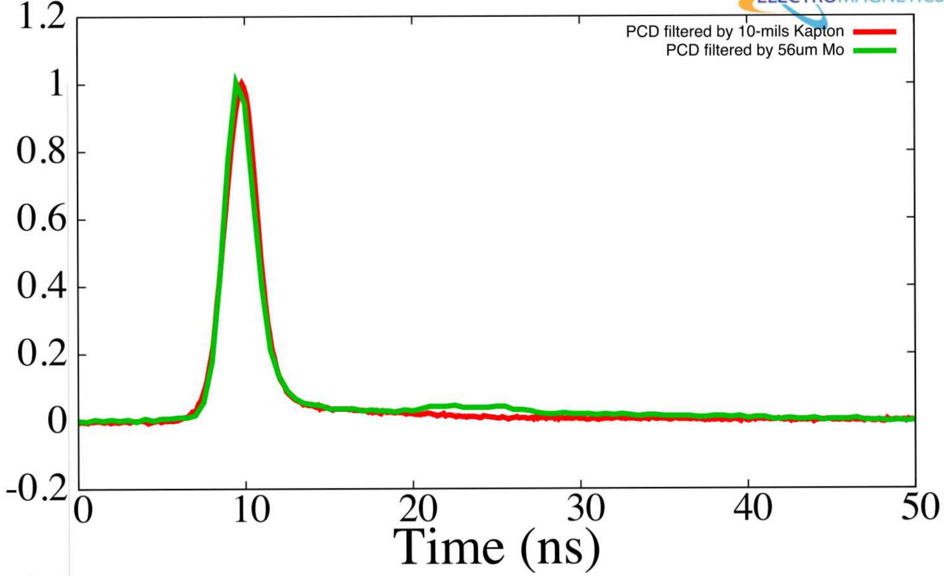
What Was Left Out

- Currently we know that
  - Blow-off / out gassing is more of an issue than was previously expected
    - Function of fluence
  - Time dependent higher energy spectrum is different than lower energy spectrum
- Indirect experimental evidence is on the next few slides

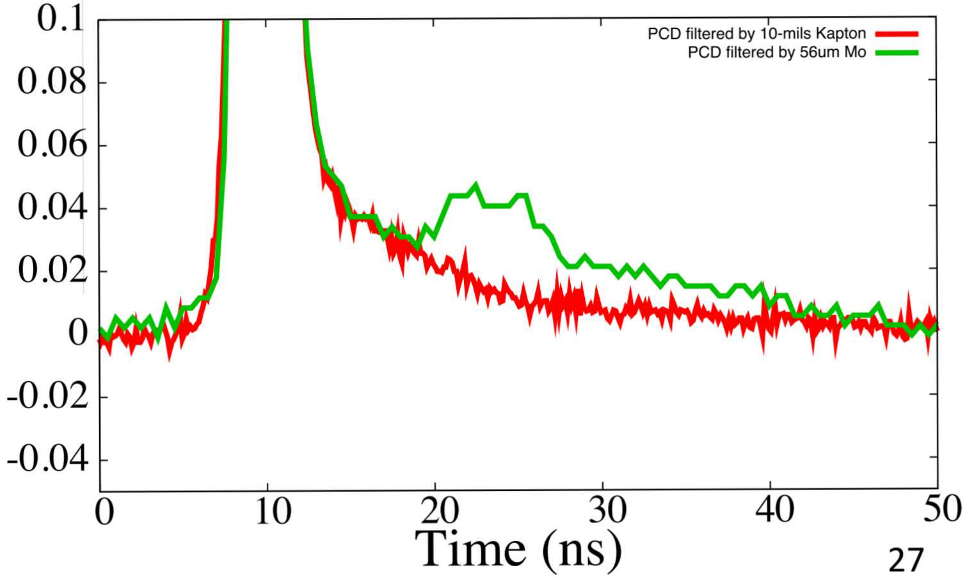
Z-Spectrum



Spectral Yield (J/eV)
Photon Energy (keV)

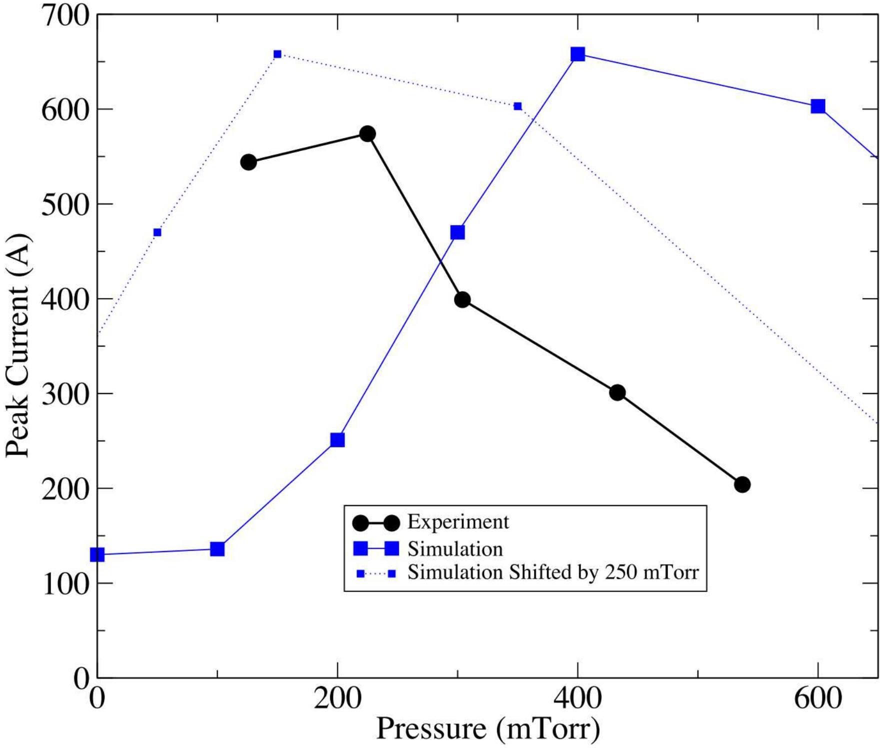


PCD filtered by 10-mils Kapton
PCD filtered by 56um Mo
Time (ns)

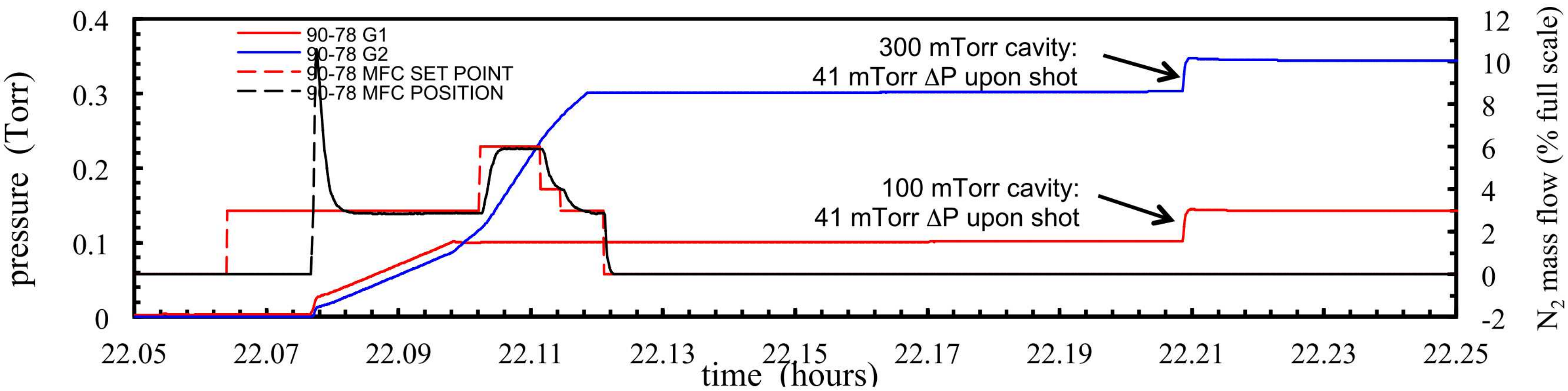


PCD filtered by 10-mils Kapton
PCD filtered by 56um Mo
Time (ns)

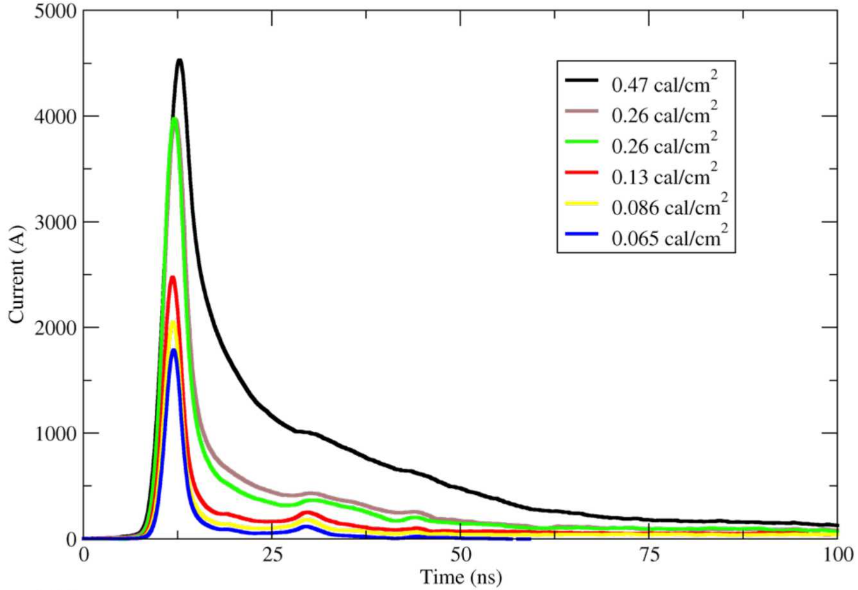
Gas Pressure

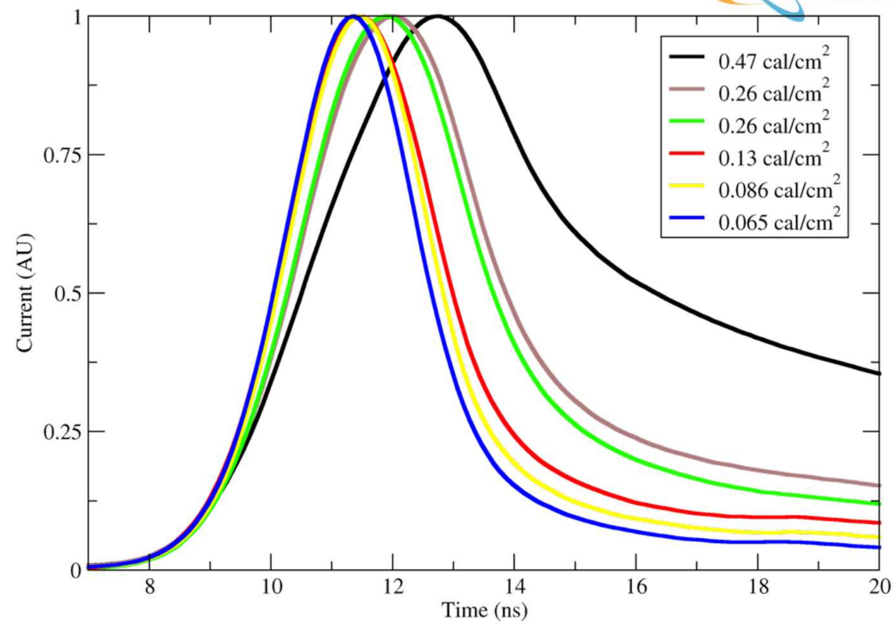


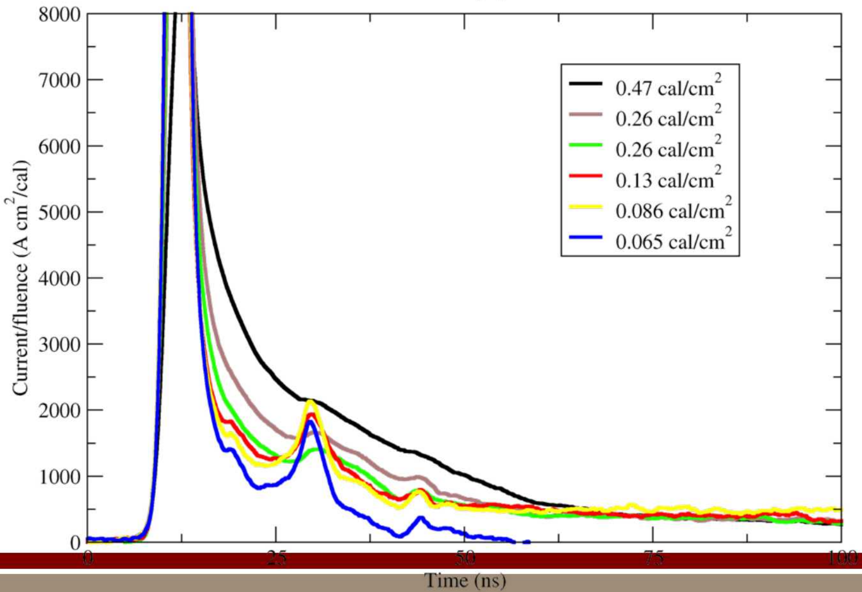
- The pressure may increase during X-ray pulse
- NIF data suggests a pressure rise of 250 mTorr or more
  - Calibration of gas pressure in progress
- The data from Z and NIF are being used together to make progress



Time Scales and Fluence for Blow Off







- Effects can be seen at ~0.25 cal/cm^2
- Tail is dominated by blow off at ~0.5 cal/cm^2
- < 1 ns before the influence of blow off can be seen in the current

Advanced Methods for Uncertainty and Error Estimation for Plasma Simulations

- Inherent difficulties:
  - Computationally expensive, large scale simulations
  - Multiple length scales, time scales, regimes
  - Multiple numerical discretization parameters
  - PIC plasma: stochastic noise $\sim 1/\sqrt{N}$ (a feature of Monte Carlo sampling)
- Embedded Sensitivity Analysis
  - Fluid plasma: forward and adjoint sensitivities
  - PIC plasma: forward sensitivities
- Numerical Error Estimation
  - Fluid plasma: existing methods (i.e. GCI)
  - PIC plasma: Stochastic Richardson Extrapolation Based Error Quantification (StREEQ)

Embedded Sensitivity Analysis

Eric Cyr, *Center for Computing Research*

- Motivation: Quantities of Interest (*Y* = QoI) can be more important than the PDE solution $u(x)$
- Examples:
  - Volume integrated quantity $Y(u,\theta) = \int_{\Omega_0 \subset \Omega} g(x,\theta)\, u(x)\, dV$
  - Surface integrated quantity $Y(u,\theta) = \int_{\Gamma_0 \subset \partial\Omega} \mathbf{F}(u,x,\theta) \cdot \mathbf{n}\, ds$
  - Point evaluated quantity $Y(u,\theta) = \int_{\Omega} \delta(x - x_0)\, u(x)\, dV$
- PDE solution has input parameter θ and satisfies: $f(u,\theta) = 0$
- Goal: find sensitivity of QoI to changes in parameter:

$$\frac{d}{d\theta} Y\left(u(\theta),\theta\right) = ?$$

- Embed sensitivity evaluation in code to evaluate concurrently with numerical solution

Forward Sensitivity Analysis

- Chain rule $\frac{d}{d\theta} Y(u,\theta) = \left(\frac{\partial Y}{\partial u}\right)^T \frac{\partial u}{\partial \theta} + \frac{\partial Y}{\partial \theta}$
- Unknown $\partial u / \partial \theta$ is computed from solution manifold $f(u,\theta) = 0$

$$\frac{d}{d\theta} f(u,\theta) = \underbrace{\frac{\partial f}{\partial u}}_{\text{Jacobian}} \cdot \frac{\partial u}{\partial \theta} + \underbrace{\frac{\partial f}{\partial \theta}}_{\text{extra computation}} = 0$$

- Forward sensitivity algorithm
  - Solve $f(u,\theta)$ for u
  - Solve $\frac{\partial f}{\partial u} \frac{\partial u}{\partial \theta} = -\frac{\partial f}{\partial \theta}$ for $\frac{\partial u}{\partial \theta}$
- One additional solve for each parameter θ
- Efficient for few parameters, costly for fields approximated on mesh
- Colleagues pursuing forward sensitivities for PIC plasma:
  Rich Lehoucq, Steve Bond, and Drew Kouri at Sandia New Mexico

Adjoint Sensitivity Analysis

- Sensitivity: $\frac{d}{d\theta} Y(u,\theta) = \left(\frac{\partial Y}{\partial u}\right)^T \frac{\partial u}{\partial \theta} + \frac{\partial Y}{\partial \theta}$ $\qquad \frac{d}{d\theta} f(u,\theta) = \frac{\partial f}{\partial u} \cdot \frac{\partial u}{\partial \theta} + \frac{\partial f}{\partial \theta} = 0$

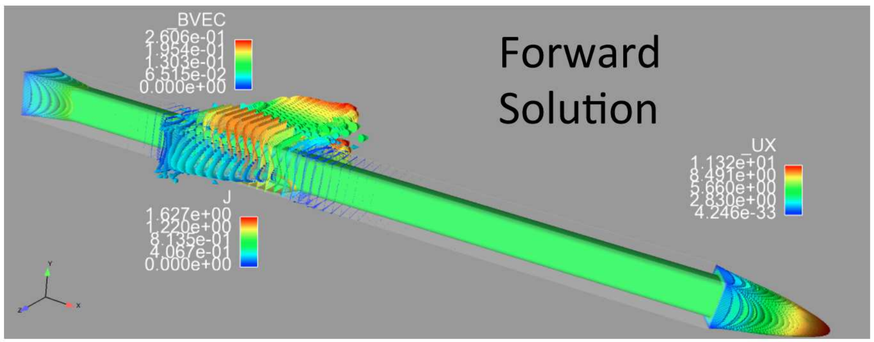
$$= -\left(\frac{\partial Y}{\partial u}\right)^T \left(\frac{\partial f}{\partial u}\right)^{-1} \frac{\partial f}{\partial \theta} + \frac{\partial Y}{\partial \theta} = -\underbrace{\left[\left(\frac{\partial f}{\partial u}\right)^{-T} \frac{\partial Y}{\partial u}\right]^T}_{\text{Adjoint solution } = w^T} \frac{\partial f}{\partial \theta} + \frac{\partial Y}{\partial \theta}$$

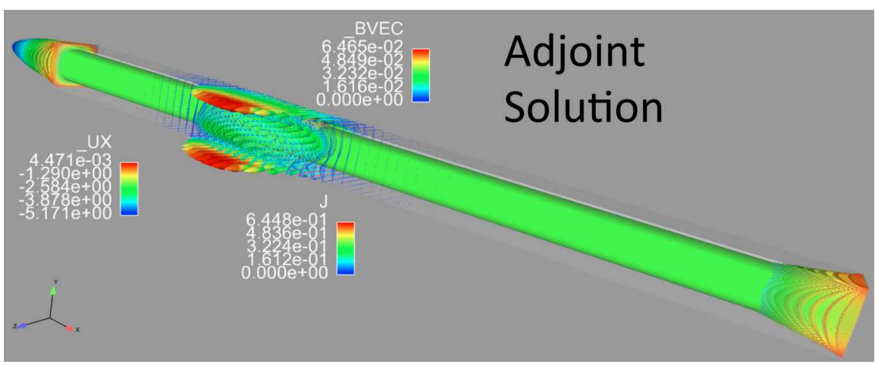
- Adjoint sensitivity algorithm
  - Solve $f(u,\theta)$ for u
  - Solve $\left(\frac{\partial f}{\partial u}\right)^T w^T = \frac{\partial Y}{\partial u}$ for w
- Must solve “dual problem” backwards in time!
- Additional solve for each QOI
- More efficient for many parameters and few QoI

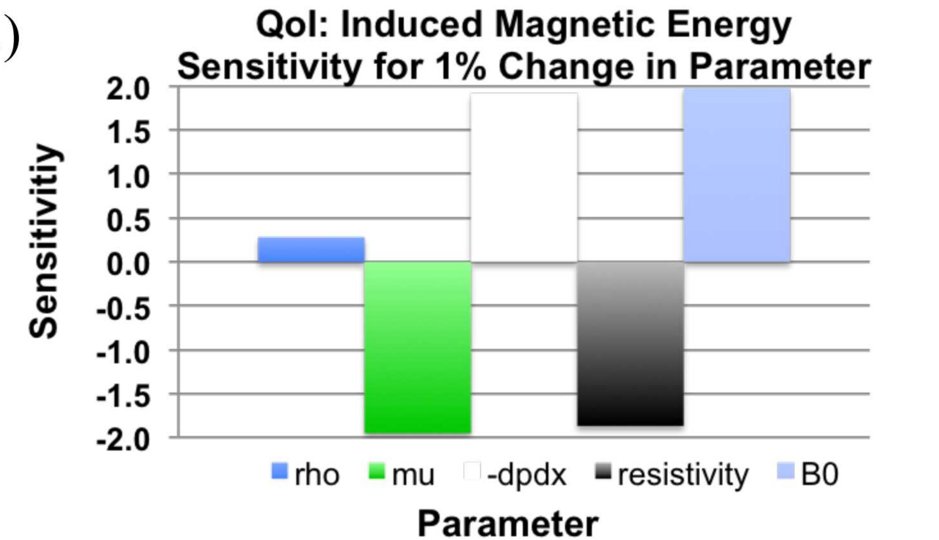
Adjoint Error-Estimation and Sensitivities for 3D MHD Generator (*Re* ~ 2500, Re_m ~ 10, *Ha* = 5)

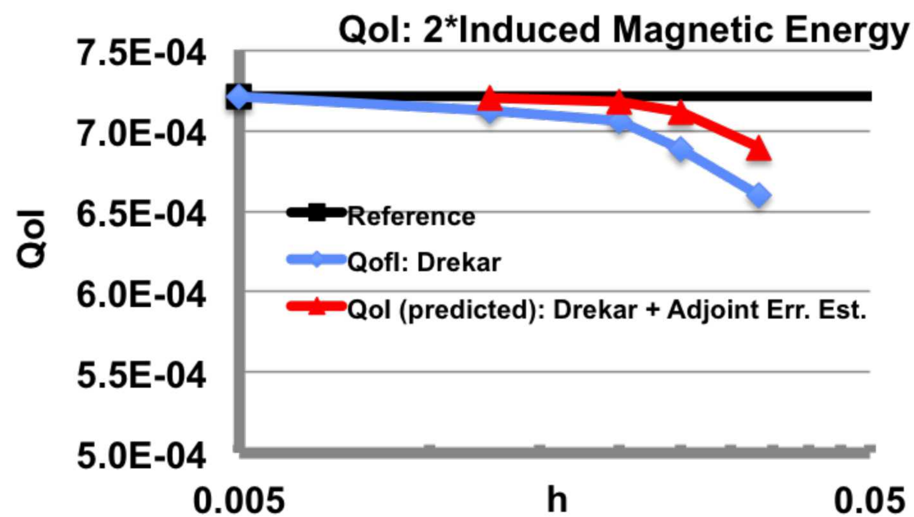
- QoI: Induced Magnetic Energy (M.E.)

$$\mathbf{M.E.} = \frac{\int_\Omega \frac{1}{2\mu_0}(B_x^2 + B_z^2)d\Omega}{\mathrm{Vol}(\Omega)}$$









Using the Drekar code

in collaboration with: John Shadid, Tim Wildey, Eric Cyr, Roger Pawlowski, Edward Phillips

MHD Duct Flow: Hartmann Analytic Solution—Uncertainty Quantification

Sandia National Laboratories
CCR Center for Computing Research

MHD Duct flow (Re = 884; Re_m = 177; Ha = 90)

- QoI: Total Energy $\text{T.E.} = \int_\Omega \frac{1}{2}(u_x^2 + u_y^2)d\Omega + \int_\Omega \frac{1}{2\mu_0}(B_x^2 + B_y^2)d\Omega$
- Compare adjoint derivative to analytic

Physical Parameter	Analytic	Drekar / Adjoint	Rel. Err.
QoI: T.E.	21.9318	21.9634	0.15%
QoI Derivatives:			
Pressure Gradient (G_0)	-20.9318	-20.9753	0.21%
Dynamic Viscosity (μ)	-3972.97	-3979.72	0.17%
Density (ρ)	0.0	3.0e-3	-----
Resistivity (η)	778.574	779.988	0.18%

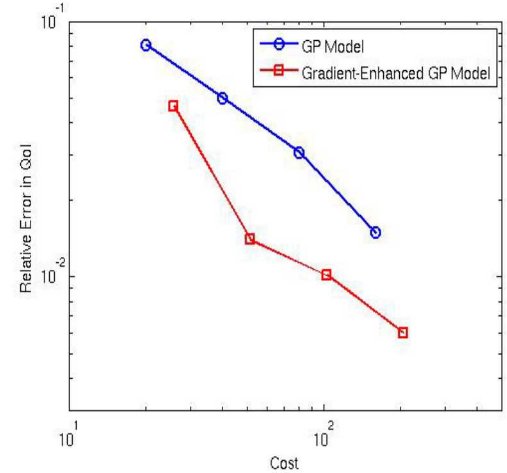
- For comparison - efficiency of FD derivative

  2pt FD derivative ~ N_θ x cost of Adjoint derivative

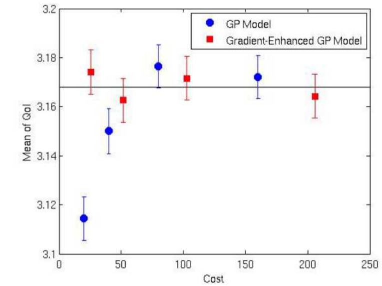
  3pt FD derivative ~ $2N_\theta$ x cost of Adjoint derivative

Using the Drekar code

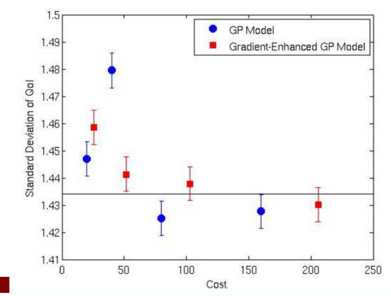
Adjoint Enhanced Surrogates



Mean



Std Dev

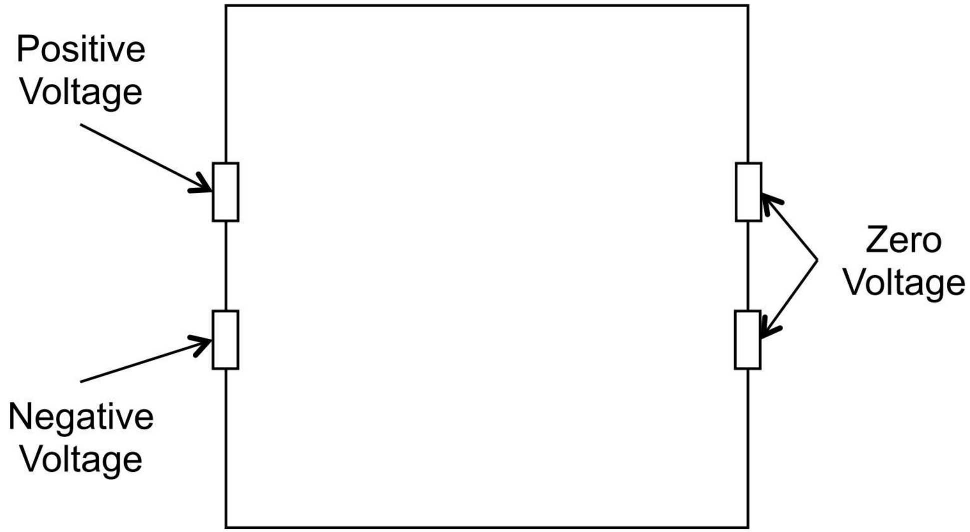


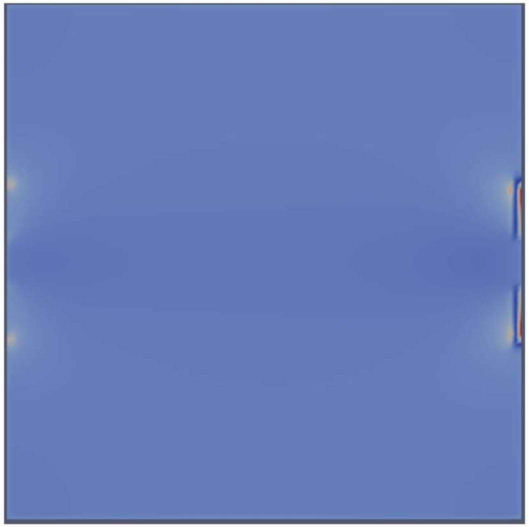
in collaboration with: John Shadid, Tim Wildey, Eric Cyr, Roger Pawlowski, Edward Phillips

Preliminary Results in Topology Optimization: Using Adjoint Sensitivities

Can also use adjoints in optimization:

- Design for plasma/electronics interactions
- Fixed amount conductive material placed to optimize current flow
- Preliminary result: find design of "two-wire" system in a box using simple electrostatic potential model





Using the Drekar code in collaboration with: Eric Cyr, G. von Winckel

Optimization library Trilinos/ROL courtesy of Ridzal, Kouri, von Winckel

Numerical Error Estimation

Gregg Radtke, *Electromagnetic Theory Group*

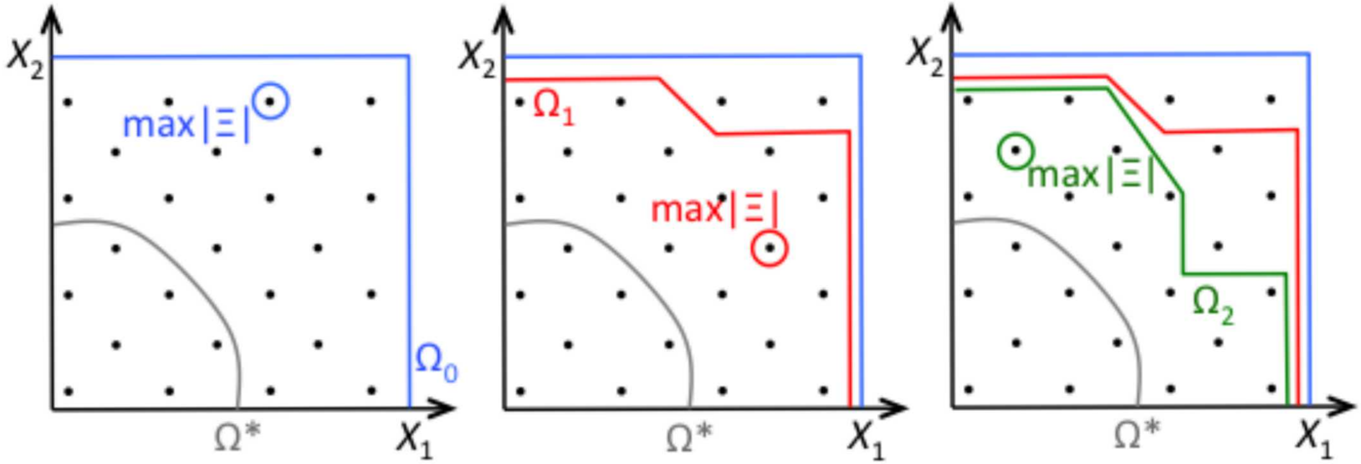
- Methods for deterministic code output
  - Grid convergence index (GCI) (Initial version Pat Roache, 1998)
    - GCI = $F_s \, |Y_1 - Y_2| \, / \, (r^{\Delta x1/\Delta x2} - 1)$
    - Convergence rate assumed, estimated by three-point-fit, or L_2 regression
    - Empirical "safety factor": $1.25 < F_s < 3$
  - Robust verification analysis (Bill Rider, et. al. 2012-)
    - Multi-fitting scheme (using nonlinear optimization) with various error norms, weighting schemes and regularizations
    - Multiple convergence parameters
    - 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 $$G(\beta,\gamma) = \left\| w \cdot \left(\beta_0 + \sum_q \beta_q X_q^{\gamma_q} + \sum_q \sum_{r>q} \beta_{qr} X_q^{\gamma_q} X_r^{\gamma_r} - \mu \right) \right\|$$
- 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

StREEQ Error Estimation

- Estimated converged result distribution $$\tilde{\beta}_{0,j}^{bm} = \beta_0^{bm} + \frac{M-1}{M-N_{\mathrm{fit}}}\varepsilon_j^{bm}$$
  - β_0^{bm} from multiple bootstrap (*b*) and fitting model (*m*) fits
  - Residuals ε_0^{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

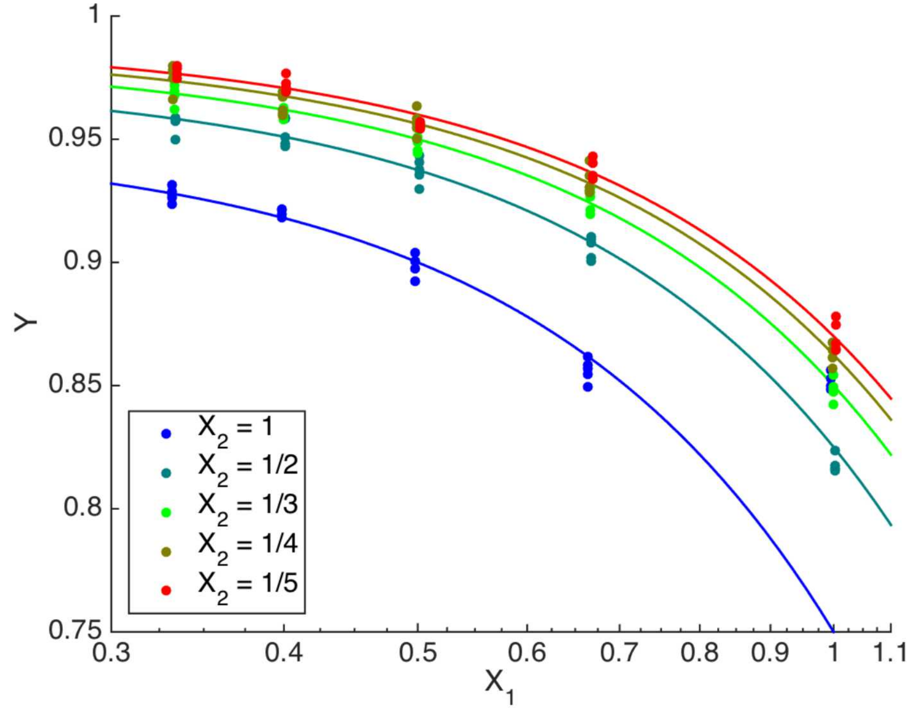


Results for Engineered Data Set

- Data set with built in bias

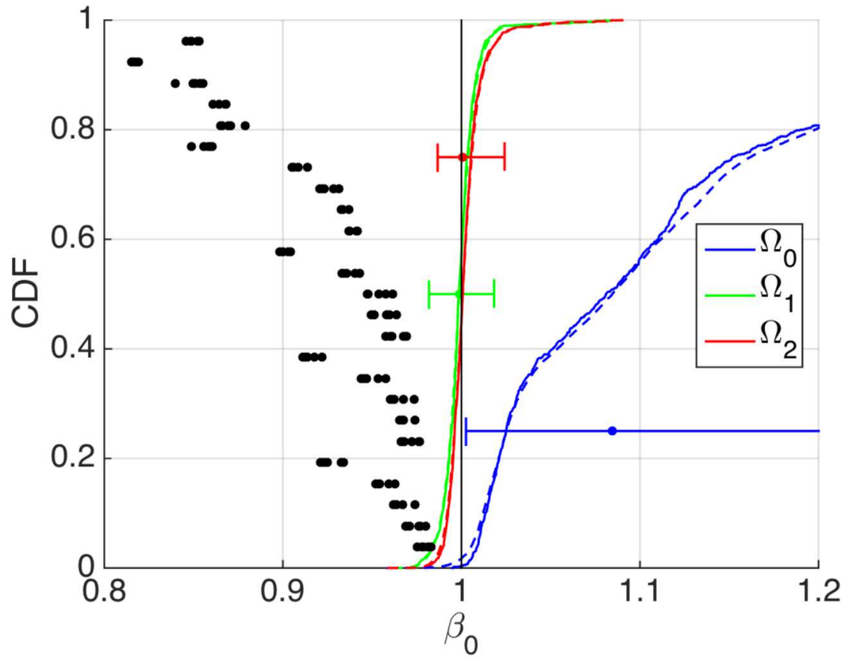
  $$Y = 1 - 0.1X_1^2 - 0.05X_2 - 0.1X_1^2 X_2 + \varepsilon + 0.1X_1^7 X_2^{7/2} \sin\left(2\pi\left[\log\left(X_1\sqrt{X_2}\right) + 0.25\right]\right)$$

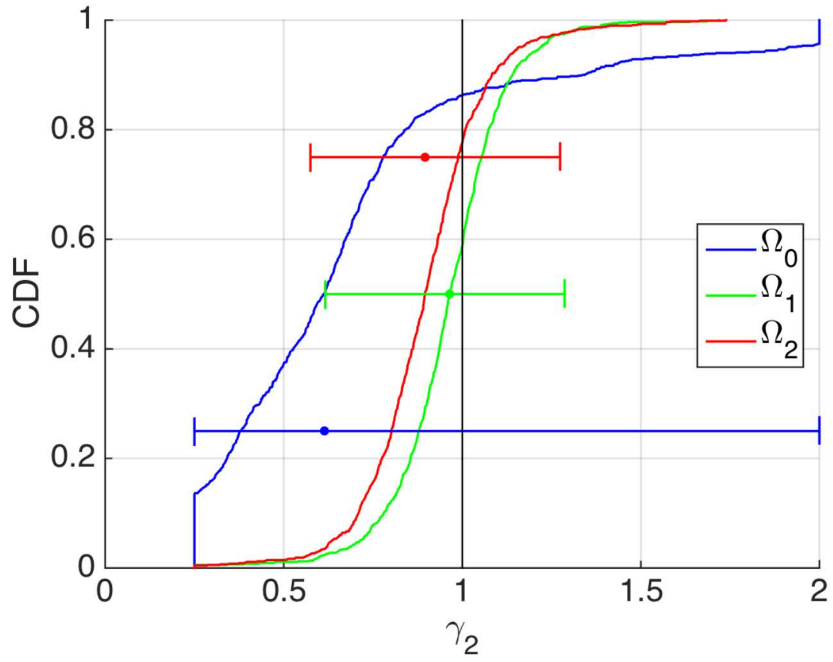
  - Random noise ε with zero mean
  - Bias is oscillatory with fast decay for *X* -> 0



Results for Engineered Data Set (II)

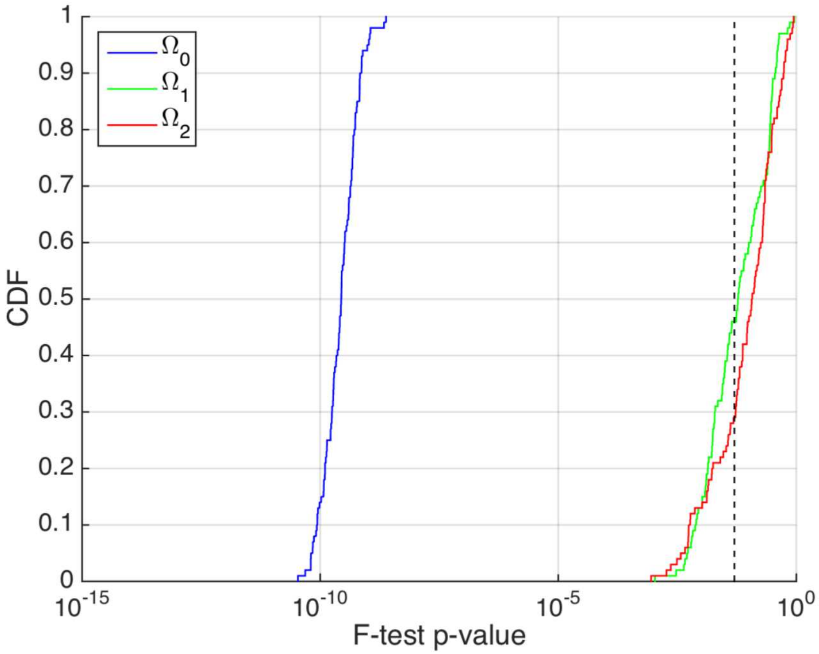
- Normally distributed, 5 samples per discretization level
  - Bias in data leads to increased uncertainty due to multiple fit models and lack-of-fit corrections
  - Minimum variance in β_0 prediction for reduced domain Ω_1

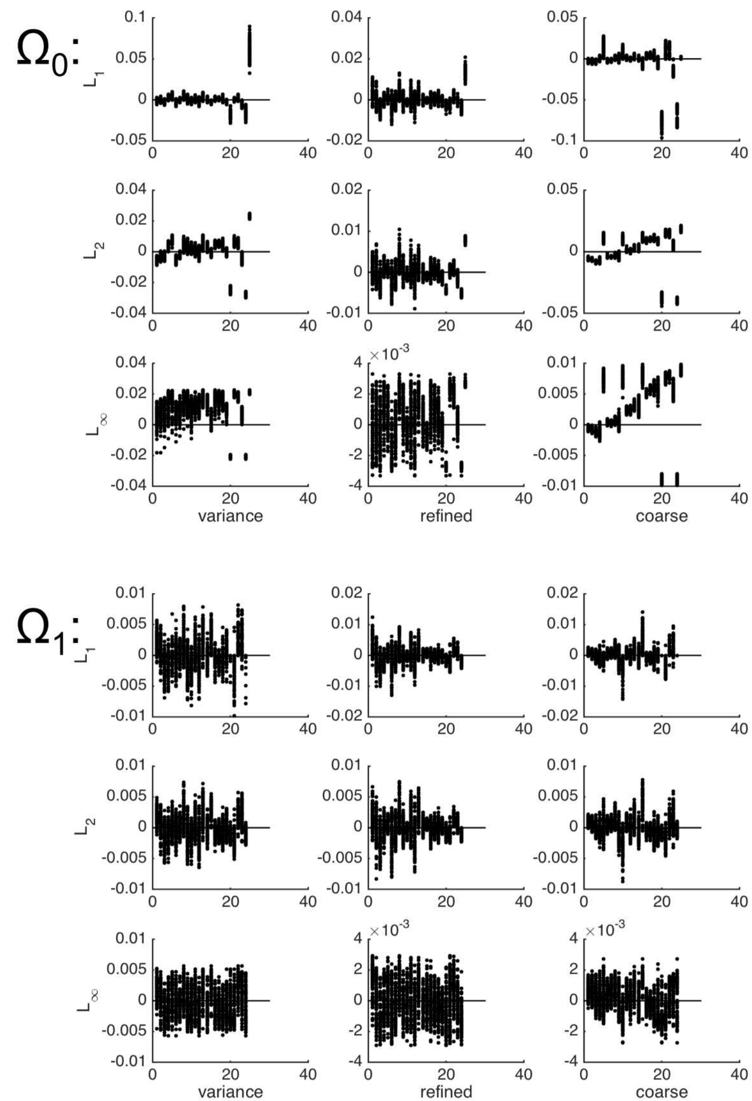




Results for Engineered Data Set (III)

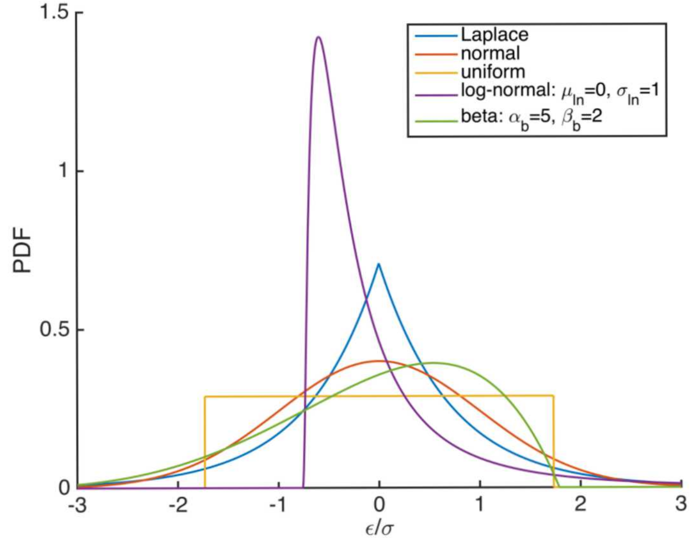
- Credibility assessment

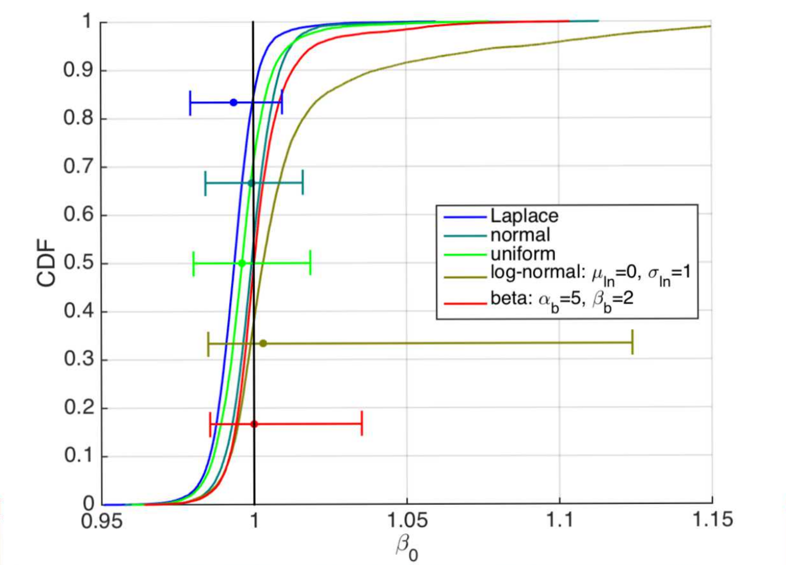




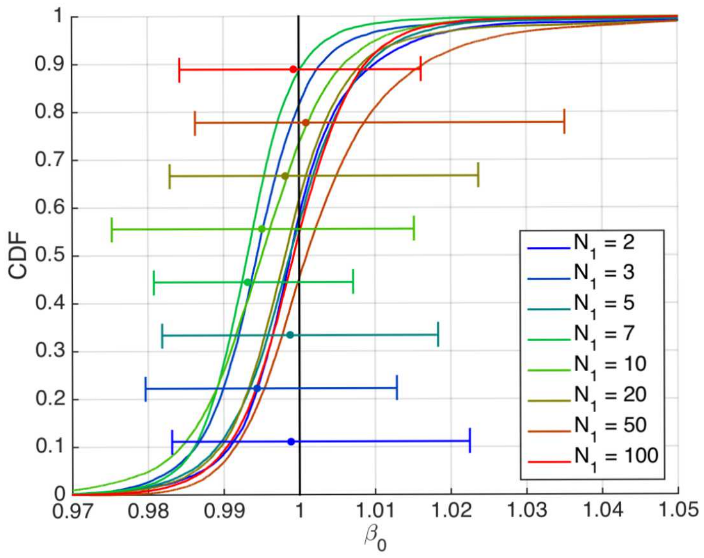
Results for Engineered Data Set (IV)

- Effect of noise distribution

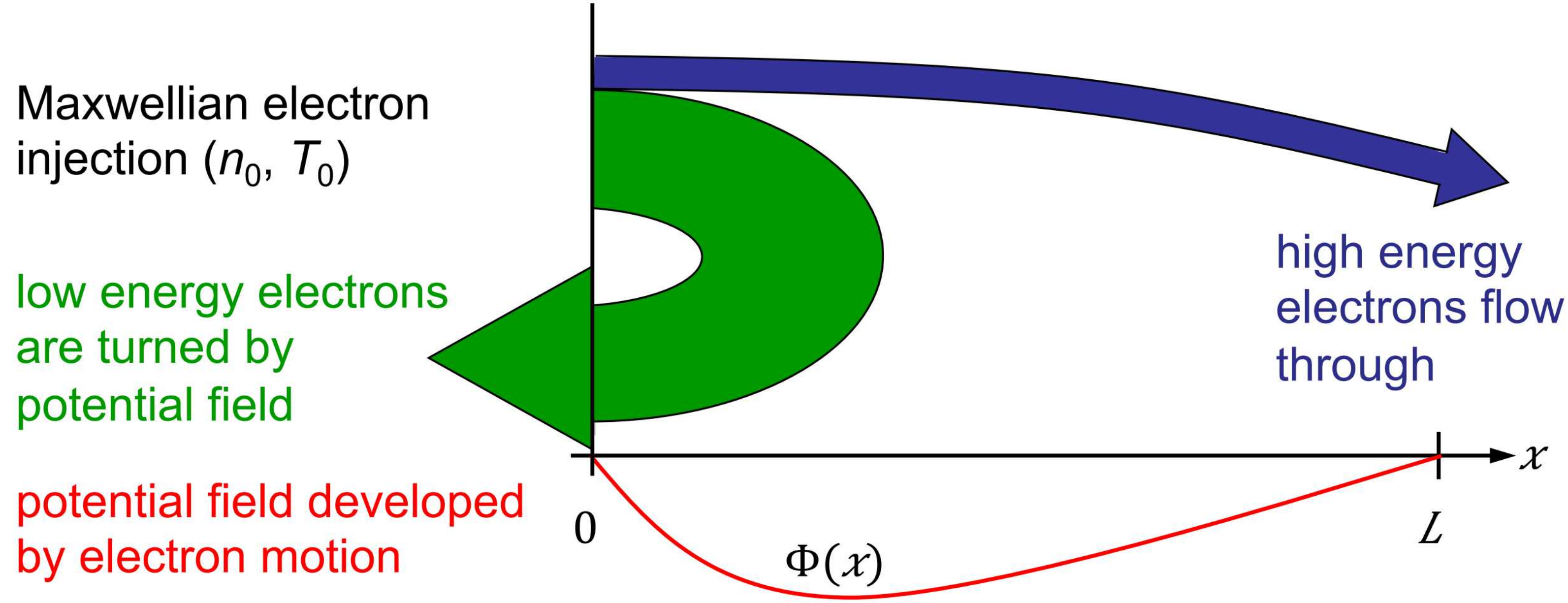




- Finite sample size effect
  - Reasonable results for only two samples per discretization level!



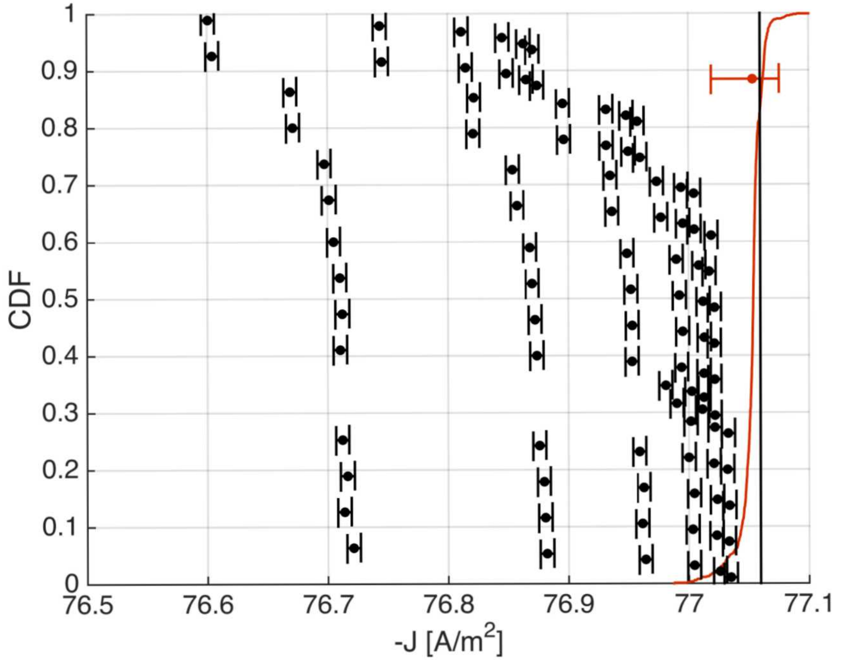
Steady Electron Diode Verification

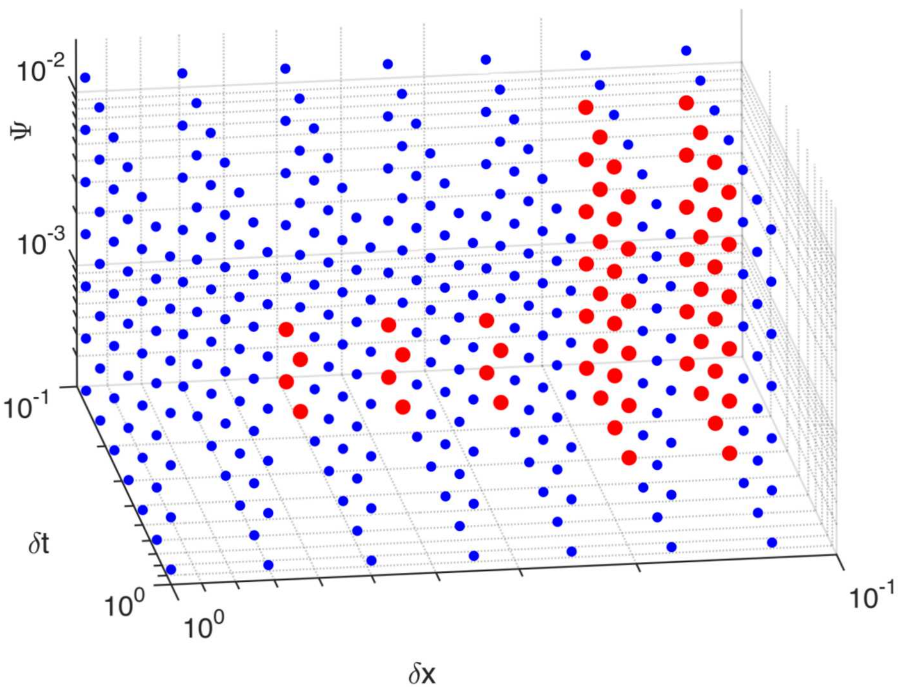


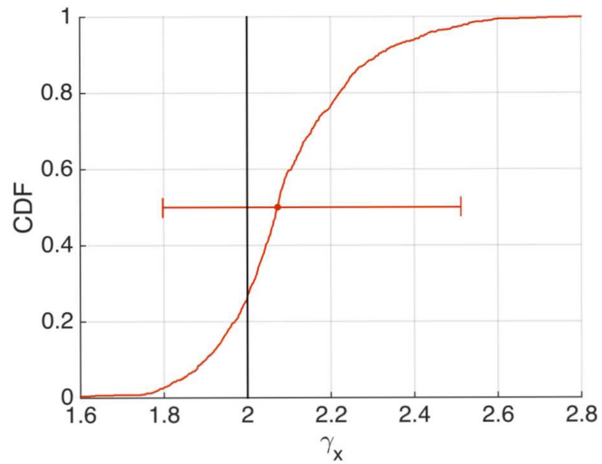
- Simulated using Sandia's Aleph electrostatic PIC plasma code
  - Quantity of interest: total current through diode (-J)
  - Input parameters: n_0 = 10^{16} m^{-3}, T_0 = 10 V, L = $20\lambda_D$
  - Exact result: -J = 77.0596 $\mathrm{A/m}^2$ (numerical quadrature)
- Dimensionless convergence parameters: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

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

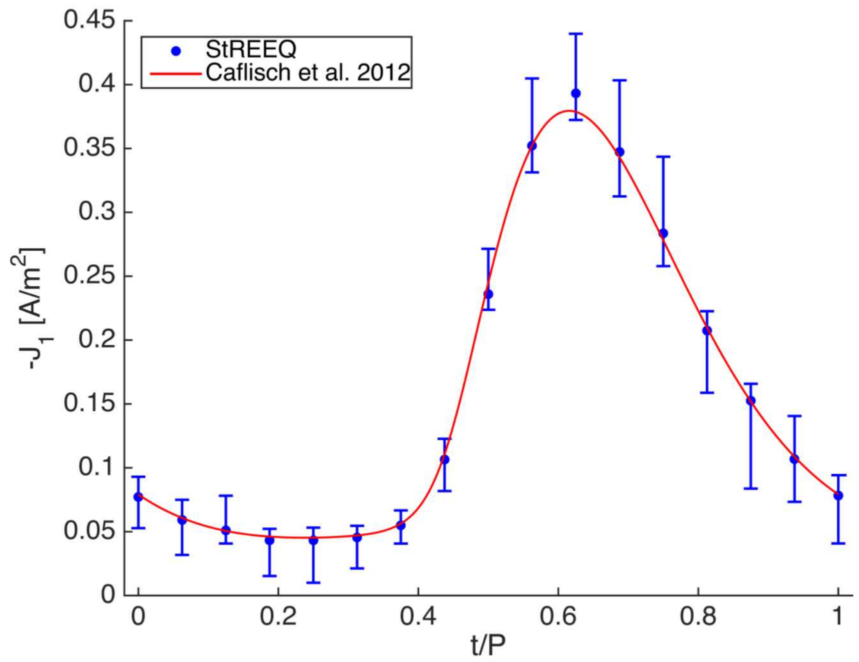






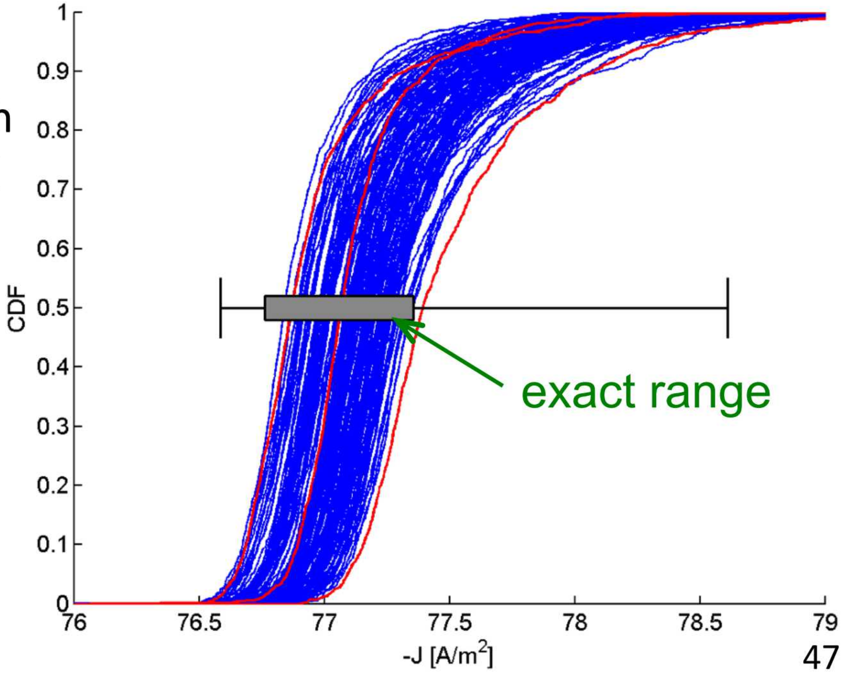
Time-Periodic Electron Diode

- 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

- For validation, numerical uncertainty is only one component of uncertainty
- 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



Conclusion

- Systematic V&V is critical for establishing simulation credibility in high consequence work
- V&V for plasma simulation has numerous challenges
- Careful validation can uncover missing physics from simulations
  - Example: radiation induced plasma validation experiment
- Advanced sensitivity and numerical error estimation
  - Forward and adjoint embedded sensitivity analysis
    - Alternate sensitivity methods for large and small parameter spaces
    - Enables efficient gradient-based optimization
  - StREEQ method for numerical error estimation for stochastic output
    - Accounts for discretization and stochastic noise using multifit approach

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