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Uncertainty quantification of beam parameters in an LIA inferred from Bayesian analysis of solenoid scans

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Outline

- Why is uncertainty quantification worth the effort?
- Old and new tools used to assess beam parameters in DARHT via the beam envelope equation
- Results from a Bayesian analysis of a solenoid scan

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Measurements are not worth much without an uncertainty

- Distinguishing between models/theories requires precision measurements (i.e. need uncertainties to be quantified)

- Distinguishing measurement methods depends on uncertainties
  - Solenoid-scan method (~10-20 shots)[1]
  - Emittance mask methods (~1 shot?)[2]
  - PIC analysis of solenoid scans (~10-20 shots)[3]

- Understanding machine variability depends on measurement precision

- Predictive tuning requires well-understood initial conditions

[1] e.g. A. Paul, NIM Phys Res. 1991. [2] S. Szustkowski, IPAC 2022. [3] A. Press, IPAC 2022.

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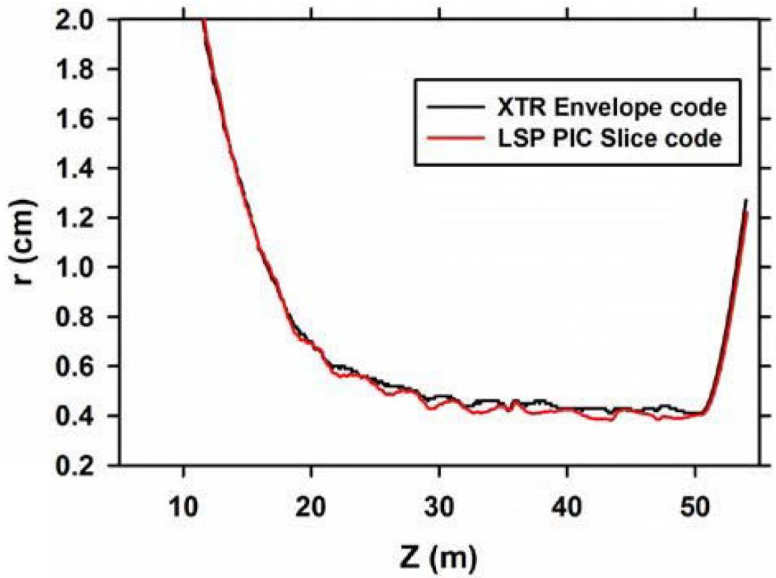
Beam envelope equation enables analysis and tuning of LIAs

- Beam radius evolution through focusing, acceleration, including space charge
- Various derivations either from beam moments[1] or paraxial equations[2]
- Use for LIA analysis developed to high degree in IDL-based xtr code[3]
- PIC comparisons with xtr show favorable results[4]

$$r_m'' + \frac{\gamma' r_m'}{\beta^2\gamma} + \frac{\gamma'' r_m}{2\beta^2\gamma} + \left(\frac{qB}{2mc\beta\gamma}\right)^2 r_m - \left(\frac{p_\theta}{mc\beta\gamma}\right)^2 \frac{1}{r_m^3} - \frac{\epsilon_n^2}{\beta^2\gamma^2 r_m^3} - \frac{K}{r_m} = 0.$$

Gap accel. effects ($\frac{\gamma' r_m'}{\beta^2\gamma}$, $\frac{\gamma'' r_m}{2\beta^2\gamma}$); Sol. focus ($\left(\frac{qB}{2mc\beta\gamma}\right)^2 r_m$); Angular momentum ($\left(\frac{p_\theta}{mc\beta\gamma}\right)^2 \frac{1}{r_m^3}$); Emittance ($\frac{\epsilon_n^2}{\beta^2\gamma^2 r_m^3}$); Self-fields ($\frac{K}{r_m}$)



Ekdahl, et al., IEEE TPS (2017)

[1]Lee and Cooper, Part. Accel. 7 (1976) 83.
[2]cf Reiser "Theory and Design…" 2008. and Humphries "Charged Particle Beams" 2002.
[3]Allison, LA-UR-01-6585 (2001)
[4]Ekdahl, et al., IEEE Trans. Plasma Sci. 45 (2017) 2962.

Actual LIAs require improvements beyond "textbook" envelope equation

- xtr and simpleEnvelope (new, python-based code) include more space-charge effects
- xtr developed w/ experimental validation; multi-person-year effort
- simpleEnvelope developing new features and undergoing code-code validation (initially)

Beam Physics Modeled	xtr	simpleEnvelope	Approximate Effect
Electrostatic neutralization	Yes	Yes	$\mathcal{O}(1)$
Current neutralization	No	Yes	$\mathcal{O}(1)$
Foil focusing	Yes	Yes	$\mathcal{O}(1)$
Beam potential depression	Yes	Yes	$\mathcal{O}(0.1)$
Beam diamagnetism	Yes	No	$\mathcal{O}(0.01)$

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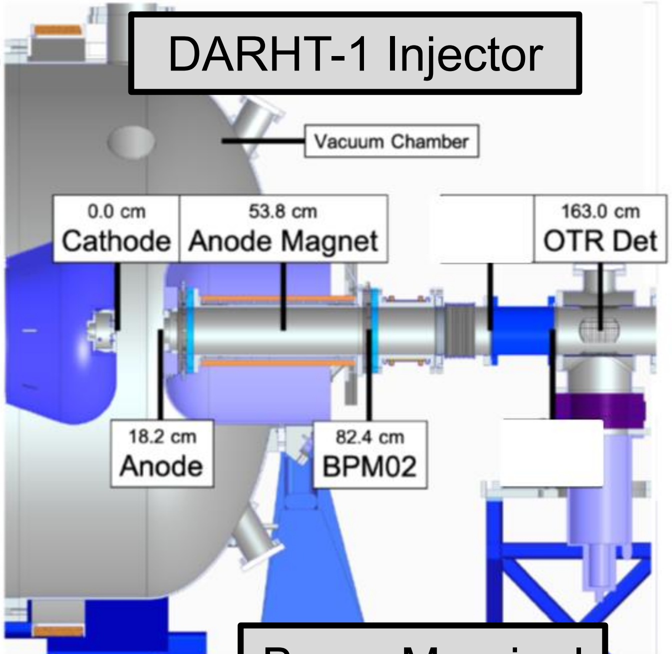
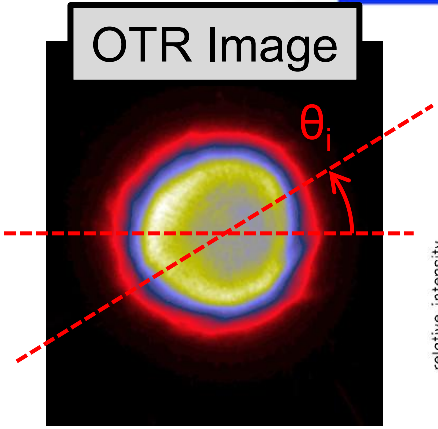
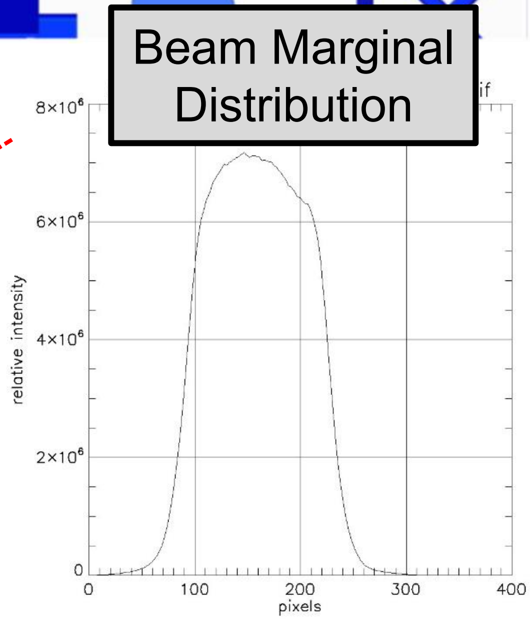
Solenoid scan at DARHT-1 injector provides experimental database for work

- Low energy, high-current beam
  - I_b=1626±3A
  - T=3.234±0.016MeV
- OTR measurements made on aluminized Kapton
  - Each image has marginal distribution at θ_i
  - RMS mean and std. dev. from N angle cuts
  - 24 cuts for each image
- Anode solenoid swept through excitations (53.73±0.1cm from cath.)



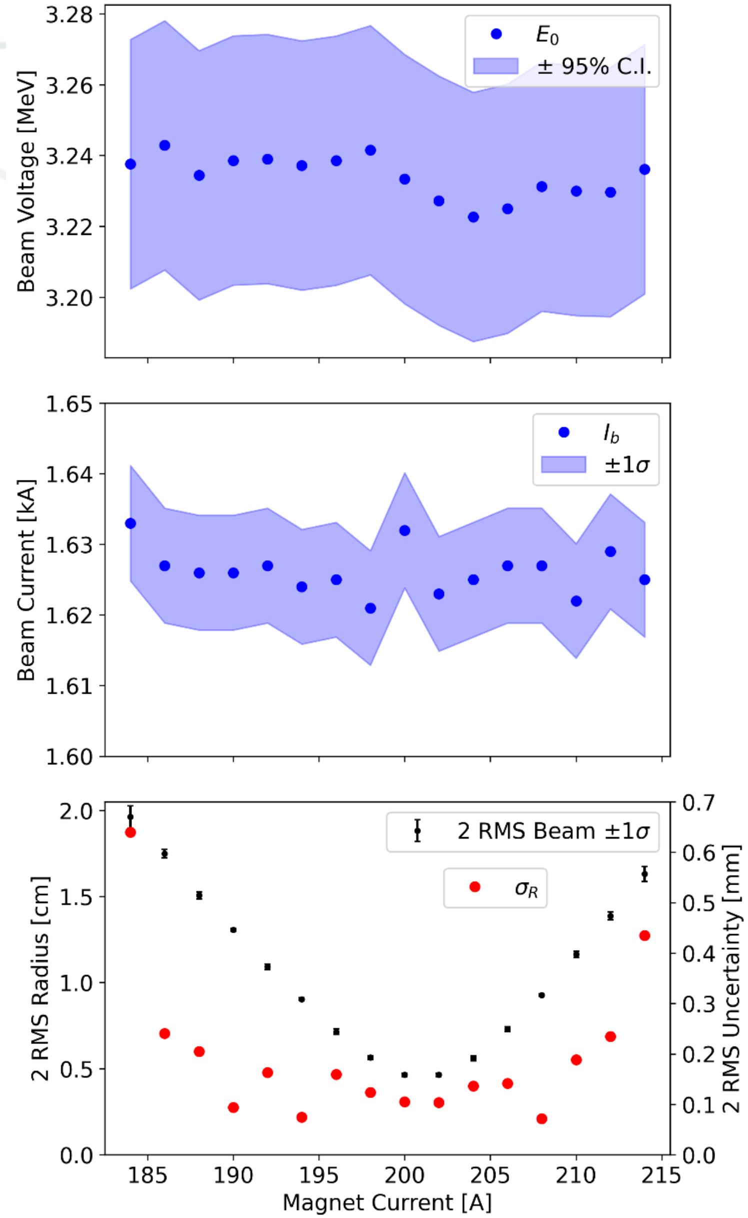




[1] S. Szustkowski, IPAC 2022. [2] DC Moir, LA-UR-21-21386

Experimental parameters for this scan

- Beam energy cross-calibration yields 95% credible interval
  - This work demonstrates the importance of this measurement precision
- Current uncertainty estimated at 0.5%
- RMS beam radius uncertainty estimated from multiple angle cuts method
- Beam initial conditions are simulated from the cathode location



xtr solution method minimizes χ^2-*like* figure-of-merit

- xtr FOM sums normalized variances
  - R_{meas}: observations
  - R_t: model value for given R_0, R_0', ε_N
- For normal distr., χ^2 is "interpretable" w.r.t. probability distribution[1]
- Xtr FOM similar to χ^2, if
  - assuming $\sigma_{meas} \sim r_t$
  - Uncertainty characterized by FOM doublings (X% increase to 2x FOM)
  - χ^2 doubling is *large* decrease in probability of a normal dist.
- Xtr solution: R_0=1.381cm, R_0'=72.6mrad, ε_N=957 mm-mrad

$$\mathrm{FOM_{xtr}} = \left[\sum_{i=1}^{N} \frac{(r_{meas,i}/r_{t,i} - 1)^2}{N}\right]^{1/2}$$

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{r_{meas,i} - r_{t,i}}{\sigma_{meas,i}}\right)^2$$

$$N \cdot \mathrm{FOM_{xtr}}^2 = \sum_{i=1}^{N} \frac{(r_{meas,i} - r_{t,i})^2}{r_{t,i}^2}$$

[1] D.S. Sivia "Data Analysis: A Bayesian Tutorial" 2006.

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LIA parameter inference accomplished with non-linear beam-envelope model

$$p(\mathbf{x}_0|\mathbf{r}_{meas},\mathbf{I}) = \frac{p(\mathbf{r}_{meas}|\mathbf{x}_0,\mathbf{I}) \times p(\mathbf{x}_0|\mathbf{I}) \times p(\mathbf{I})}{p(\mathbf{r}_{meas},\mathbf{I})}$$

$$\mathbf{x}_0 = (R_0, R_0', \epsilon_N) \quad \mathbf{r}_{meas} = (r_{meas,i}, \sigma_{meas,i})$$

$$\mathbf{I} = (T_i, I_{b,i}, z_{AM}, \ldots)$$

- Likelihood function assumed to be normally distributed about beam-envelope solution: f($\mathbf{x}_0$,$\mathbf{I}$)

$$p(\mathbf{r}_{meas}|\mathbf{x}_0,\mathbf{I}) \propto \exp\left[-\frac{1}{2}\left\|\frac{(f(\mathbf{x}_0,\mathbf{I}) - \mathbf{r}_{meas})}{\sigma_{meas}}\right\|^2\right]$$

- Input variables include I_b, T, z_{AM}
  - σ_T varies with absolute instrument precision (~16keV)
  - σ_z varies by reasonable estimate (1mm)
  - σ_I varies as 0.5% precision

$$\sigma_T, \sigma_I, \sigma_Z \cdots \sigma_\alpha \sim \mathcal{N}(0, \sigma_\alpha^2)$$

$$I_\alpha = \mu_{0,\alpha} + \sigma_\alpha$$

- Uninformative priors used to avoid biases

$$R_0, R_0', \epsilon_N \sim \mathcal{U}(x_{\beta,min}, x_{\beta,max})$$

or

$$p(x_\beta, T) = p(x_\beta|T) \times p(T)$$

$$x_\beta|T \sim \mathcal{N}\left(\mu_{x_\beta} + \frac{\Sigma_{x_\beta,T}}{\Sigma_{T,T}}(T - \mu_T), \Sigma_{x_\beta x_\beta} - \frac{\Sigma_{x_\beta,T} \cdot \Sigma_{T,x_\beta}}{\Sigma_{T,T}}\right)$$

- Strong correlation with varying energy
  - Markov-Chain Monte Carlo (MCMC) solutions generally less efficient
  - Hierarchical model employed to break correlations
  - Sampled as conditional bivariate normal distributions
  - PYMC4 library used for sampling

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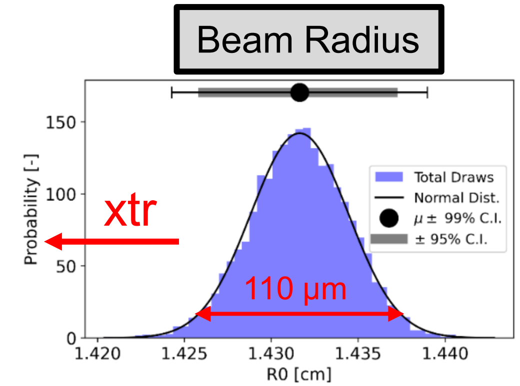
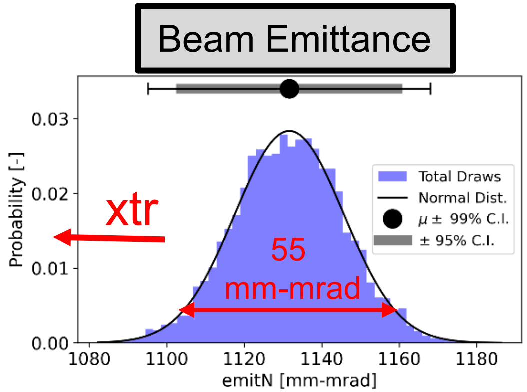
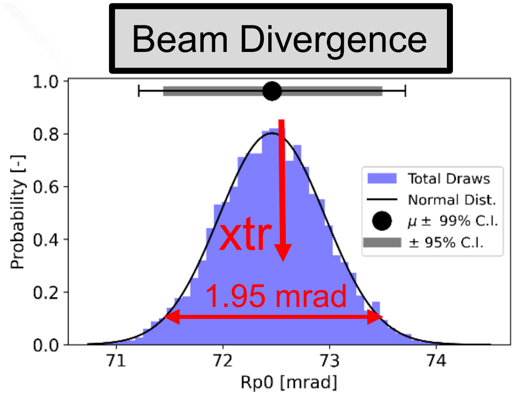
Single energy simulation provides point-comparison to xtr results

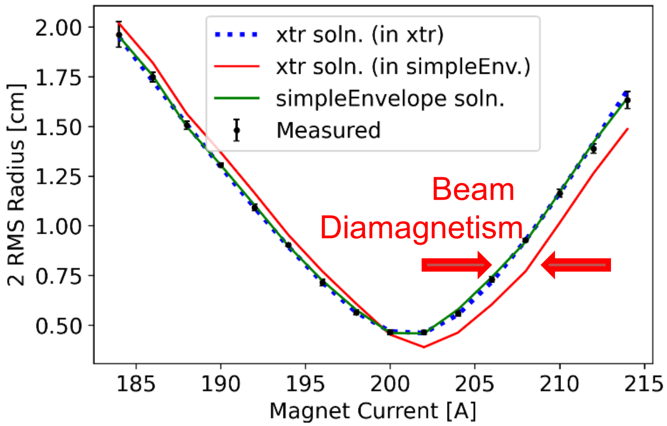
- Perfectly known energy assumption provides comparison
- Xtr solution is OUTSIDE the uncertainty bounds
  - Beam diamagnetism not included in simpleEnvelope
  - Approx. 1% reduction in solenoid strength (~2A)
  - FOM doubling metric in xtr is pessimistic given the data quality
- UQ demonstrates the ability to distinguish beam physics models







	simple-Envelope	xtr	Units
R_0	1.432±0.003	1.38±0.02	cm
R_0’	72.5±0.5	72.6±3.5	mrad
ε_N	1132±14	957±96	mm-mrad



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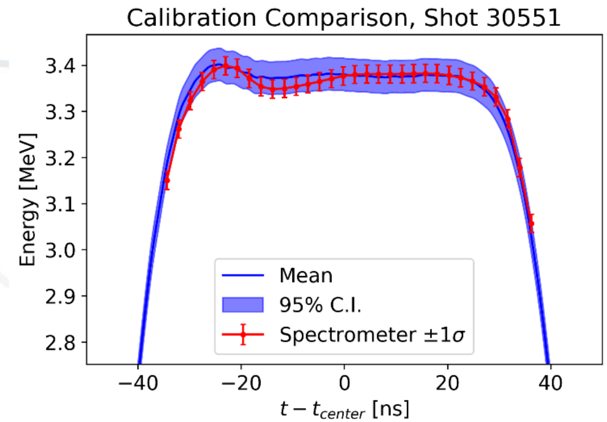
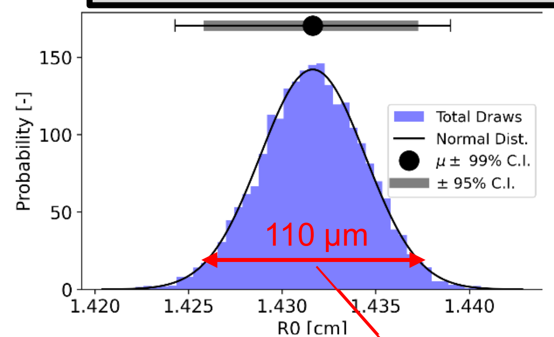
Finite, absolute precision of energy measurement affects uncertainties

- Gap voltage monitored with e-dot
  - Recently recalibrated against electron spectrometer [1]
  - Uncertainty in absolute calibration is ±17keV at 3.4MeV (~0.5%)
  - Pulse-to-pulse variability only ~0.2%

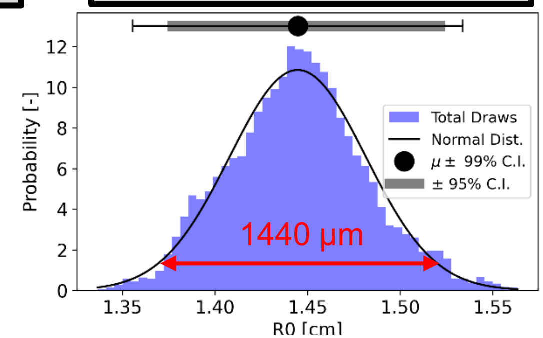
- Energy variation expands uncertainty
  - 1% energy change leads to 6.5% R_0 variation
  - Strongly affects accelerator transport and matching

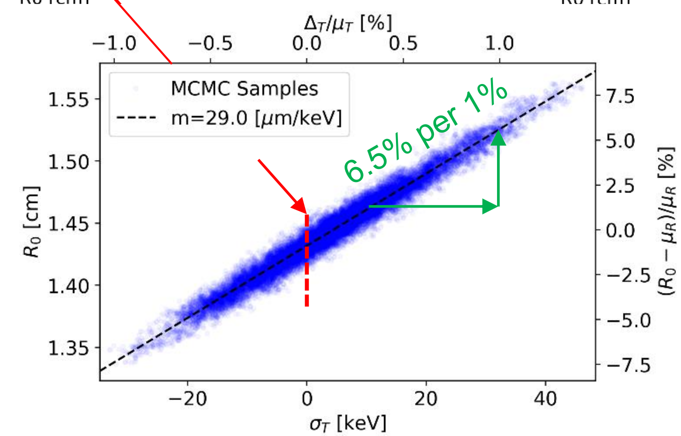


R_0 w/ Single Energy



R_0 w/ Energy Dist.





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Results indicate applicability for further parameter and machine inferences

- New experiments and measurements are being devised to better constrain lab kinetic energy, T
- Basic methodology can be extended to include
  - Magnet misalignments, positioning errors
  - Charge and current neutralization effects
  - Further space-charge and beam distribution effects
- UQ approach will continue to depend on high-quality data for credible inferences and constraints

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Summary

- Rigorous approach to uncertainty enables scientific discovery through model differentiation and efficient data use
- Comparison of MAP-like solution in xtr with Bayesian simpleEnvelope allows model differentiation for a ~1% effects
  - Solenoid scan method strongly constrains solutions for a given lab kinetic energy value
  - xtr uncertainty estimates are pessimistic w.r.t. data quality
- Absolute energy variation greatly expands uncertainty of beam inlet radius, but basic methodology has potential in further studies

Thank you for your attention!

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Backup

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Mix of proven and development methods are used to characterize LIAs like DARHT

- Beam envelope models used for tuning require beam radius, convergence, and emittance
- Long-established method is the solenoid scan (~10-20 shots)[1]
- Developing interpretation of emittance-mask methods (a.k.a. pepper-pots) (~1 shot?)[2]
- Also examining the use of full 2D and 3D PIC simulations for regular solenoid scan interpretation (~10-20 shots)[3]
- UQ is necessary for method comparisons

[1] e.g. A. Paul, NIM Phys Res. 1991. [2] S. Szustkowski, IPAC 2022. [3] A. Press, IPAC 2022.

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Understanding the sources of machine variability can also come from UQ studies

- DARHT and similar light sources must perform reliably and repeatably
- Measurement precision (i.e. uncertainty) determines the degree to which variations can be observed (“Is it out of the noise floor?”)
- Separating instrumental “noise” from real variations in machine parameters often requires understanding entire system (or facility)

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Bayesian analysis works by deriving probabilities of parameters given the observables

$$p(\mathbf{x}_0, \mathbf{r}_{meas}, \mathbf{I}) = p(\mathbf{x}_0|\mathbf{r}_{meas}, \mathbf{I}) \times p(\mathbf{r}_{meas}, \mathbf{I})$$

- Bayes rule derived from manipulating joint distribution
- Solution of probability distribution gives uncertainty bounds automatically
- Practical problems do not assume functional form – not tractable analytically
- Markov-Chain Monte Carlo (MCMC) provides a numerical solution for the posterior distribution

posterior likelihood prior(s)

$$p(\mathbf{x}_0|\mathbf{r}_{meas}, \mathbf{I}) = \frac{p(\mathbf{r}_{meas}|\mathbf{x}_0, \mathbf{I}) \times p(\mathbf{x}_0|\mathbf{I}) \times p(\mathbf{I})}{p(\mathbf{r}_{meas}, \mathbf{I})}$$

$$p(\mathbf{r}_{meas}, \mathbf{I}) = \int_{-\infty}^{\infty} p(\mathbf{x}_0, \mathbf{r}_{meas}, \mathbf{I}) \mathrm{d}\mathbf{x}_0$$

$$\mathbf{x}_0 = (R_0, R_0', \epsilon_N)$$

$$\mathbf{I} = (T_i, I_{b,i}, z_{AM}, \ldots)$$

$$\mathbf{r}_{meas} = (r_{meas,i}, \sigma_{meas,i})$$

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