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Title:	Proof-of-Concept Study for Uncertainty Quantification and Sensitivity Analysis using the BRL Shaped-Charge Example
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LA-UR-16-25183

Proof-of-Concept Study for Uncertainty Quantification and Sensitivity Analysis using the BRL Shaped-Charge Example

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Outline

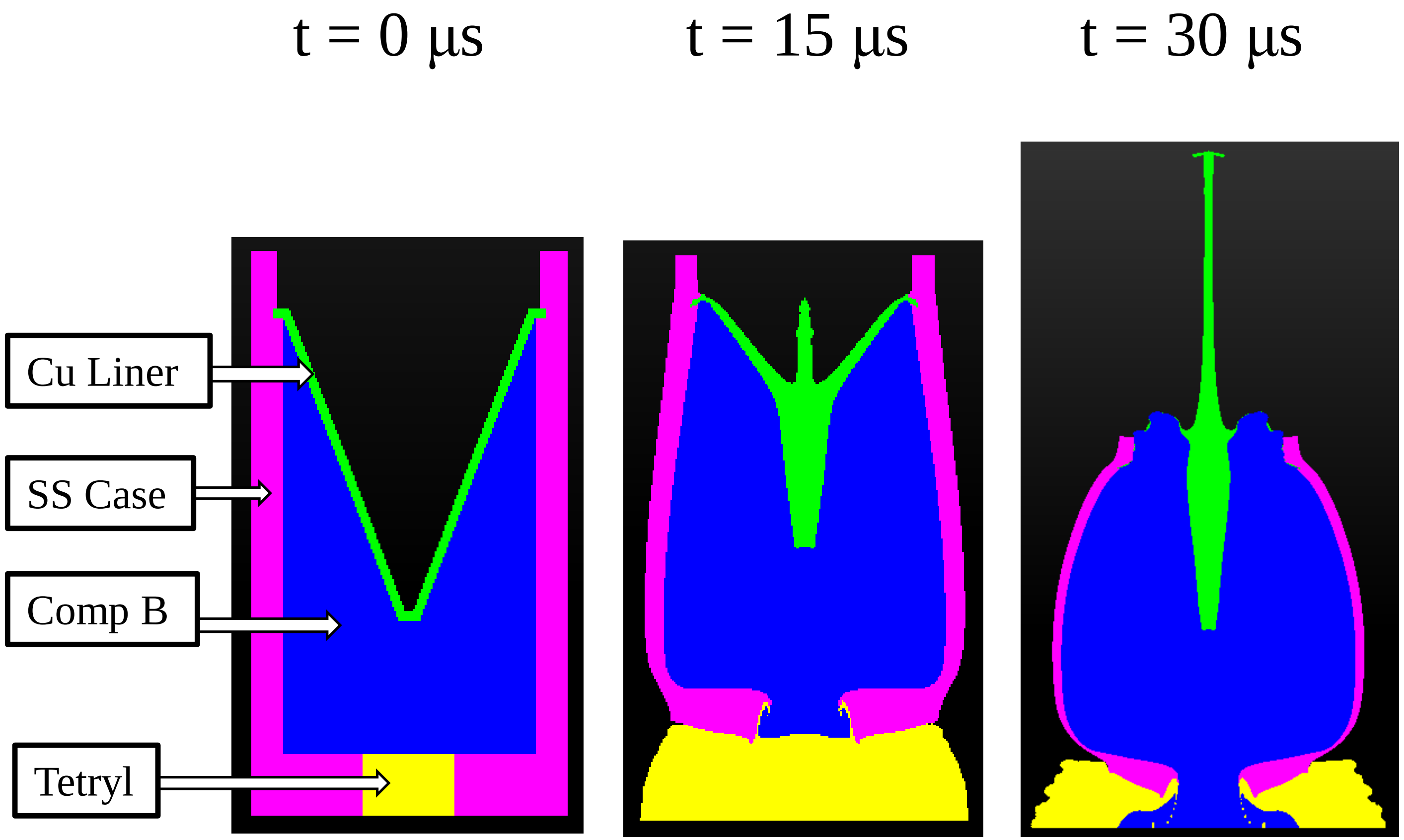
- The BRL Shaped-Charge Geometry in PAGOSA
- Mesh Refinement Study
- Surrogate Modeling using a Radial Basis Function Network (RBFN)
- Ruling out parameters using Sensitivity Analysis
  - Equation of State Study
    - Design of Experiments
    - Accuracy Study for Minimizing Prediction Error
    - Sensitivity Analysis using the Fourier Amplitude Sensitivity Test (FAST)
- Uncertainty Quantification (UQ) Methodology
  - Forward Propagation Using Monte Carlo Simple Random Sampling
- Sensitivity Analysis (SA) Methodology
  - Fourier Amplitude Sensitivity Test (FAST) for First Order Sensitivity Indices

LA-UR-16-25183

The BRL Shaped-Charge Geometry and Materials

Materials of the BRL Shaped-Charge

Material	Strength Model	Equation of State
Copper	Modified Steinberg-Guinan	U_s - U_p
Stainless Steel	Modified Steinberg-Guinan	U_s - U_p
Composition B	-----	Jones-Wilkins-Lee
Tetryl	-----	Jones-Wilkins-Lee



- To decrease simulation time, the problem is constructed as 2-D with symmetry about the z-axis
- Since this a shaped-charge with a projectile, the jet tip velocity was chosen as the output metric-of-interest

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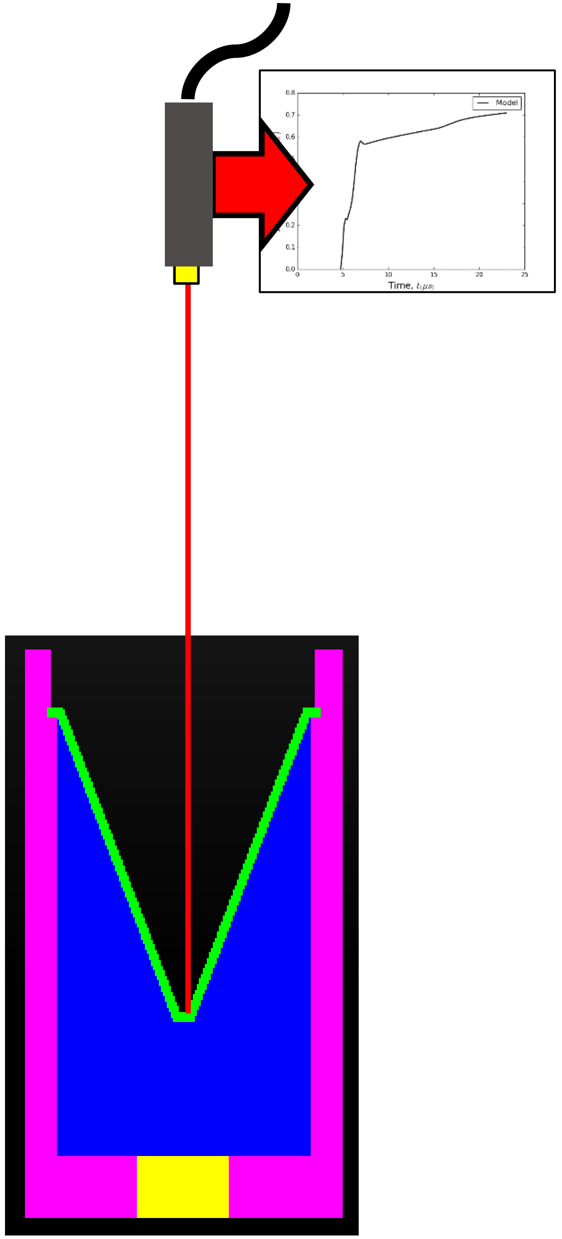
Mesh Refinement Study

Comparing Simulations

- For **Uncertainty** and **Sensitivity** Analyses, results must be within a **numerically stable solution** region to reduce the influences of mesh size and numerical noise.

- The effect of mesh size was investigated at **1000 μm**, **600 μm**, **200 μm**, **100 μm**.

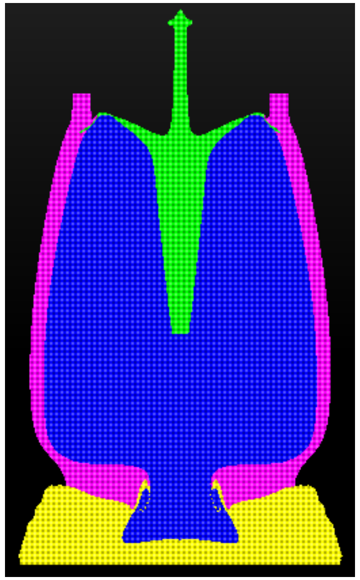
- A simulated Photon Doppler Velocimeter (**PDV**) positioned parallel to the z-axis at a 0.5 mm offset was used to quantify the **jet tip velocity** and compare simulations.



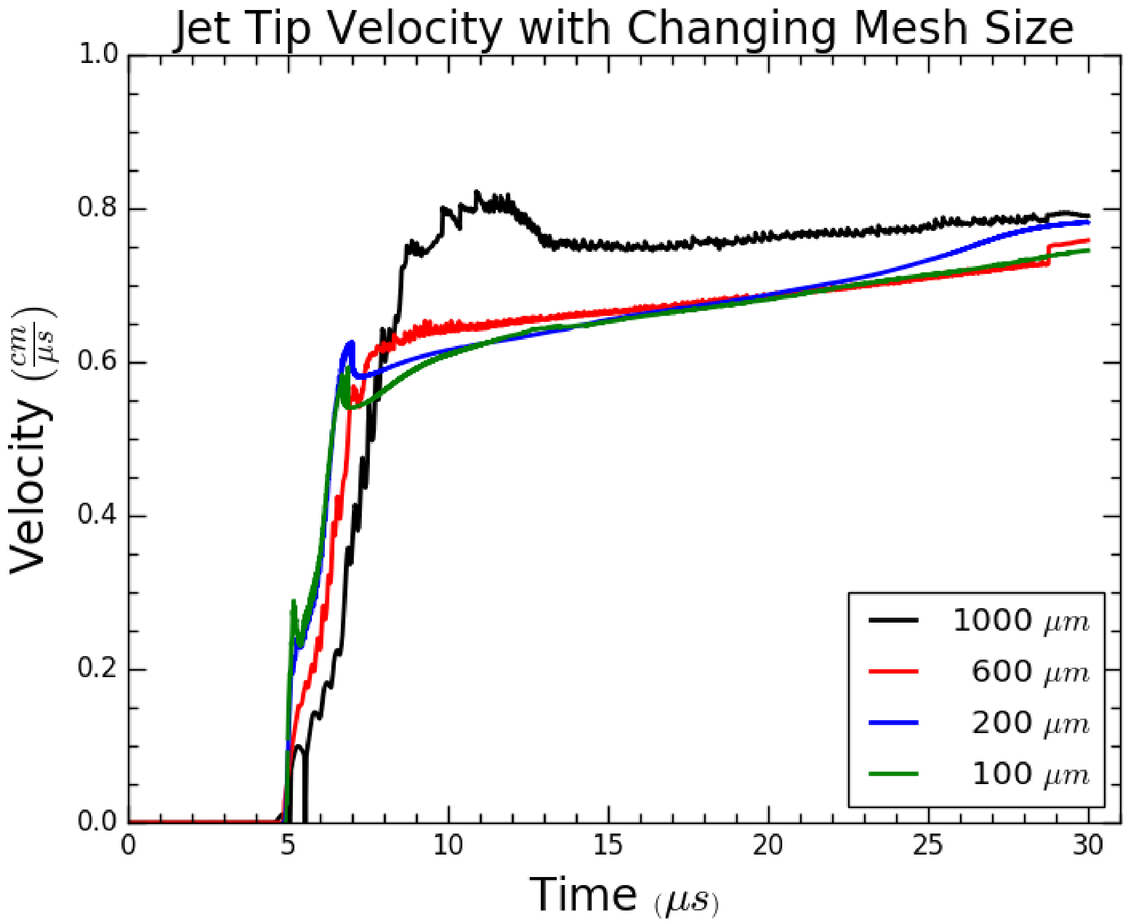
Results of the Mesh Refinement Study

- Simulations at 1000 μm and 600 μm ejected a small particle near the PDV axis while at 200 μm and 100 μm the jet tip forked.

1000/600 μm



200/100 μm

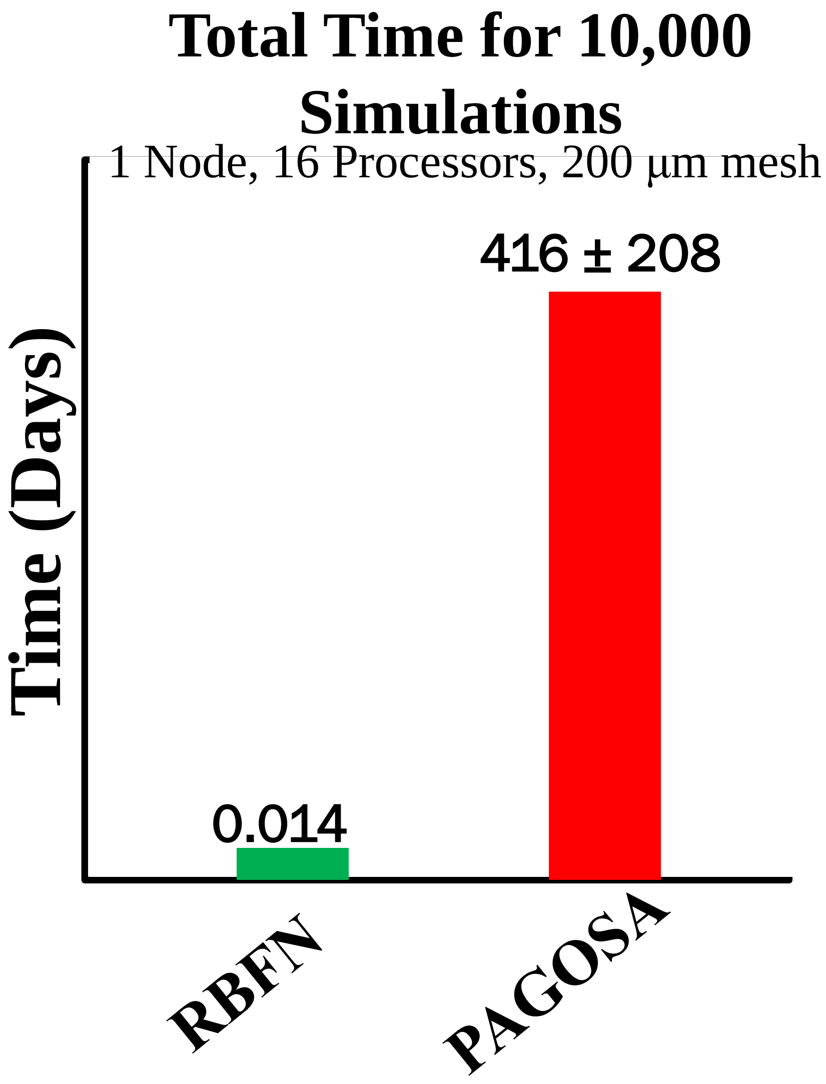


extract_pdv.py

Surrogate Modeling using a Radial Basis Function Network (RBFN)

Surrogate Modeling of PAGOSA Simulations

- For both **Uncertainty and Sensitivity** Analyses, **thousands of computations** are necessary and is **not feasible** for **large-scale simulations** of complex processes.
- **Surrogate models** allow for the **approximation** of **simulation output** with a much **lower** computational **cost** with the trade-off of **less accuracy**.
- A **Radial Basis Function Network (RBFN)** was used for the shaped-charge data due to its ability to model nonlinear responses [1].



[1] Fang, H., Rais-Rohani, M., Liu, Z., Horstemeyer, M.F., "A Comparative Study of Metamodeling methods for Multiobjective Crashworthiness Optimization," Computers and Structures, 83, pp2121-2136, 2005.

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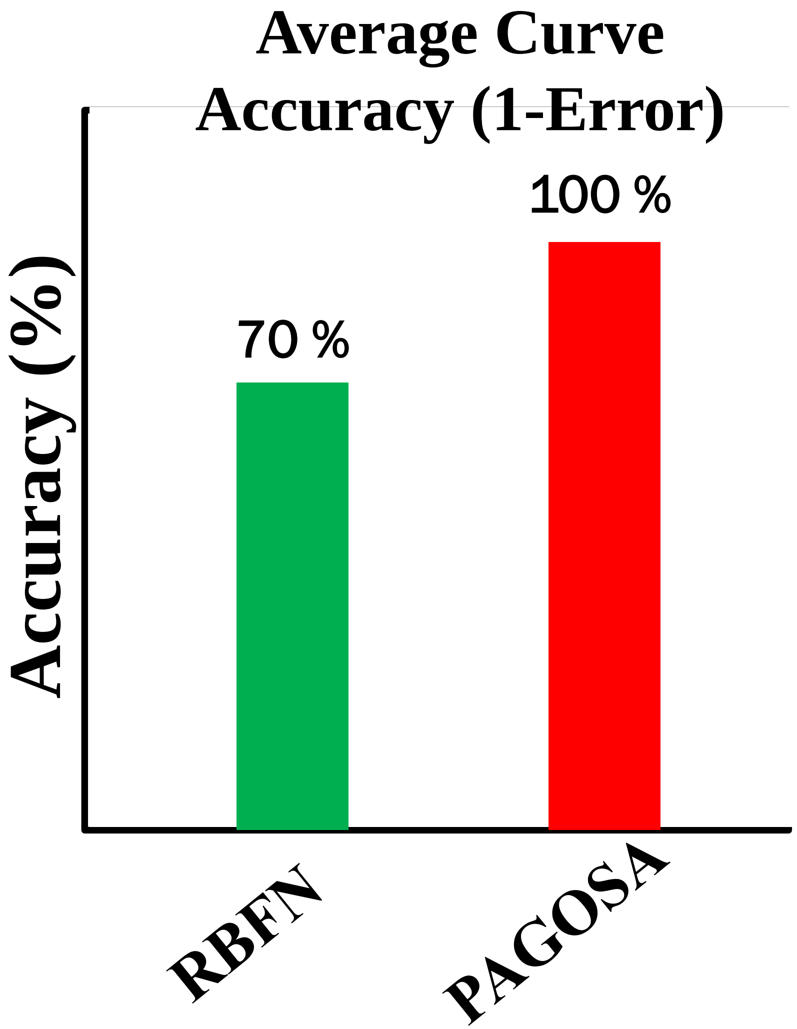


[1] Fang, H., Rais-Rohani, M., Liu, Z., Horstemeyer, M.F., "A Comparative Study of Metamodeling methods for Multiobjective Crashworthiness Optimization," Computers and Structures, 83, pp2121-2136, 2005.

Radial Basis Function Network (RBFN) Theory

- Model is approximated with the function [1,2]:

$$f_{RBF}(\underline{x}) = \sum_{i=1}^{n} \lambda_i \varphi(||\underline{x} - \underline{x}_i||) = \sum_{i=1}^{n} \lambda_i \varphi(\underline{r}_i)$$

Where,

- $\underline{x}$ is the vector of sample points
- $\underline{x}_i$ is the vector of design points at the ith sampling point
- $||\underline{x} - \underline{x}_i||$ is the Euclidean distance of the sample point from the design point (radius, $\underline{r}_i$)
- λ_i is the unknown weighting factor for each design point at each sampling point
- φ is a user-defined basis function

[1] Fang, H., Rais-Rohani, M., Liu, Z., Horstemeyer, M.F., “A Comparative Study of Metamodeling methods for Multiobjective Crashworthiness Optimization,” Computers and Structures, 83, pp2121-2136, 2005.
[2] Mai-Duy, N., Tran-Cong, T., “Approximation of Function and its Derivatives using Radial Basis Function Networks,” Applied Mathematical Modeling, 27, pp197-220, 2003.

Radial Basis Function Network (RBFN) Basis Functions

- Thin Plate: $\varphi(r) = r^2 log(cr^2)$
- Gaussian: $\varphi(r) = e^{-cr^2}$
- Multiquadric: $\varphi(r) = \sqrt{r^2 - c^2}$
- Inverse Multiquadric: $\varphi(r) = \frac{1}{\sqrt{r^2 - c^2}}$

- Where:
  - $r = ||\underline{x} - \underline{x_i}||$ is the Euclidean distance (vector magnitude)
  - c is an RBFN constant that can be tuned to minimize error

Computing the Lambda Matrix for the Radial Basis Function Network (RBFN)

- The RBFN formula is solved for λ using a simple matrix inversion:

$$f_i = \varphi_{ij}\lambda_i$$
$$\lambda_i = \varphi_{ij}^{-1} f_i$$

- This calculation is performed at each time step, producing a set of weighting factors for each training data set (f_i).
- If the phi matrix is singular, the Moore-Penrose Pseudoinverse is used.

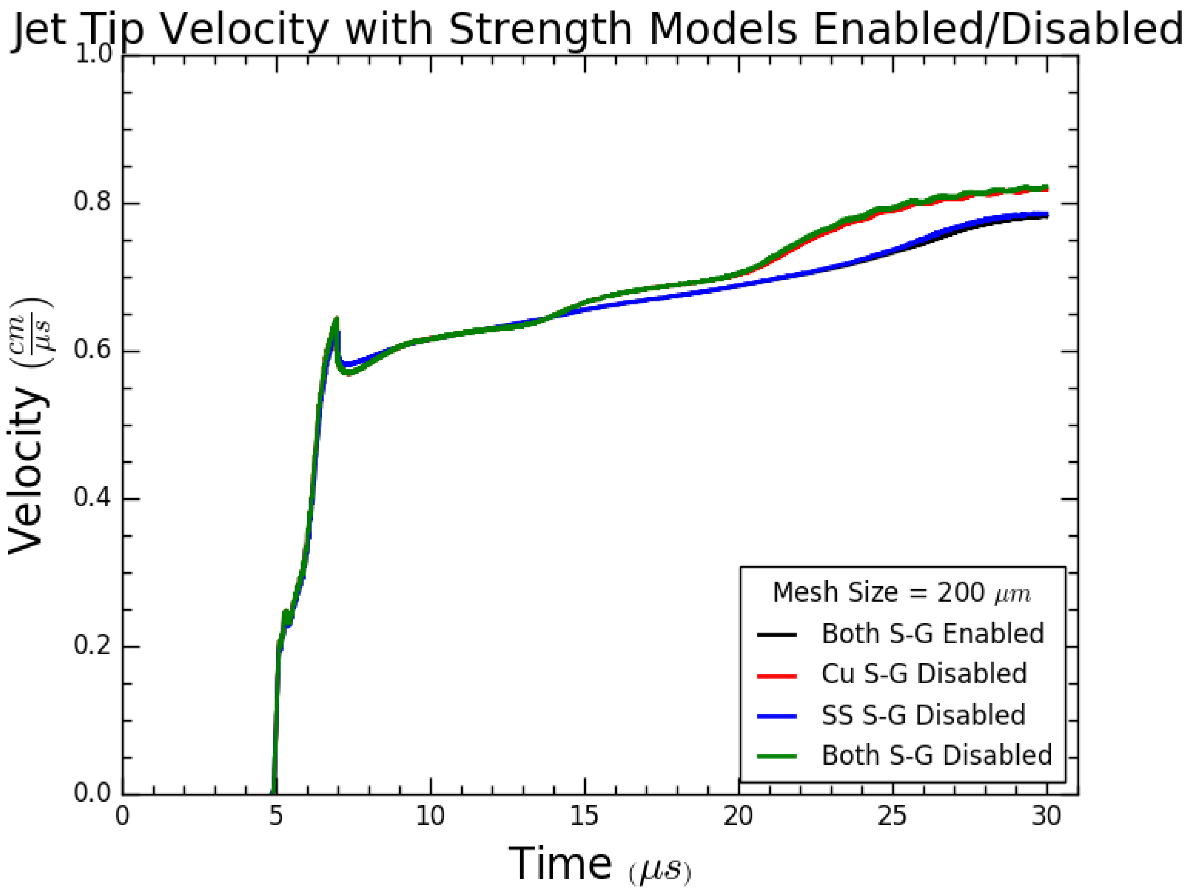
$$\varphi_{ij}^{-1} \approx \varphi_{ij}^{T}\left(\varphi_{ij}\varphi_{ij}^{T}\right)^{-1}$$

Training the Radial Basis Function Network (RBFN)

- In order to use the **surrogate model**, data to **train** the **RBFN** are needed.
- The **number** of simulations to **fully describe** the model behavior **scales** as **Levels^Parameters**. (2 Levels, 8 Parameters = 256 Simulations)
- To **reduce** the number of needed **simulations**, the **parameter space** is **explored** systematically using a **Design of Experiments** (DOE) methodology.
- A **Fractional Factorial** design **method** is employed in **Matlab** using the script **Fractional.m**.
- The method reduced the number to **12 simulations** for the Equation of State study instead of 256.

Ruling Out Strength Model Parameters

- For a first pass, a simple **On/Off** analysis was used determine overall effect on jet tip velocity.
- 4 Simulations: Both On, Cu Off, SS Off, Both Off
- The **copper liner** overwhelmingly **controlled** the jet tip velocity **response**.
- The **stainless steel** confinement will be **ignored** for later parameter studies.



Testing for Non-Physical Parameter Combinations of the Jones-Wilkins-Lee (JWL) Equation of State (EOS)

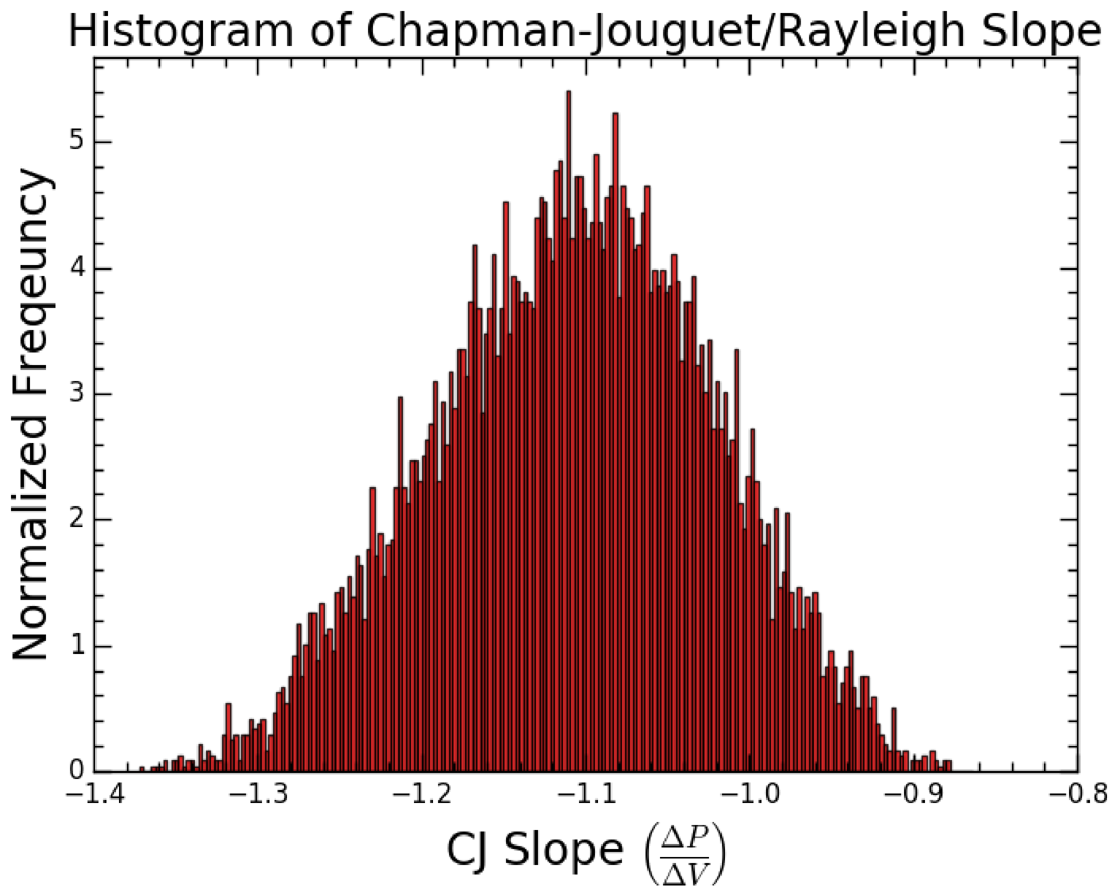
- The Monte Carlo sampling routine must not pick a non-physical parameter set to ensure appropriate uncertainty analysis.
- The Chapman-Jouguet slope was estimated to determine if the parameter set was physically possible (slope < 0).
- JWL parameters estimated from Composition B experiments were used as a basis for sampling [1] (assuming $P_0 = 0$, $V_0 = 1$)

Set	ρ_0	e_0	W	B1	C1	B2	C2	DetVel	CJ Slope
1	1.718	0.0617	0.28	5.849288	7.731	0.149834	2.577	0.7954	-1.04
2	1.694	0.064935	0.28	5.797578	7.623	0.114037	2.541	0.7876	-0.99
3	1.583	0.060095	0.28	4.652022	7.1235	0.130651	2.3745	0.751	-0.85
4	1.717	0.049505	0.34	5.242	7.2114	0.07678	1.8887	0.798	-1.08

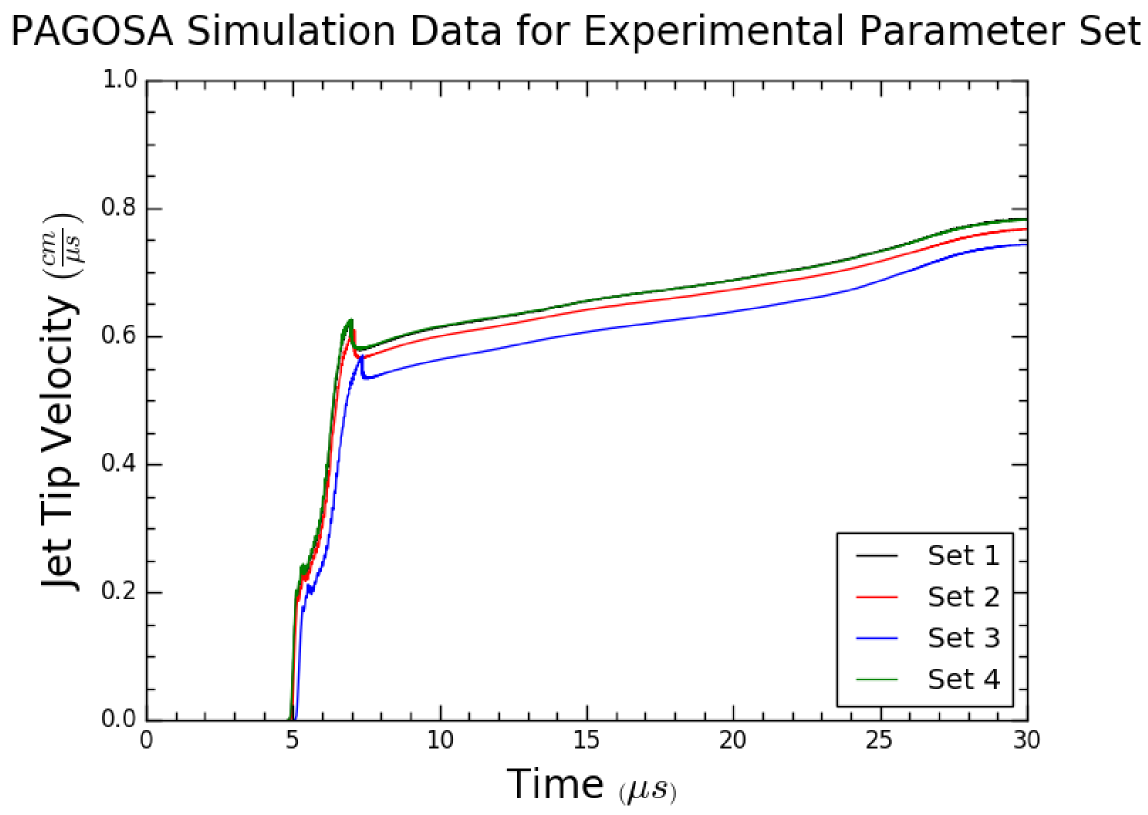
[1] Weseloh, W., “JWL in a Nutshell (rev.1),” PAGOSA Technical Note, Los Alamos National Laboratory XTD-SS, LA-UR-14-24318.

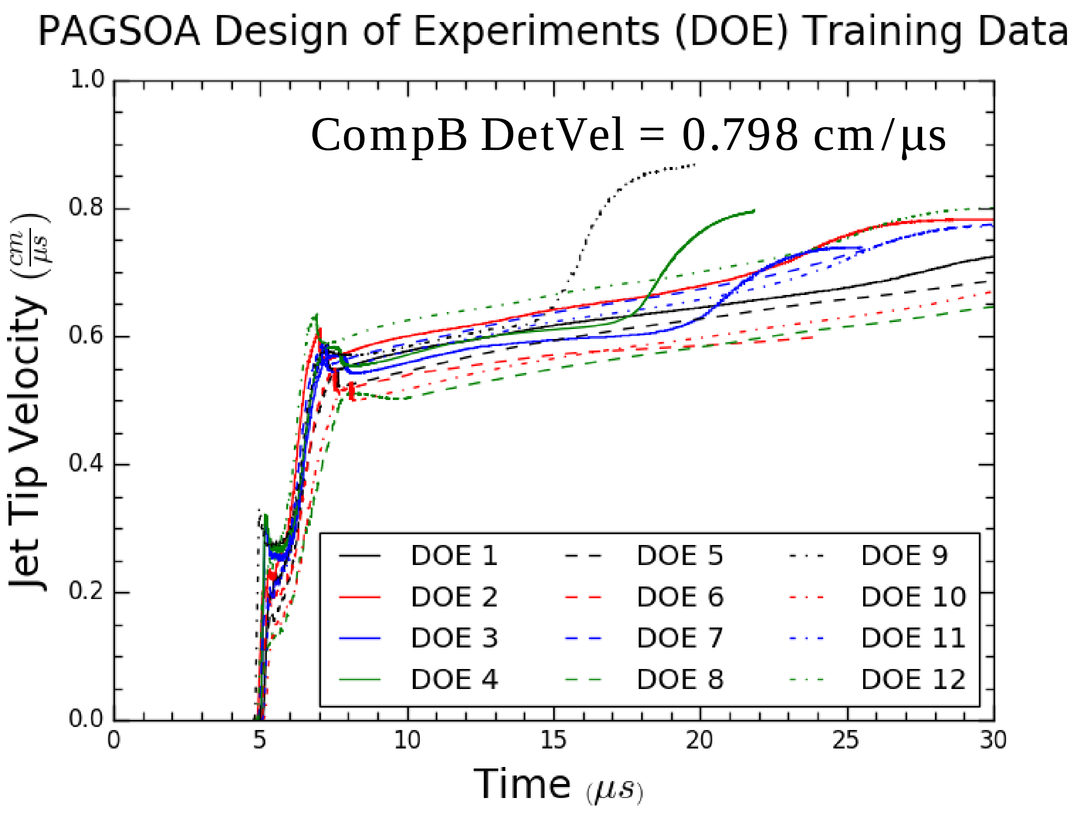
Monte Carlo Results of Chapman-Jouguet (CJ) State For Composition B

- Each parameter is sampled as a Uniform distribution from its minimum to maximum observed
- CJ State estimated for 10,000 samples
- All samples were determined to produce a negative slope (physical).



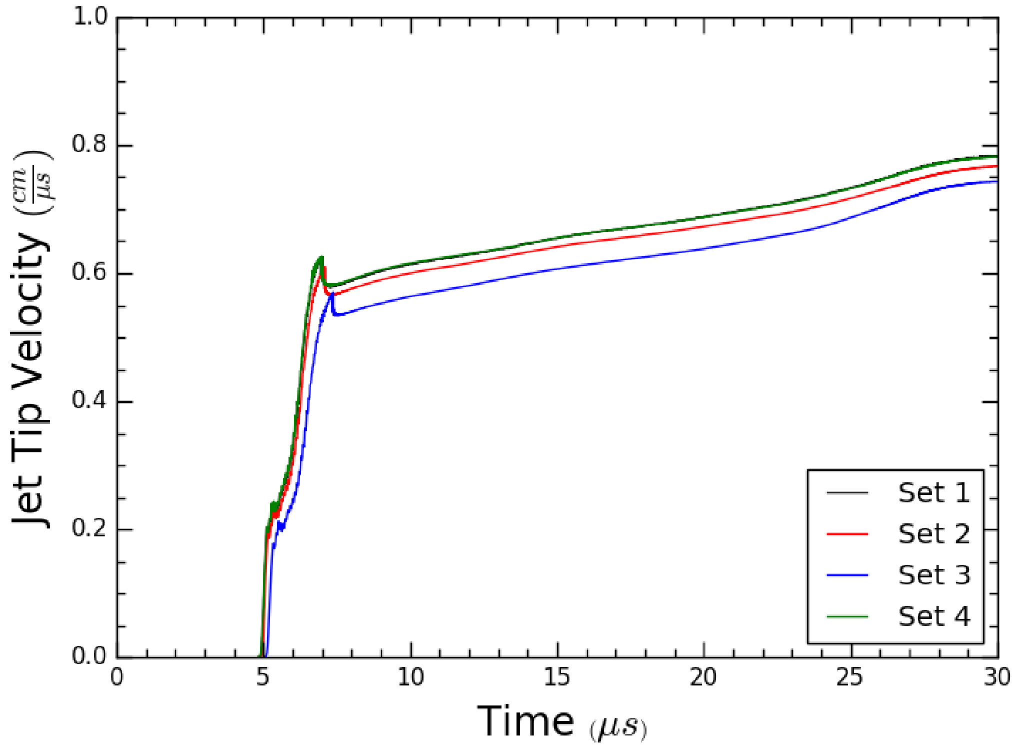
PAGOSA Jet Tip Velocity Data for Experimental Parameter Sets and Design of Experiments (DOE)



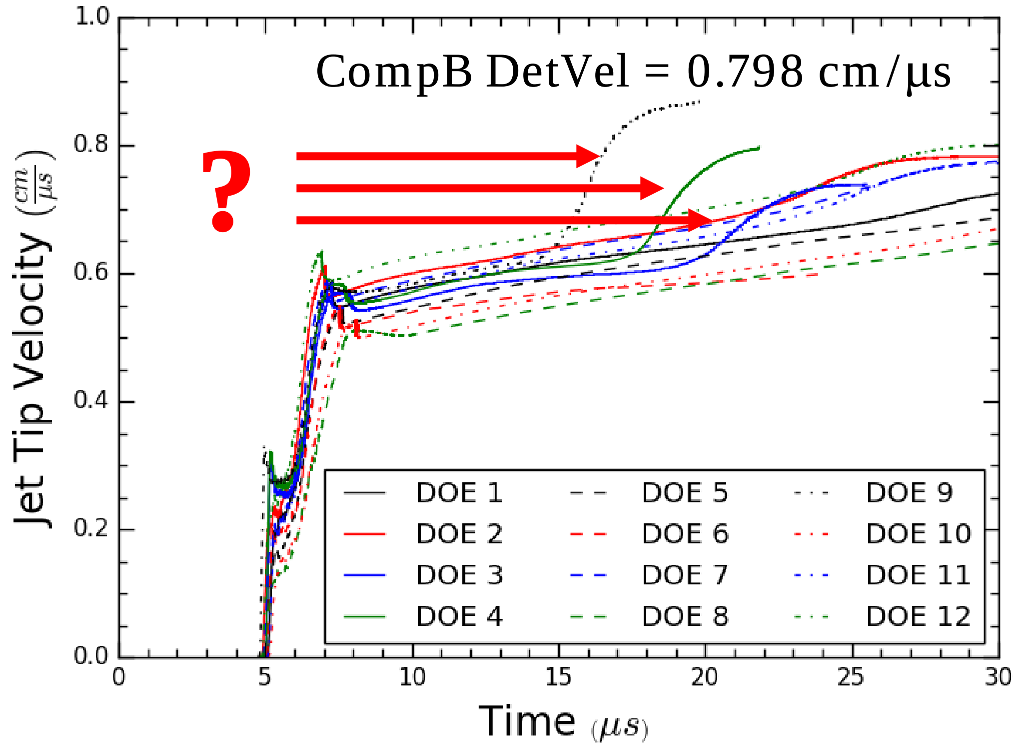


PAGOSA Jet Tip Velocity Data for Experimental Parameter Sets and Design of Experiments (DOE)

PAGOSA Simulation Data for Experimental Parameter Set



PAGSOA Design of Experiments (DOE) Training Data



Set	ρ_0	e_0	W	B1	C1	B2	C2	DetVel	CJ Slope
DOE 3	1.718	0.064935	0.34	4.652022	7.124	0.14983	2.577	0.751	-1.06
DOE 4	1.718	0.064935	0.28	4.652022	7.124	0.14983	1.889	0.751	-1.12
DOE 9	1.718	0.049505	0.28	5.849288	7.124	0.14983	2.577	0.798	-1.28

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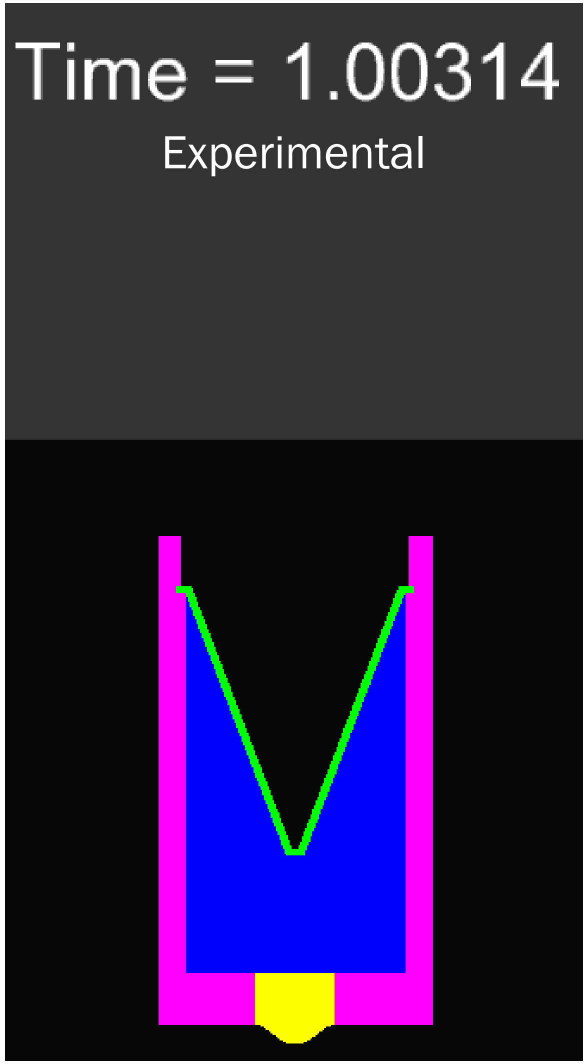
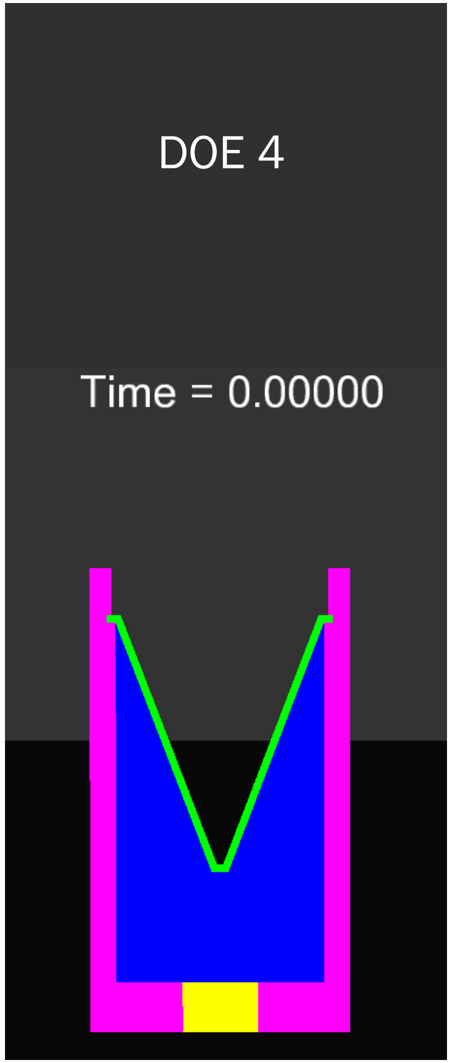
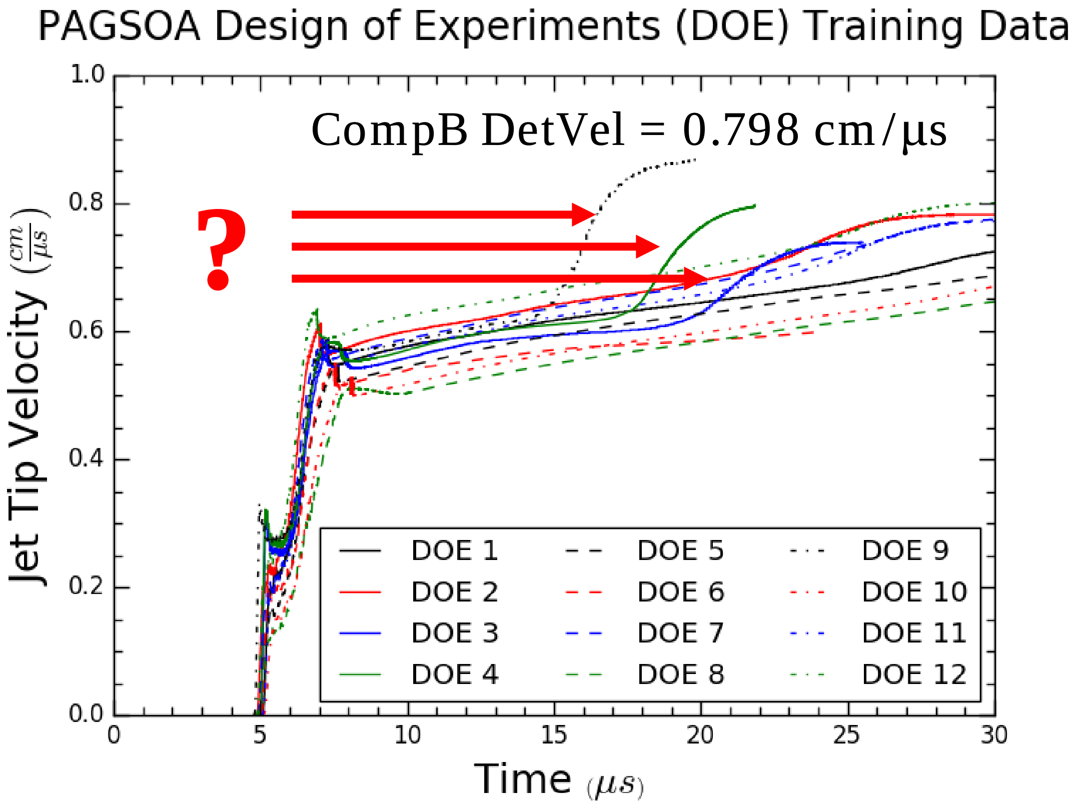
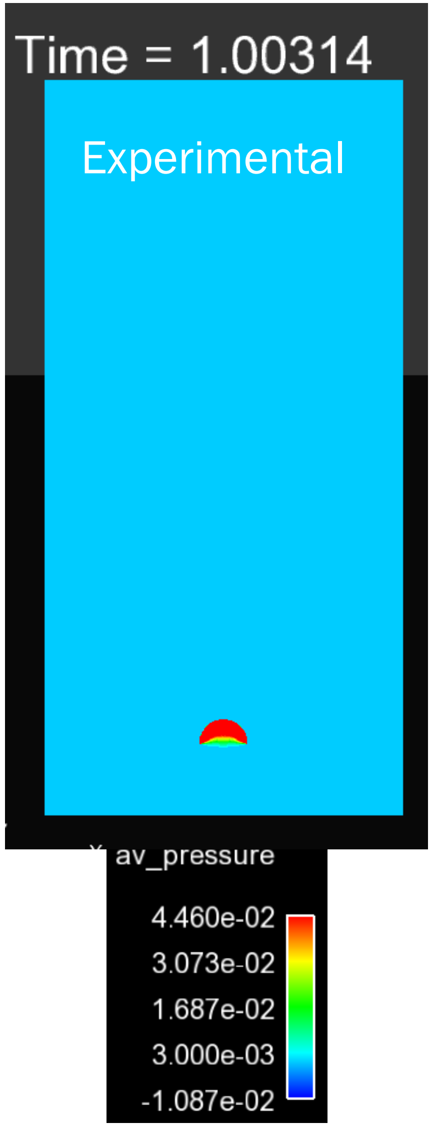


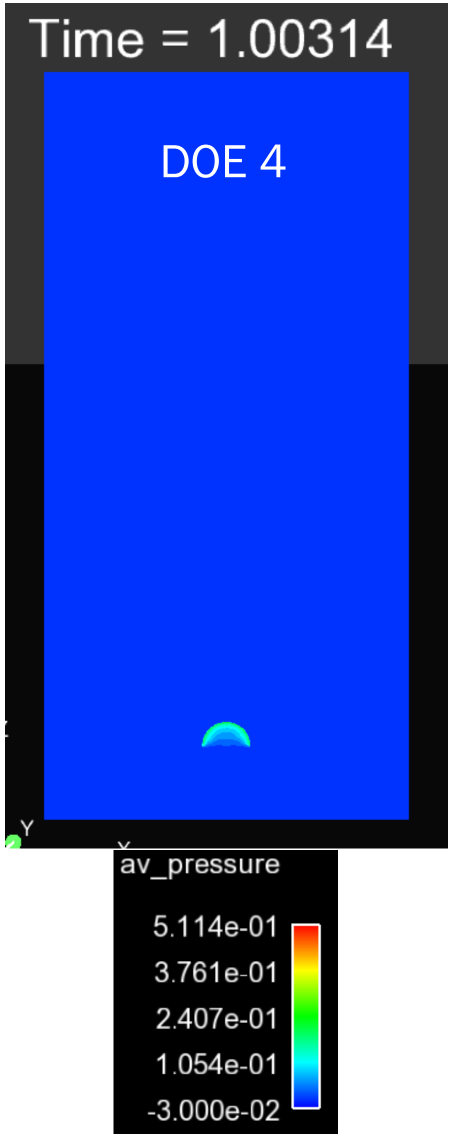


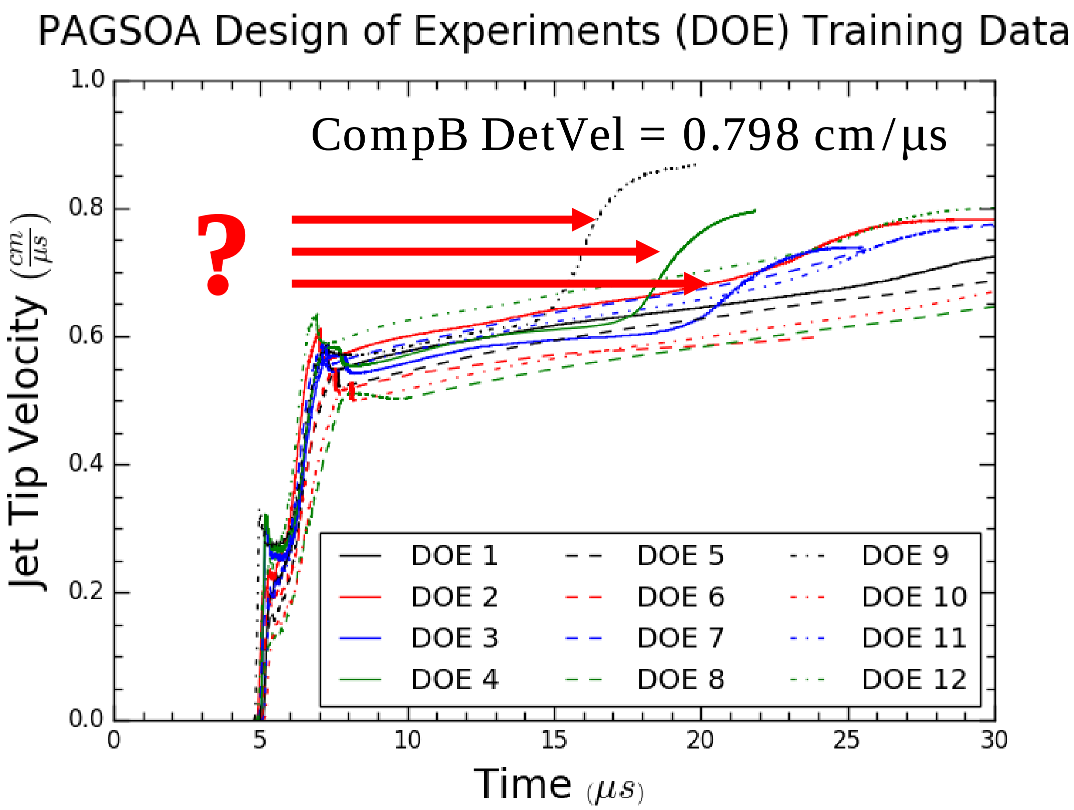


DOE 4: Copper liner disconnects from confinement canister

PAGOSA Jet Tip Velocity Data for Experimental Parameter Sets and Design of Experiments (DOE)







*Uncertainty and Sensitivity Analyses will be limited to less than 20 μs to use all data sets.

Radial Basis Function Network (RBFN) Error Study for the Inverse Multiquadric Basis Function

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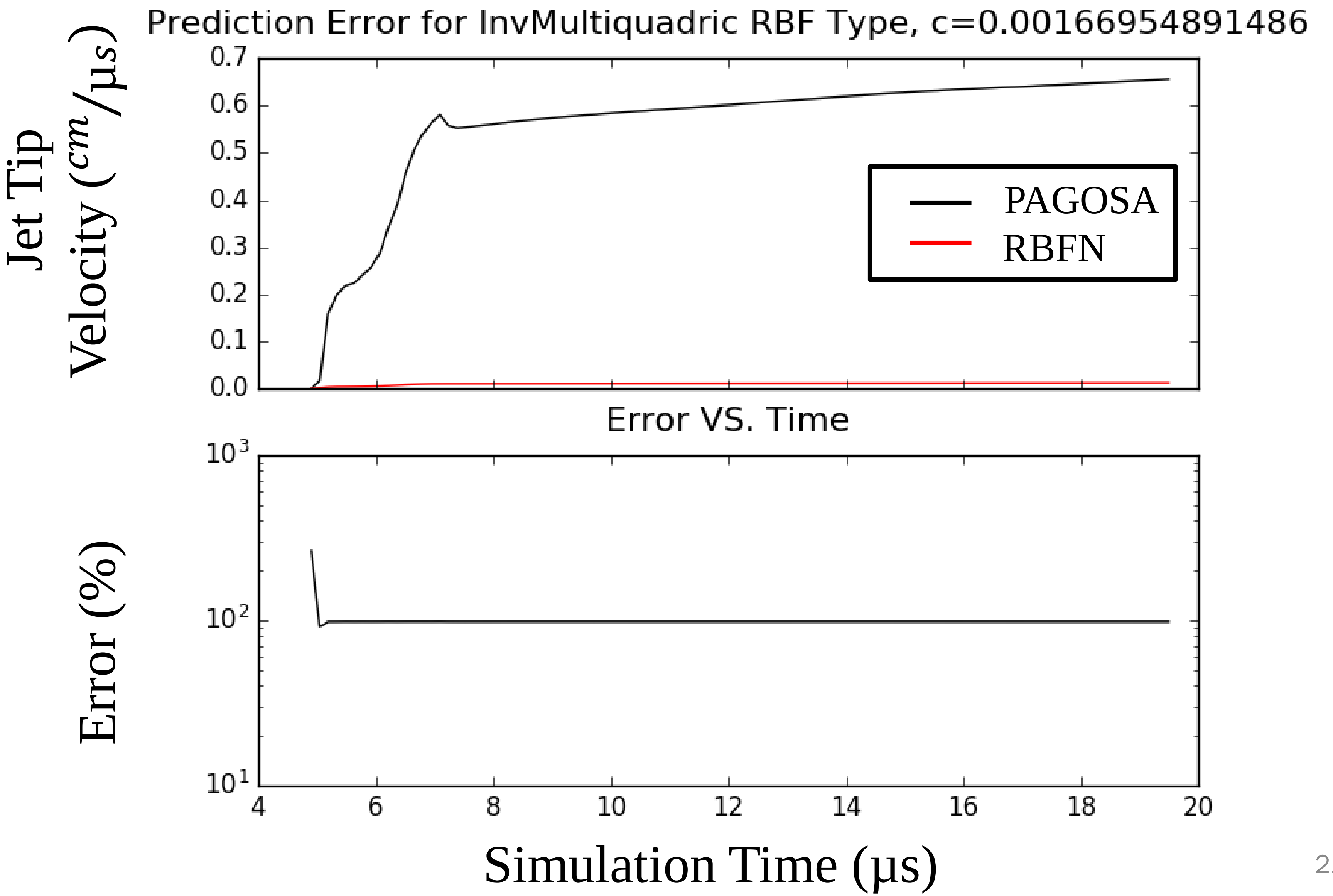
Basis Function

$$\varphi(r) = \frac{1}{\sqrt{r^2 - c^2}}$$



Radial Basis Function Network (RBFN) Error Study for the Multiquadric Basis Function

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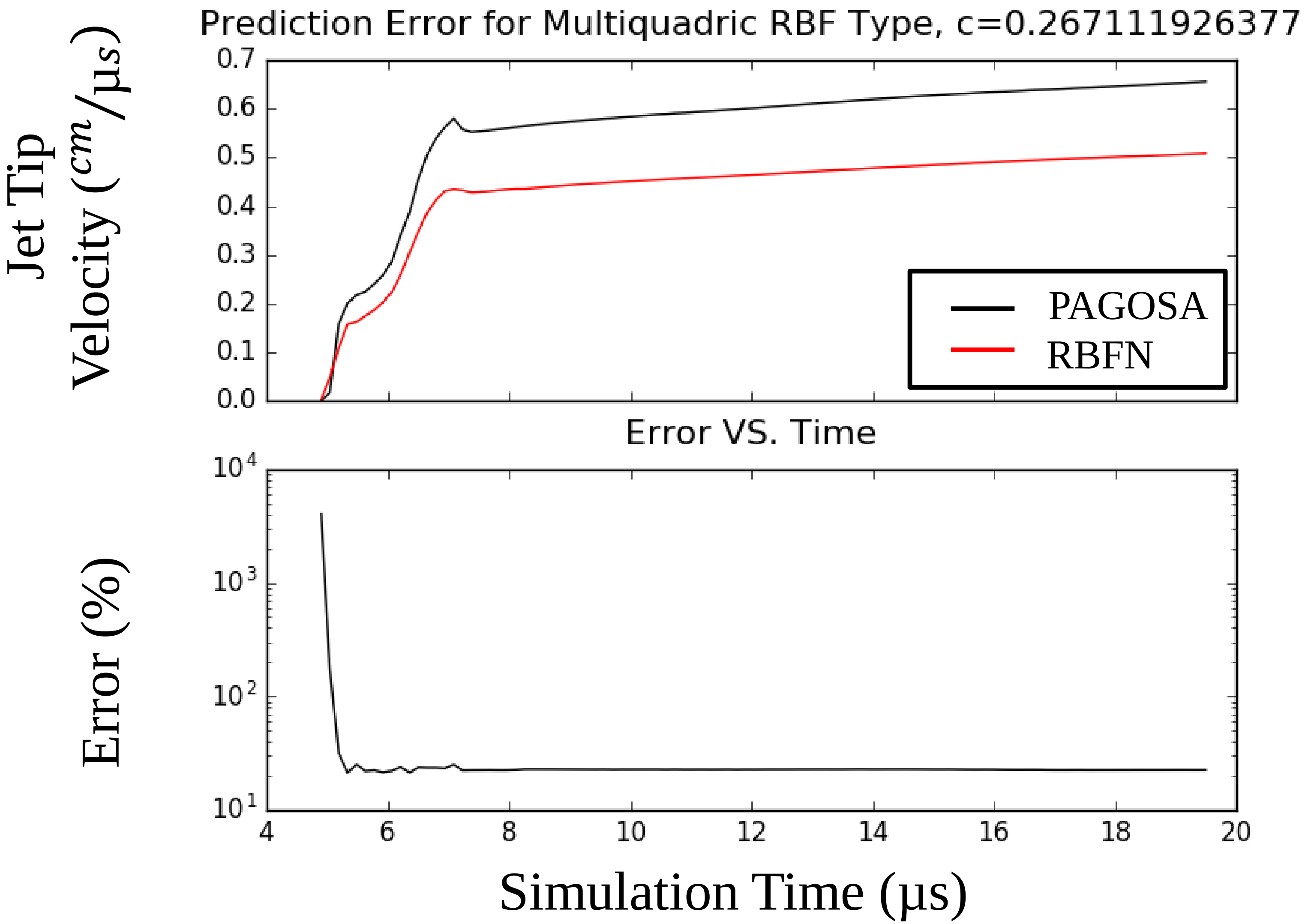
Basis Function

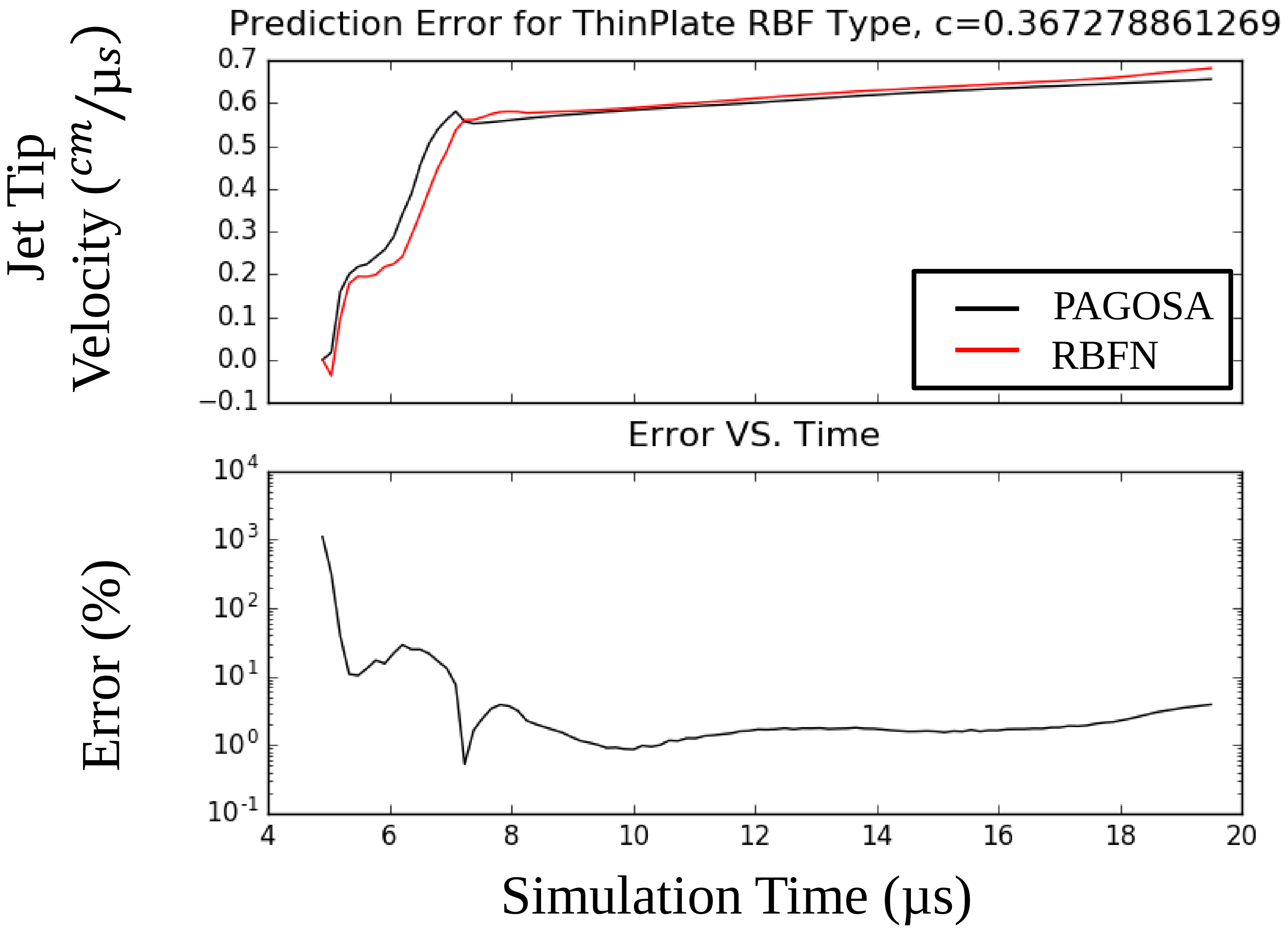
$$\varphi(r) = \sqrt{r^2 - c^2}$$



Radial Basis Function Network (RBFN) Error Study for the Thin Plate Basis Function

Basis Function

$$\varphi(r) = r^2 log(cr^2)$$



Radial Basis Function Network (RBFN) Error Study for the Gaussian Basis Function

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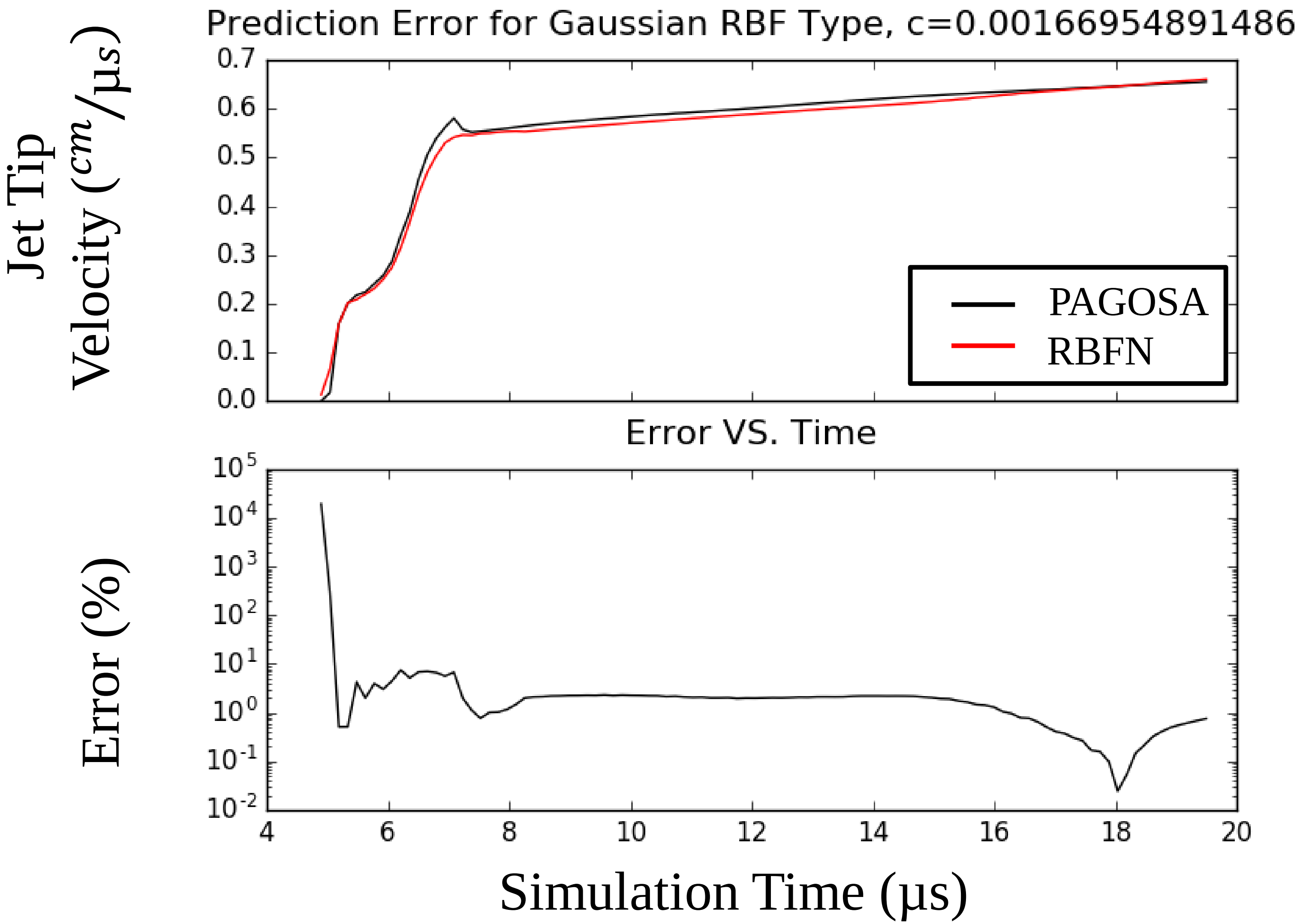
Basis Function

$$\varphi(r) = e^{-cr^2}$$



Uncertainty Quantification (UQ) for the BRL Shaped-Charge Jet Velocity

What is uncertainty?

- Qualitatively, **Uncertainty** is the **possibility of error** in experimentation and modeling.
- Quantitatively, **uncertainty** is a **mathematical description** of the **expected range of values** due to natural variation in experimentally measured quantities due to **imprecision** of **measurement systems** and material **manufacturing methods**.
- Since models are **calibrated** with **uncertain** experimental **data**, models will **inherit** this uncertainty.
- We can use various computational techniques to quantify the effects of uncertainty on modeling (forward propagation).
- If the distribution of the output is known (posterior), then a parameter's uncertainty can be approximated (inverse method)

Uncertainty Quantification Methods for Experiments and Modeling

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- Experimental Uncertainty
  - Statistical Confidence Intervals
- Modeling Uncertainty
  - Propagation of Uncertainty
    - Truncated Taylor Series Expansion Method [1]
  - Monte Carlo (MC) Methods
    - Random Sampling (Forward Propagation Method)
    - Acceptance/Rejection Sampling [2]
    - Markov-Chain Monte Carlo (MCMC) (Inverse Method) [3]
  - Generalized Polynomial Chaos (gPC) [4]
  - Latin Hypercube Sampling (Stratified Systematic Sampling)

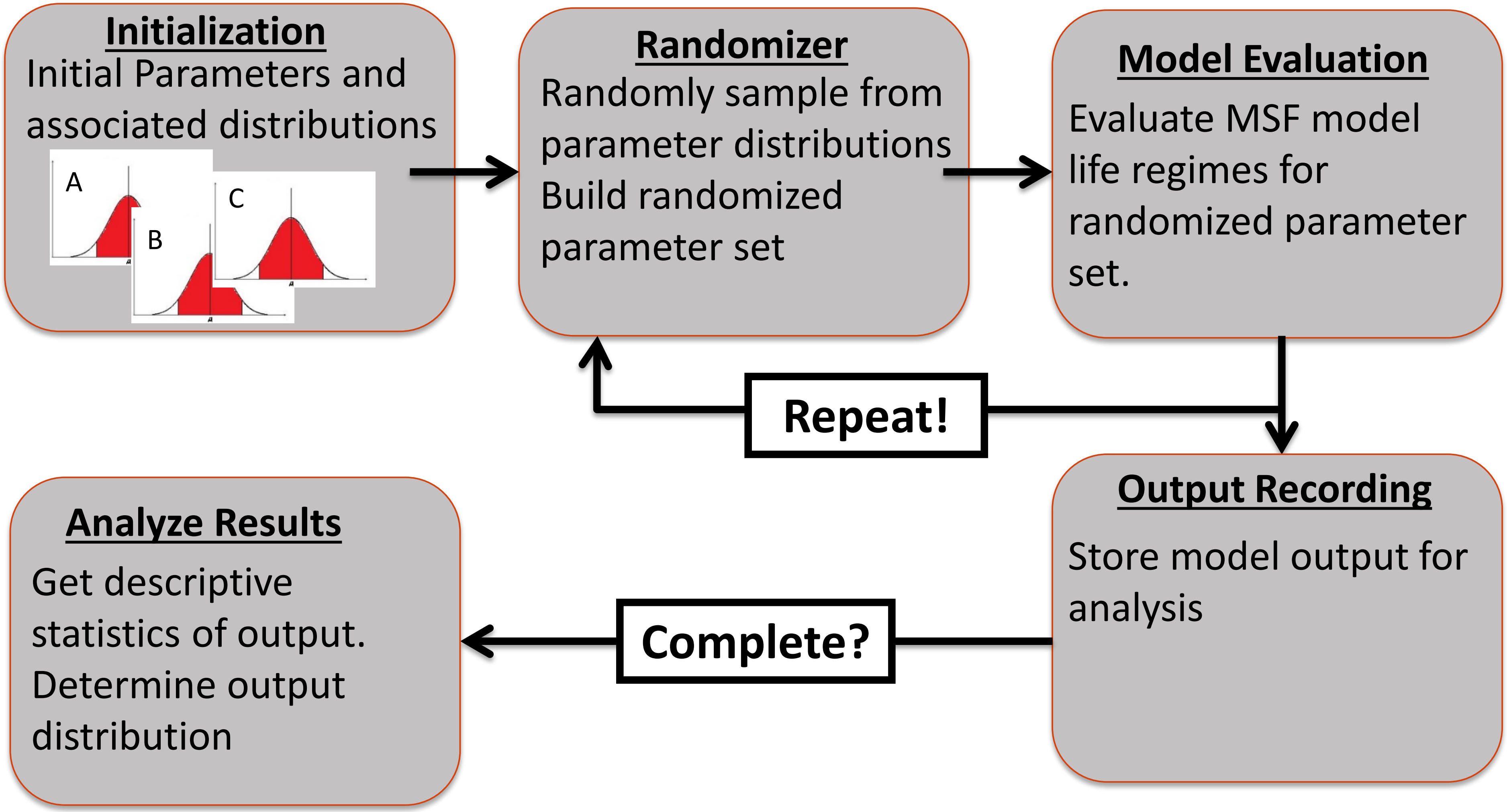
*Large-scale simulations rely on surrogate models to lower computational costs

[1] Coleman HW, Steel WG. *Experimentation and Uncertainty Analysis for Engineers*. 2nd Ed. New York: John Wiley and Sons; 1999.
[2] Martino, L, Miguez, J. Generalized rejection sampling schemes and applications in signal processing. Signal Processing. V90:11, 2981-2995. 2010.
[3] Moral, PD, Doucet, A, Jasra, A. Sequential Monte Carlo Samplers, Journal of the Royal Statistical Society: Series B (Statistical Methodology), V68:3, 411-436. 2006.
[4] D. Xiu, *Numerical Methods for Stochastic Computations: A Spectral Method Approach*. Princeton University Press, 2010.

Monte Carlo (MC) Simple Random Sampling for Uncertainty Propagation

- MC methods seek to propagate known (or assumed) statistical distributions through a model to determine the amount of variance in output
- This is done by sampling randomly from representative statistical distributions (priors) for each parameter of interest in a model
- Parameter sets are mapped through the model and descriptive statistics and histograms are collected to quantify the posterior statistical distribution.

Monte Carlo Random Sampling Method Workflow



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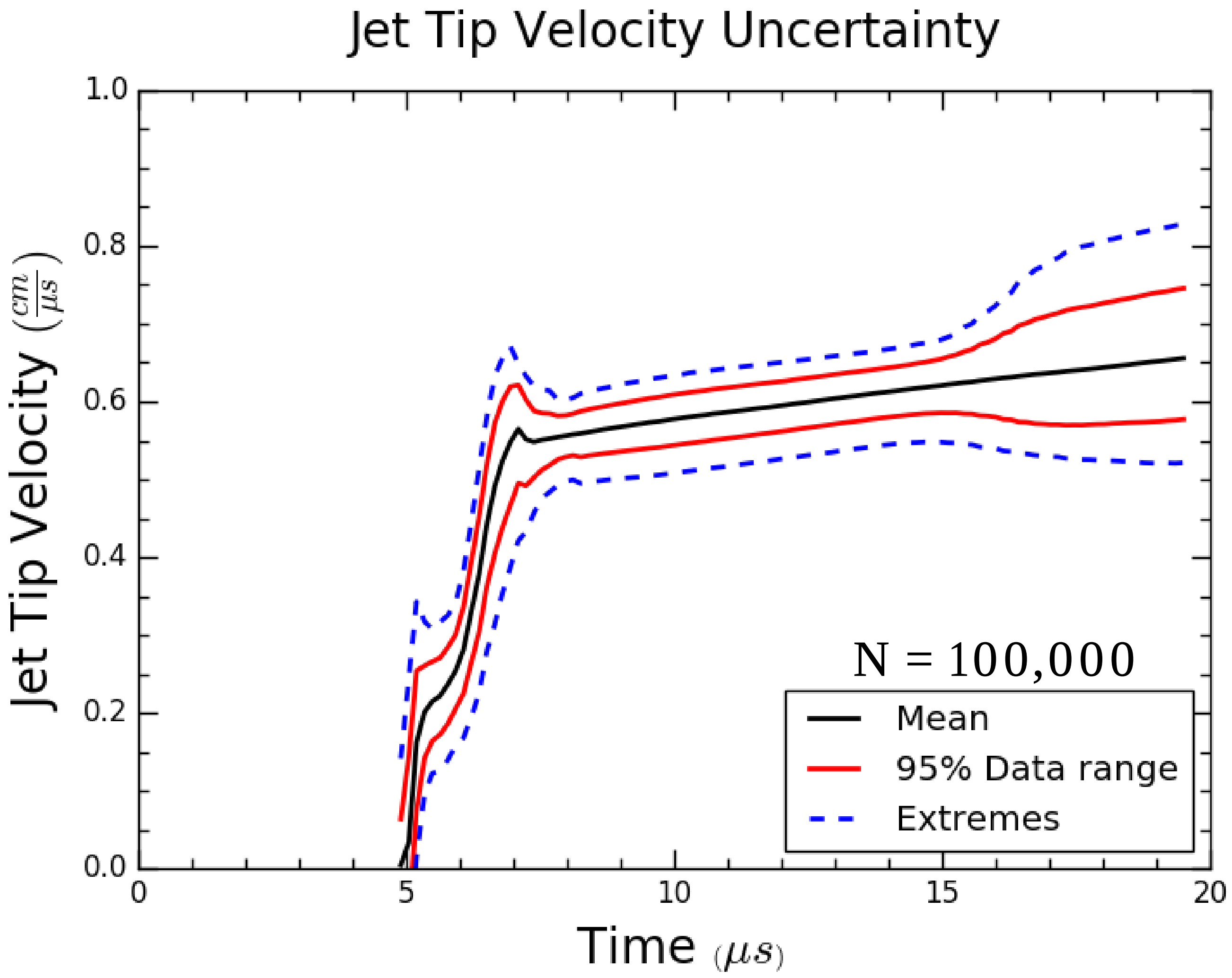
Uncertainty Resulting from Variation in Jones-Wilkins-Lee Parameters for Composition B



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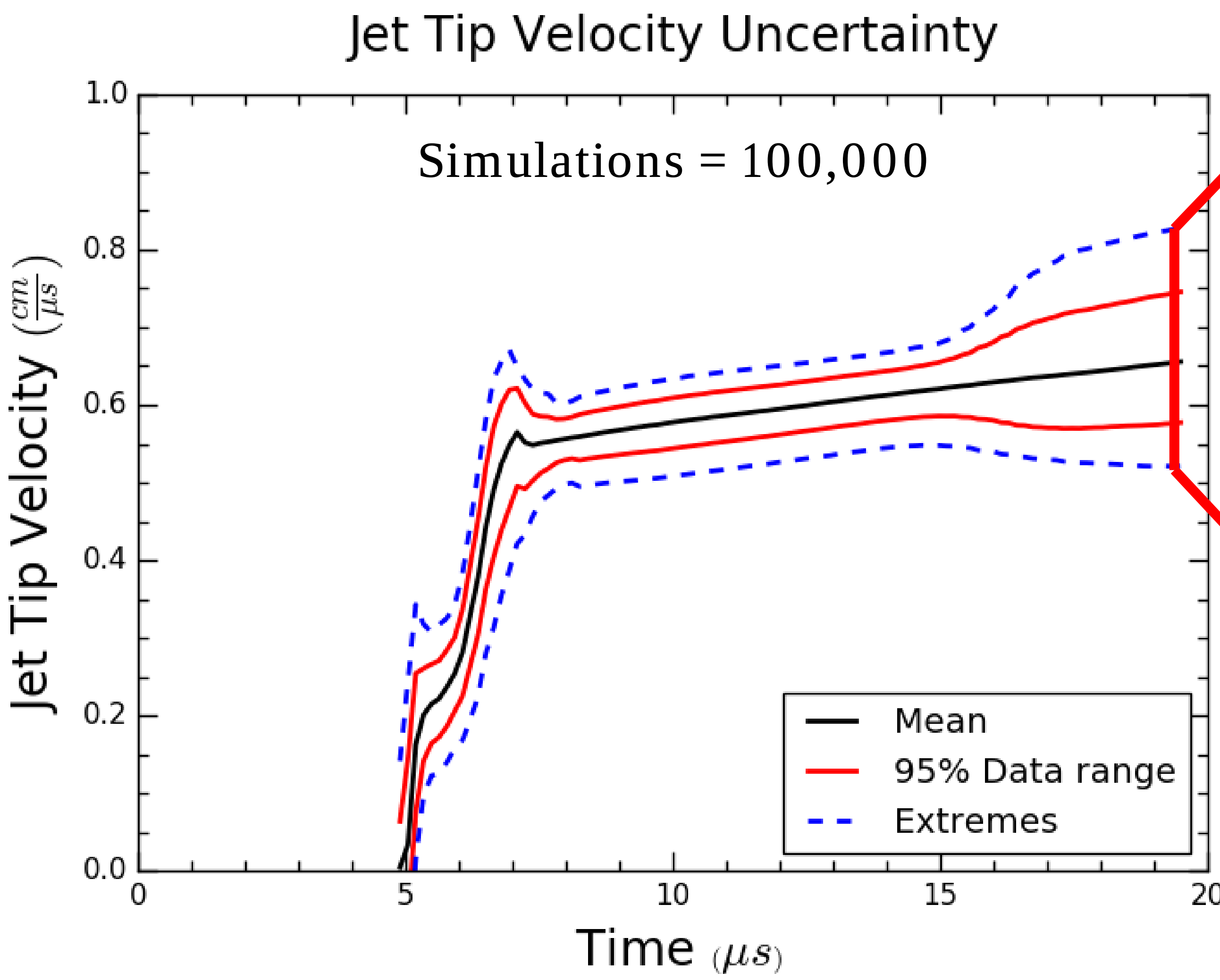
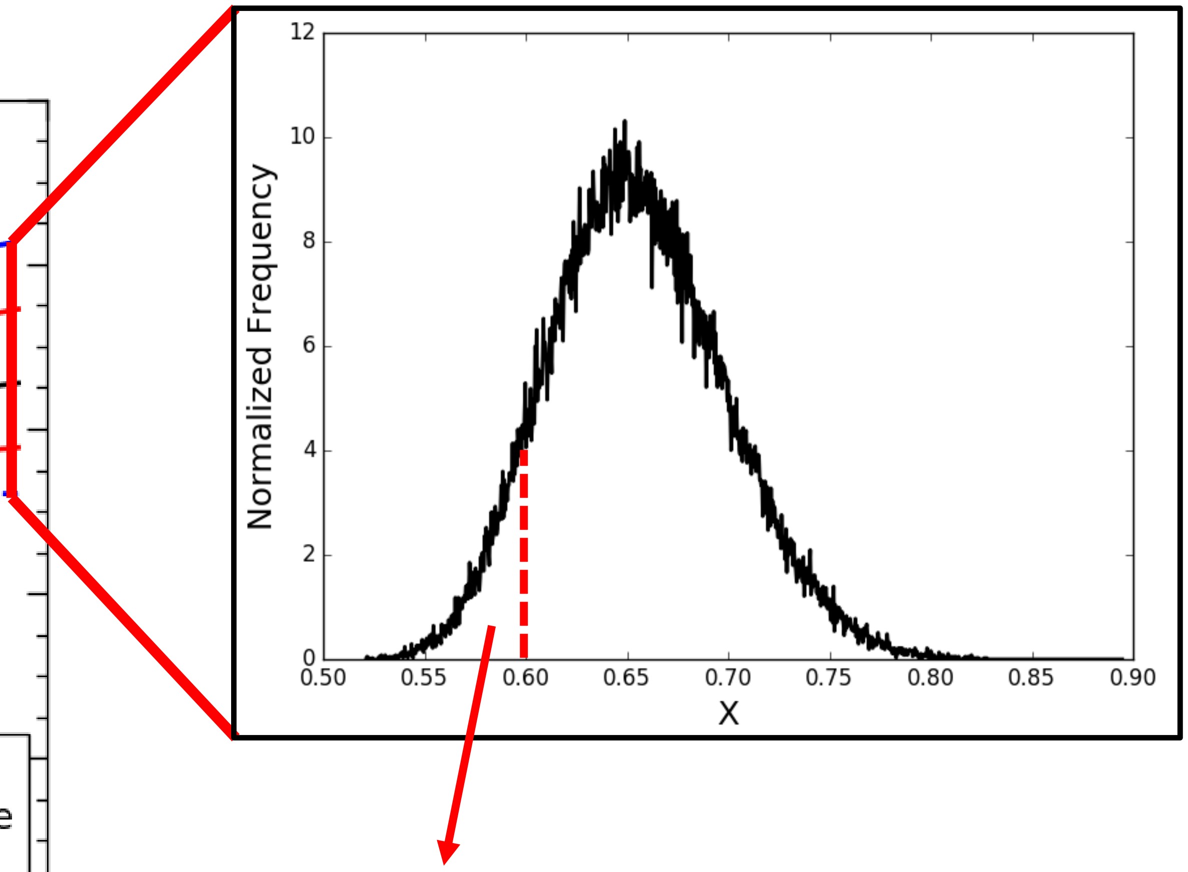
Uncertainty Resulting from Variation in Jones-Wilkins-Lee Parameters for Composition B





$$P\left(V_{jet} < V_{Critical}\right)$$

Sensitivity Analysis (SA) for the BRL Shaped-Charge Jet Velocity

What is meant by "Sensitivity Analysis"?

- **Sensitivity Analysis (SA)** is a general idea for **measuring** a parameter's **influence** on modeling **output**.
- Two main **analysis** types: **Local** and **Global**
- **Local methods** can give an idea of a how influential a parameter is but only examines a **single point** within the entirety of the a model's N-dimensional input space.
- Analysis of Variance (ANOVA) **global methods** seek to describe the **contribution** of a given parameter to the **total variance** of model **output** by passing the parameter's distribution through the model.

Sensitivity Analysis Methods for Modeling

- Local Methods
  - Partial derivatives [1] via perturbation method
- Global Methods
  - First Order Effects Index [2]
    - Monte Carlo method
    - Fourier Amplitude Sensitivity Testing (FAST) [2]
  - Total Effects Index [3]

Large-scale simulations rely on surrogate models to lower computational costs

[1] Coleman HW, Steel WG. *Experimentation and Uncertainty Analysis for Engineers*. 2nd Ed. New York: John Wiley and Sons; 1999.
[2] Saltelli, A., Tarantola, S., Chan, K.P.-S., "A Quantitative Model-Independent Method for Global Sensitivity Analysis of Model Output", Technometrics, Vol 41, No 1, Feb 1999.
[3] Saltelli, A., Paola, A., Azzini, I., Campolongo, F., Ratto, M., Tarantola, S., "Variance-based sensitivity analysis of model output. Design and estimator for the total sensitivity index," Computer Physics Communications, Vol 181, pp 259-270, 2010.

Global Methods: First Order Effects Index

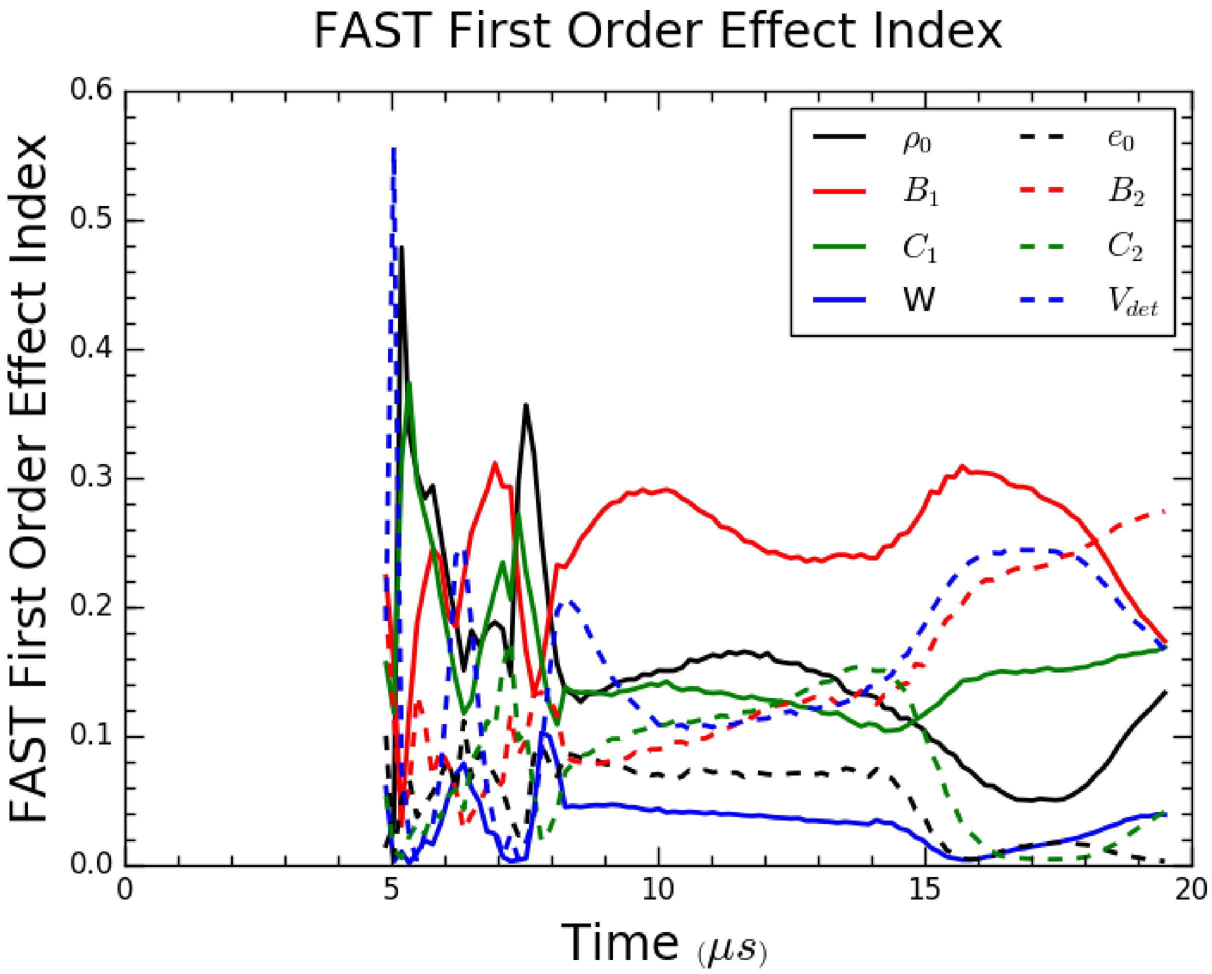
- Analysis of Variance (ANOVA) method
- First order effects indices measure a parameters direct contribution to the overall model variance

$$S_i = \frac{Var(Y|x_i)}{Var(Y)}$$

- Where,
  - $Var(Y|x_i)$ is the variance of model Y by varying parameter x_i alone
  - $Var(Y)$ is the total variance of model Y by varying all parameters together
- Monte Carlo methods can be used to get these quantities directly, however this can be very computationally expensive ($9\text{x}10^4$ versus 1704 function evaluations)

Fourier Amplitude Sensitivity Test (FAST) First Order Effects Indices for Jones-Wilkins-Lee Parameters of Composition B

- Detonation Velocity (V_{det}), Initial Density (ρ_0), and C_1 controls initial liner velocity
- B_1 controls majority of initial jet formation while B_2 controls late time formation
- W will be ignored as insignificant ($S < 0.1$)



$$P = f\left[\frac{WE}{V} + B_1\frac{C_1V - W}{C_1V} + B_2\frac{C_2V - W}{C_2V}\right]$$

Uncertainty and Sensitivity for PAGOSA Simulations Due to Variation in Jones-Wilkins-Lee Parameters

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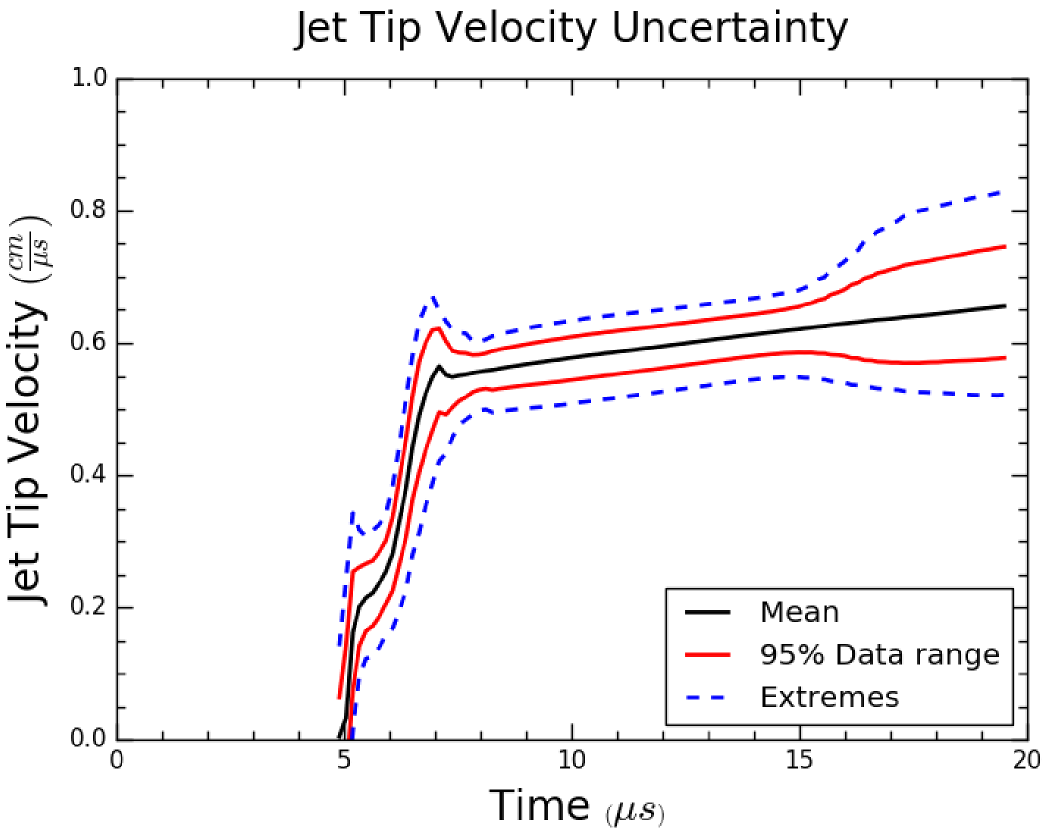

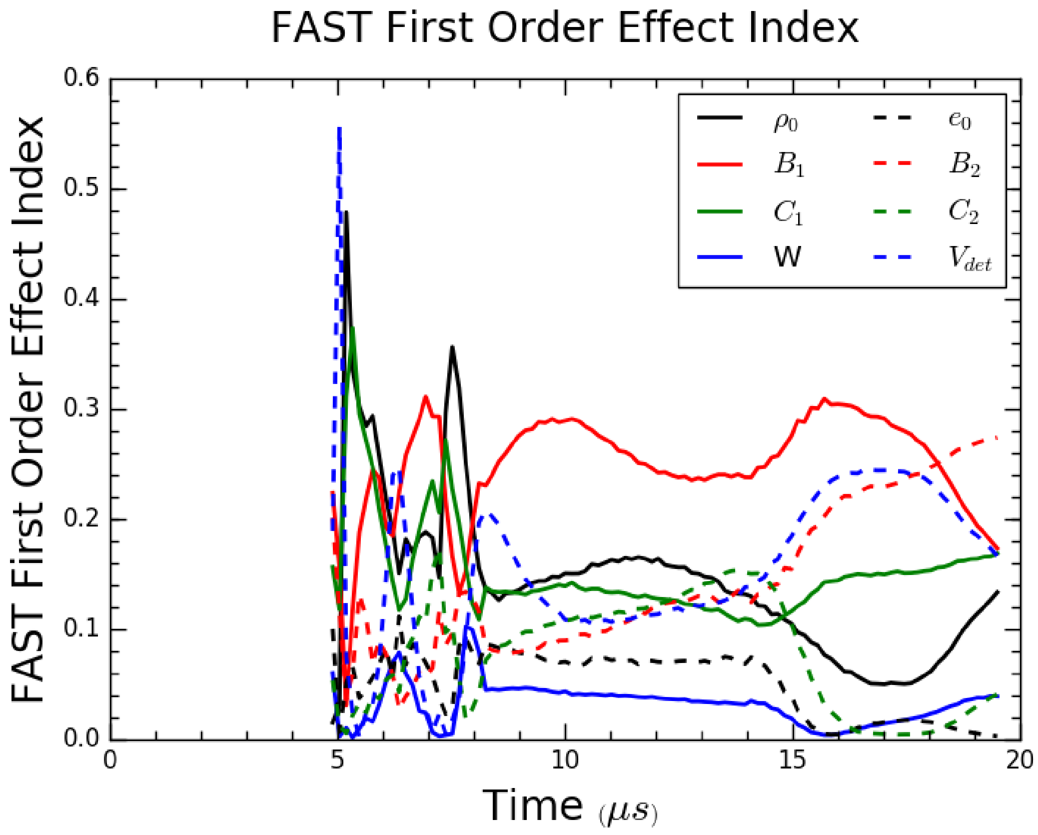

Summary

- A mesh convergence study was used to ensure that solutions were numerically stable by comparing PDV data between simulations.
- A Design of Experiments (DOE) method was used to reduce the simulation space to study the effects of the Jones-Wilkins-Lee (JWL) Parameters for the Composition B main charge.
- Uncertainty was quantified by computing the 95% data range about the median of simulation output using a brute force Monte Carlo (MC) random sampling method.
- Parameter sensitivities were quantified using the Fourier Amplitude Sensitivity Test (FAST) spectral analysis method where it was determined that detonation velocity, initial density, C1, and B1 controlled jet tip velocity.

Future Work/Improvements

- Improve parameter sampling method to ensure thermodynamical consistency for the Jones-Wilkins-Lee (JWL) Equation of State (EOS) (Implement rejection criterion)
- Investigate effects of variation in parameters from both EOS's and strength models together (EOS: Copper Liner, CompB, Steel, Tetryl Booster; Strength: Copper Liner)

Questions?

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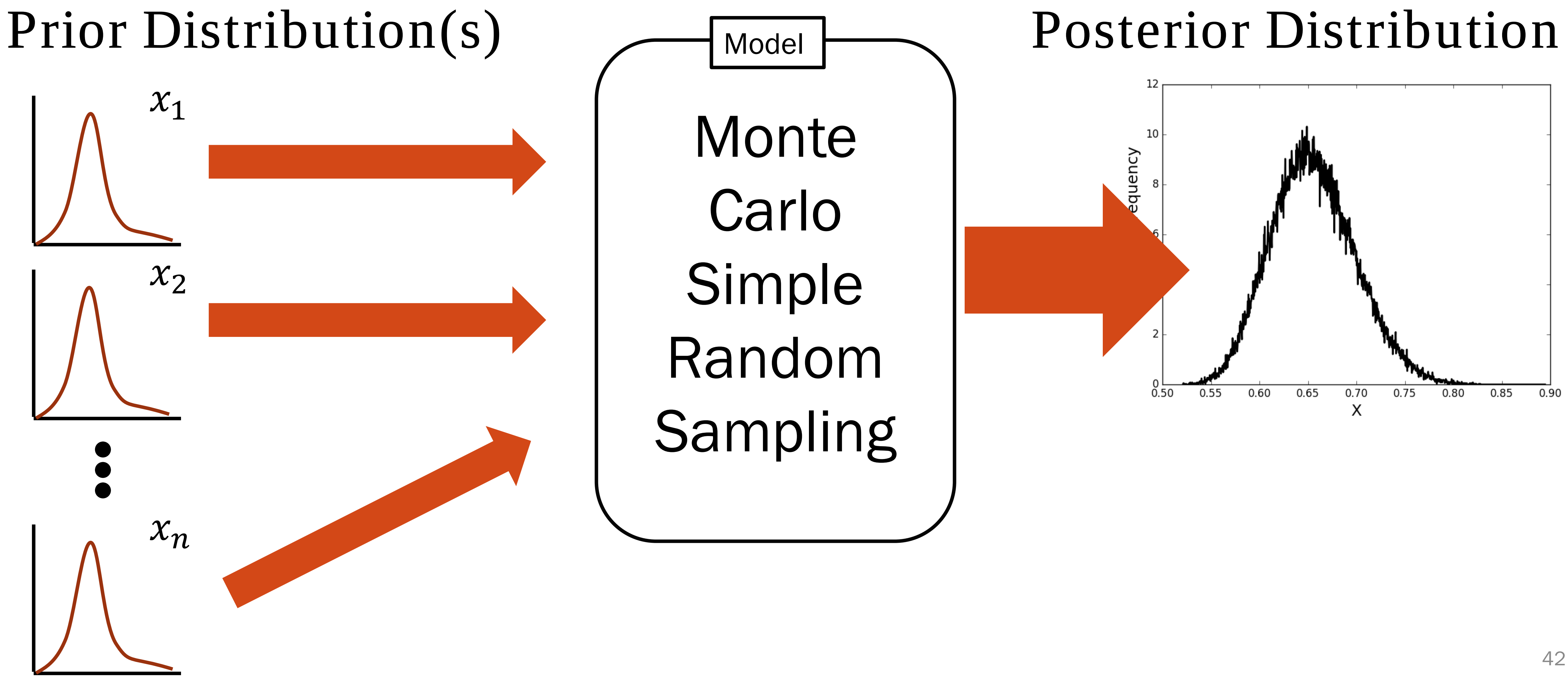
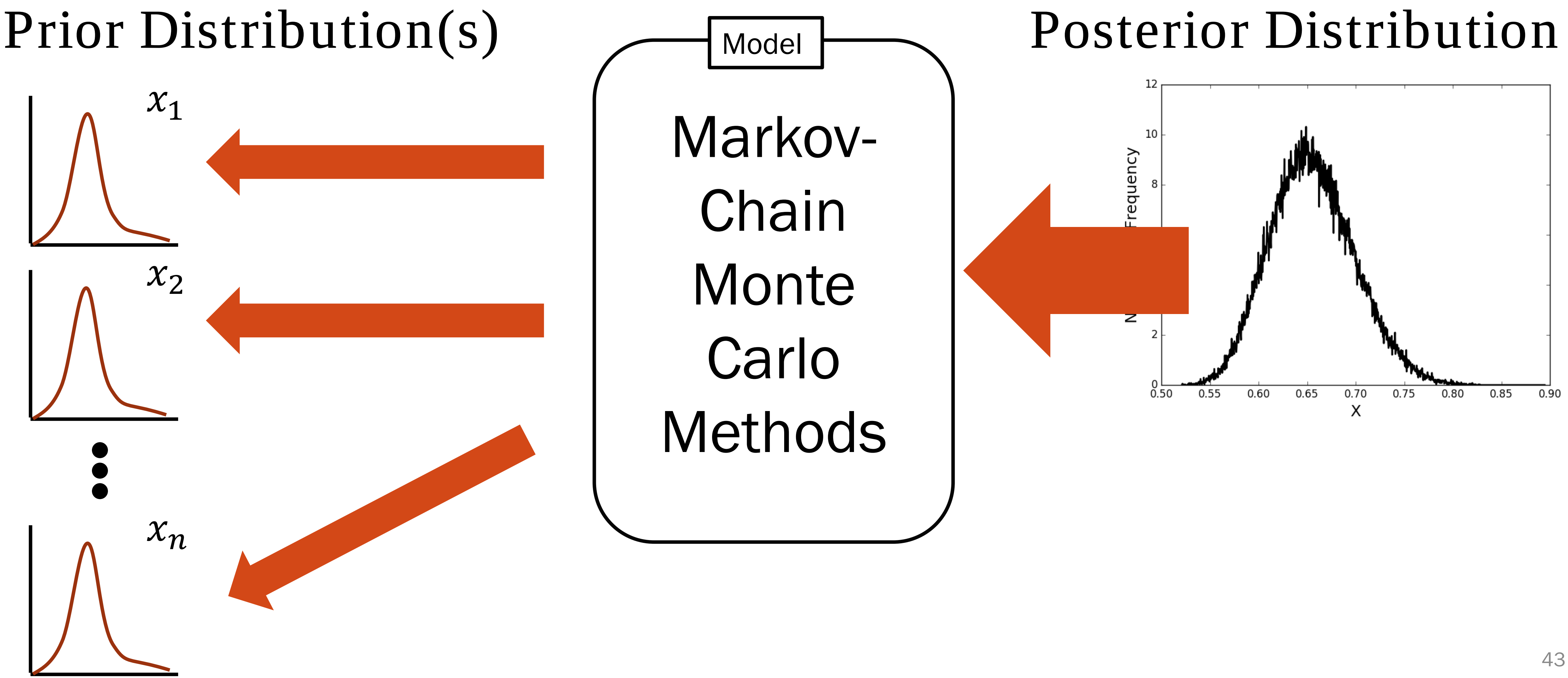
Appendix

Forward Propagation Monte Carlo Method



Inverse Monte Carlo Method



Required Python Packages for the Included Analysis Scripts

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- NumPy – multi-dimensional array support
- SciPy – library of scientific tools
- MatPlotLib – Matlab-like plotting package

The installation method will vary depending on your platform (Windows, Unix) and Python installation (basic, Anaconda).

Summary of Scripts Used

- Fractional.m – Fractional Factorial Design of Experiments (DOE)
- Taguchi.m – Taguchi Design of Experiments (DOE)
- pdv_read.py – Python extractor for PAGOSA PDV data
- xy_interp.py – Linear interpolator to ensure that all datasets are in the same x coordinates. Can also be used to shorten datasets.
- sgfilter.py – Savitsky-Golay smoothing algorithm for noisy datasets
- rbfTrain.py – Training script for investigating error using four implemented basis functions
- UQSA.py – Automated routines for uncertainty quantification and sensitivity analysis

Design of Experiments (DOE) Matrix for BRL Shaped-Charge Simulation Study

Set	ρ_0	e_0	W	B1	C1	B2	C2	DetVel	CJ Slope
1	1.718	0.049505	0.34	5.849288	7.731	0.07678	1.889	0.751	-0.98
2	1.583	0.064935	0.34	5.8492888	7.124	0.07678	1.889	0.798	-0.97
3	1.718	0.064935	0.34	4.652022	7.124	0.14983	2.577	0.751	-1.06
4	1.718	0.064935	0.28	4.652022	7.124	0.14983	1.889	0.751	-1.12
5	1.718	0.049505	0.28	4.652022	7.731	0.07678	1.889	0.798	-0.81
6	1.583	0.049505	0.28	5.849288	7.124	0.07678	2.577	0.751	-0.94
7	1.583	0.049505	0.34	4.652022	7.124	0.14983	1.889	0.798	-0.92
8	1.583	0.064935	0.28	4.652022	7.731	0.07678	2.577	0.798	-0.61
9	1.718	0.049505	0.28	5.849288	7.124	0.14983	2.577	0.798	-1.28
10	1.583	0.049505	0.34	4.652022	7.731	0.14983	2.577	0.751	-0.7
11	1.583	0.064935	0.28	5.849288	7.731	0.14983	1.889	0.751	-0.89
12	1.718	0.064935	0.34	5.849288	7.731	0.14983	2.577	0.798	-1.04

The Fourier Amplitude Sensitivity Test (FAST) Method

Analysis of Variance (ANOVA)

- Total Variance breakdown:

$$V_T = \sum_{i=1}^{n} V_i + \sum_{i=1}^{n} \sum_{j=i+1}^{n} V_{ij} + \sum_{i=1}^{n} \sum_{j=i+1}^{n} \sum_{k=i+2}^{n} V_{ijk} + \cdots + H.O.T.$$

First Order — Second Order — Third Order

The total number of variance terms scales as:

$$Evaluations = (2^{Factors} - 1) * Simulations$$

To put this in perspective, for capturing these effects for the PAGOSA simulations:

$$(2^8 - 1) * 10000 * \frac{0.5\ hr}{1\ sim} \frac{1\ day}{24\ hr} \frac{1\ year}{365\ days} = 145.6\ years\ cpu\ time$$

Fourier Amplitude Sensitivity Test (FAST) for First Order Effects Indices

- Divide by the total variance to obtain all the sensitivity indices:

$$1 = \sum_{i=1}^{n} S_i + \sum_{i=1}^{n} \sum_{j=i+1}^{n} S_{ij} + \sum_{i=1}^{n} \sum_{j=i+1}^{n} \sum_{k=i+2}^{n} S_{ijk} + \cdots + H.O.T.$$

First Order Effects Index

Method	Scales as	Evalutations Needed
Monte Carlo	$Factors * Simulatons$	80000 (8, 10k)
FAST	$(2M\omega_{max} + 1)$	1697 (M=16, ω_{max}=53)

Fourier Amplitude Sensitivity Testing (FAST) for First Order Effects Indices

- FAST is a much quicker method for computing sensitivity measures over a Monte Carlo approach
- Each parameter is represented by a cyclic function known as a search curve that approximates a statistical distribution when sampled.
- For uniformly distributed variables [1]:

$$x(\theta) = (x_{max} - x_{min})\left[\frac{1}{2} + \frac{1}{\pi}\text{asin}(\sin(\omega\theta + \varphi))\right] + x_{min}$$

[1] Saltelli, A., Tarantola, S., Chan, K.P.-S., "A Quantitative Model-Independent Method for Global Sensitivity Analysis of Model Output", Technometrics, Vol 41, No 1, Feb 1999.

Uniform Distribution Search Curve

$$x(\theta) = (x_{max} - x_{min})\left[\frac{1}{2} + \frac{1}{\pi}\operatorname{asin}(\sin(\omega\theta + \varphi))\right] + x_{min}$$

- Where

  x_{max} is the maximum value of the parameter

  x_{min} is the minimum value of the parameter

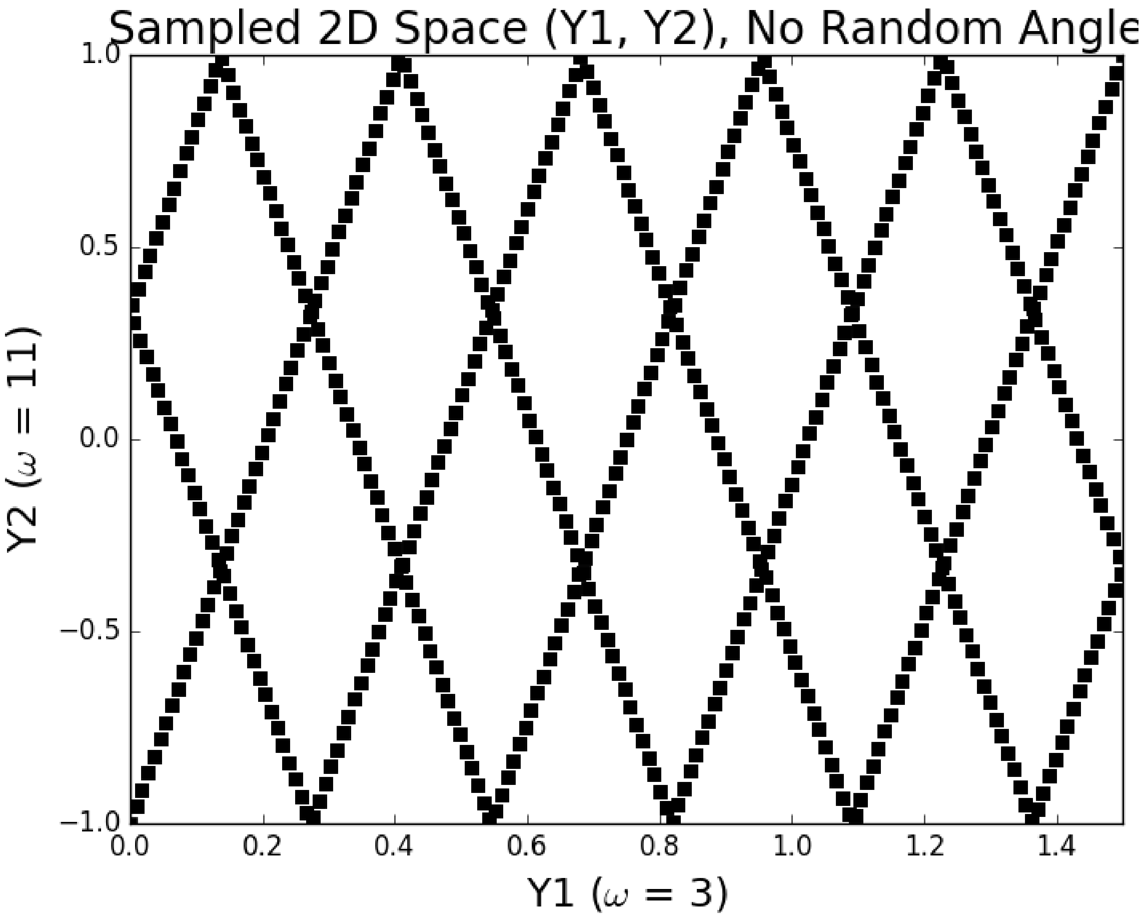
  ω is the parameter frequency

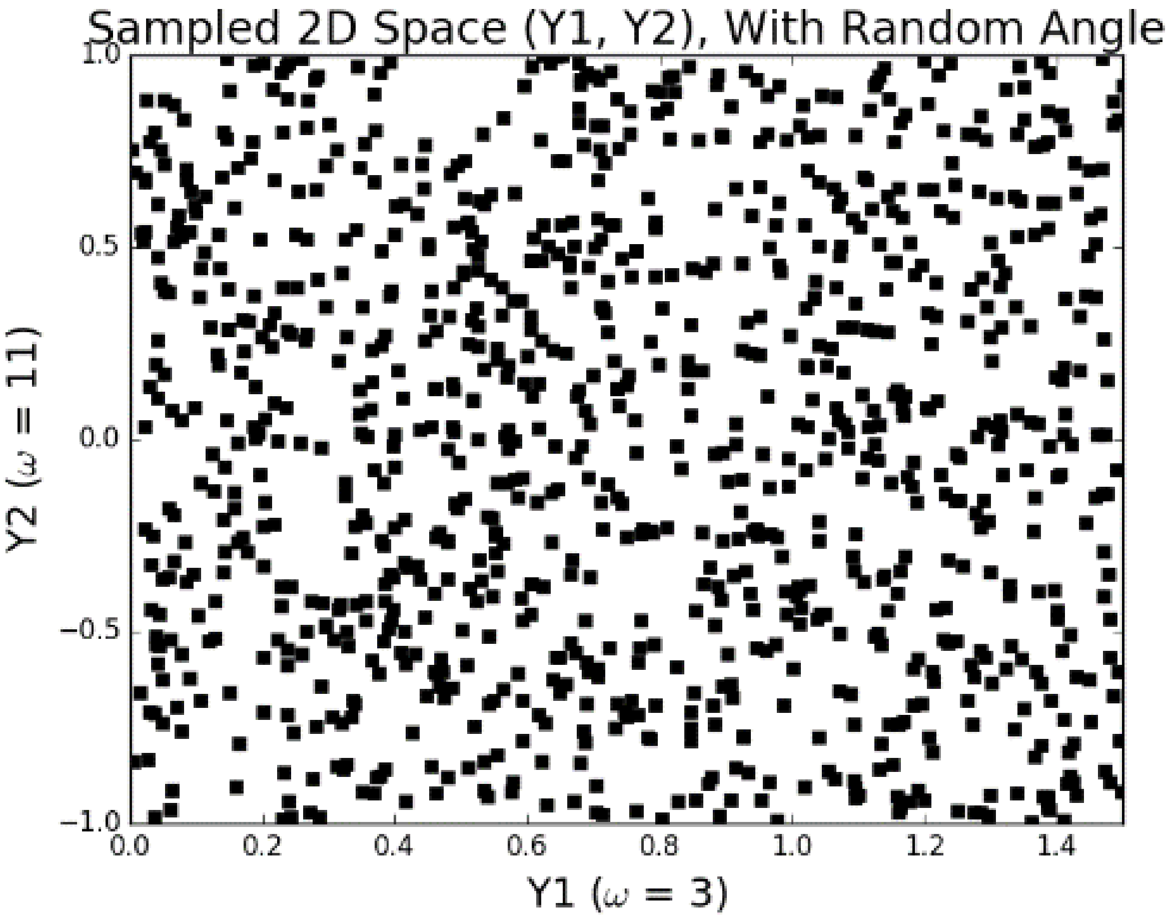
  φ is a random value from a uniform distribution from 0 to 1

- The phase angle, φ, serves to improve the sampling of parameter space and make sampling less regular.
- For each variable of a model, each frequency must be incommensurate (orthogonal) such that they do not share higher order resonant frequencies. (e.g. primes)

Uniform Distribution Search Curve With and Without a Random Phase Angle

- Inclusion of the random phase angle makes the sampling more "space filling"





Fourier Amplitude Sensitivity Testing (FAST) Theory

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- The FAST method is essentially applying multiple Fourier filters to a single data set.
- For an N-dimensional model, the complex Fourier transform is:

$$\underline{x} = (x_1, x_2, \dots, x_N)$$

$$f(\underline{s}) = \int_{\boldsymbol{R}^N} e^{-2\pi i \underline{x}} f(\underline{x}) d\underline{x} = \iint \dots \int e^{-2\pi i (x_1 s_1 + x_2 s_2 + \cdots x_N s_N)} f(\underline{x}) dx_1 dx_2 \dots dx_N$$

Condensing the N-Dimensional Fourier Transform

- Since each parameter can be represented as a cyclic function $x = f(\theta)$, this simplifies the N-dimensional Fourier transform to a transform over a single variable.

$$f(s) = \int_{\boldsymbol{R}^N} e^{-2\pi i \underline{x}(\theta)} f\left(\underline{x}(\theta)\right) d\theta$$

- The transform is applied to the numerical data of the sampled function to produce f(s).

Fourier Amplitude Sensitivity Testing (FAST) Discrete Fourier Transform Coefficients

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- Now that f(s) is obtained, the sensitivity measures are comprised of the coefficients of the discrete Fourier transform as:

$$A_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(s) \, cos(js) \, ds \qquad B_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(s) \, sin(js) \, ds$$

$$\Lambda_j = A_j^2 + B_j^2 \text{ where j=1,2,...,N}$$

- This gives the total variance from a single parameter for each j^{th} higher order resonance frequency.

Fourier Amplitude Sensitivity Testing (FAST) Sensitivity Measures

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- Next, sum the Λ_j over each higher order resonance to get the variance contributed by the i[th] parameter and the total model variance:

$$D_i = 2\sum_{p=1}^{n} \Lambda_{p\omega} \qquad D = 2\sum_{j=1}^{n} \Lambda_j$$

- The first order effects sensitivity measure by FAST is then simply:

$$S_i^{FAST} = \frac{D_i}{D}$$