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Form Approved
OMB No. 0704-0188

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1. REPORT DATE (DD-MM-YYYY) 17 September 2015		2. REPORT TYPE Briefing Charts		3. DATES COVERED (From - To) 24 August 2015 – 17 September 2015	
4. TITLE AND SUBTITLE Verification of DSMC Simulations Using Spectral Analysis				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) S. J. Araki and R. S. Martin				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER Q0A5	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Air Force Research Laboratory (AFMC) AFRL/RQRS 1 Ara Drive Edwards AFB, CA 93524-7013				8. PERFORMING ORGANIZATION REPORT NO.	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Research Laboratory (AFMC) AFRL/RQR 5 Pollux Drive Edwards AFB, CA 93524-7048				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S) AFRL-RQ-ED-VG-2015-349	
12. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; distribution unlimited					
13. SUPPLEMENTARY NOTES For presentation at DSMC15; Kapaa, Kauai, Hawaii; 13-17 Sep 2015 PA Case Number: #15556; Clearance Date: 9/15/2015					
14. ABSTRACT Viewgraphs/Briefing Charts					
15. SUBJECT TERMS N/A					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT SAR	18. NUMBER OF PAGES 18	19a. NAME OF RESPONSIBLE PERSON J. Koo
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified			19b. TELEPHONE NO (include area code) N/A



Verification of DSMC Simulations Using Spectral Analysis

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SEPTEMBER 13-17, 2015

DISTRIBUTION A: APPROVED FOR PUBLIC RELEASE;
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AFTC/PA CLEARANCE NO. TBD





Outline



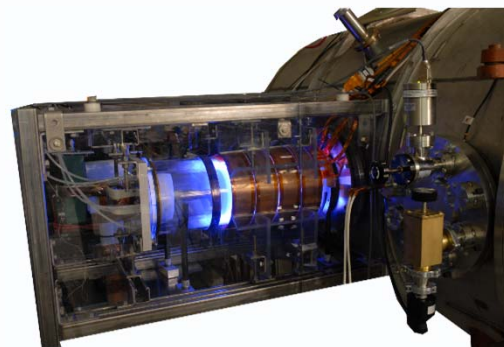
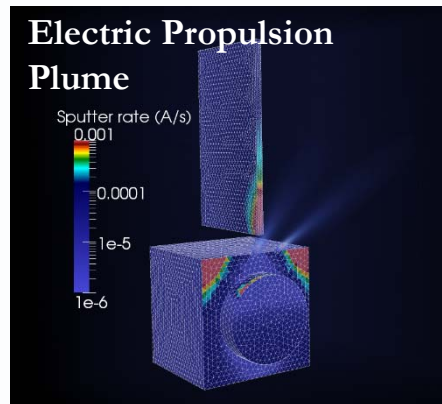
- Introduction
- Test Problem
- Chi-Square Test
- Spectral Analysis
- Conclusion / Future Work



TURF: Thermodynamics Universal Research Framework



- Unifies multiple research codes from group
 - Models of spacecraft propulsion relevant plasma at different spatial scales (1 μ m-100m)
 - Single fluid Magnetohydrodynamics (MHD) solver
 - Unstructured multi-fluid solver
 - Vlasov solver
 - Particle-In-Cell (PIC) with DSMC
 - Combined redundant functionality in those codes
 - Unified GPU support



Field Reversed Configuration
Plasma

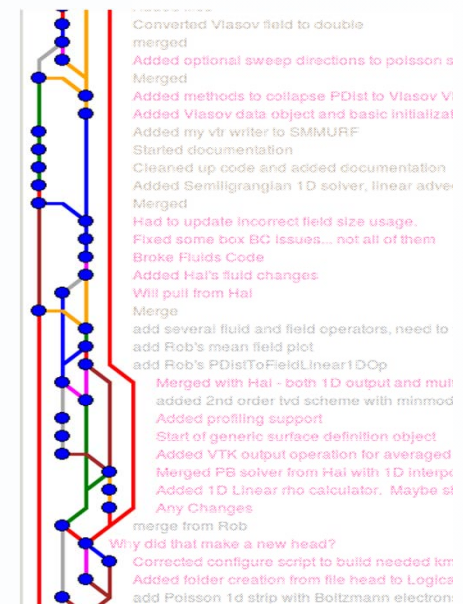




Motivation

- Multiple developers of TURF
 - Changes to core class objects required by one model can break the others.
 - Merging different heads and making sure all the models work properly
- Automated test suites for different models

Multiple heads in Mercurial



Objectives

- Set up simple problem for testing DSMC part of TURF
- Development of efficient procedure in verifying the results



Test Problem: 1D Normal Shock



- Standalone DSMC code run on GPU
- Initial State
 - Upstream and downstream flow properties according to Rankine-Hugoniot relations
 - Discontinuous profile at $t=0$

$$M_2^2 = \frac{1 + \frac{\gamma-1}{2} M_1^2}{\gamma M_1^2 - \frac{\gamma-1}{2}}$$

$$\frac{n_2}{n_1} = \frac{u_1}{u_2} = \frac{(\gamma+1)M_1^2}{(\gamma-1)M_1^2 + 2}$$

$$\frac{T_2}{T_1} = 1 + \frac{2(\gamma-1)}{(\gamma+1)^2} \frac{\gamma M_1^2 + 1}{M_1^2} (M_1^2 - 1)$$

	Upstream ₁	Downstream ₂
Mach Number, M	1.20	0.85
Density, n (m⁻³)	1.00×10²²	1.30×10²²
Temperature, T (K)	293.0	350.1



Test Problem: 1D Normal Shock

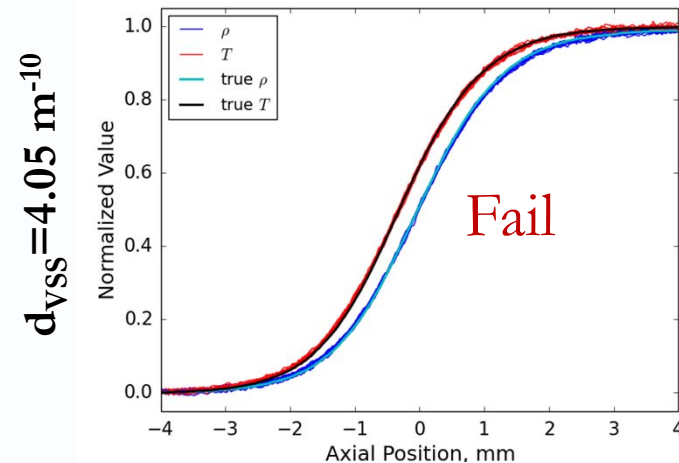
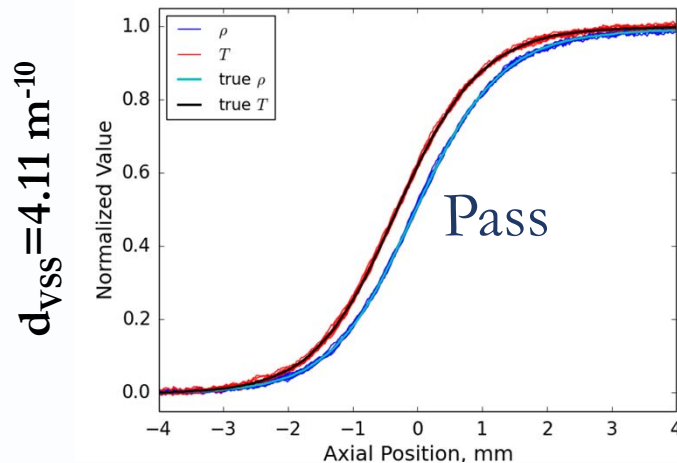


Requirements

- Fast simulation (at least < 5 hours) – less particles
- Smooth solution – more particles and time-steps

Baseline inputs: (40 mins)

- 8,000,000 Ar particles, 10,000 time-steps, 1,000 sampling cells



How can we systematically accept/reject results ?

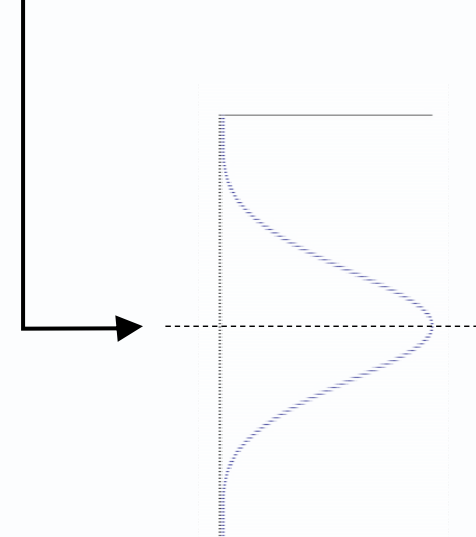
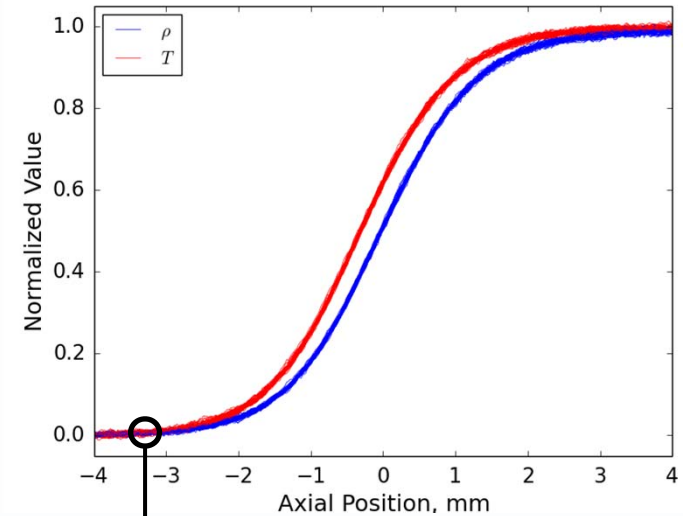


Chi-Square Test: Normal Distribution



1. Run the test problem M times with different random number seed
2. Deviation of results is expected to fall under normal distribution

$$f(x, \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$



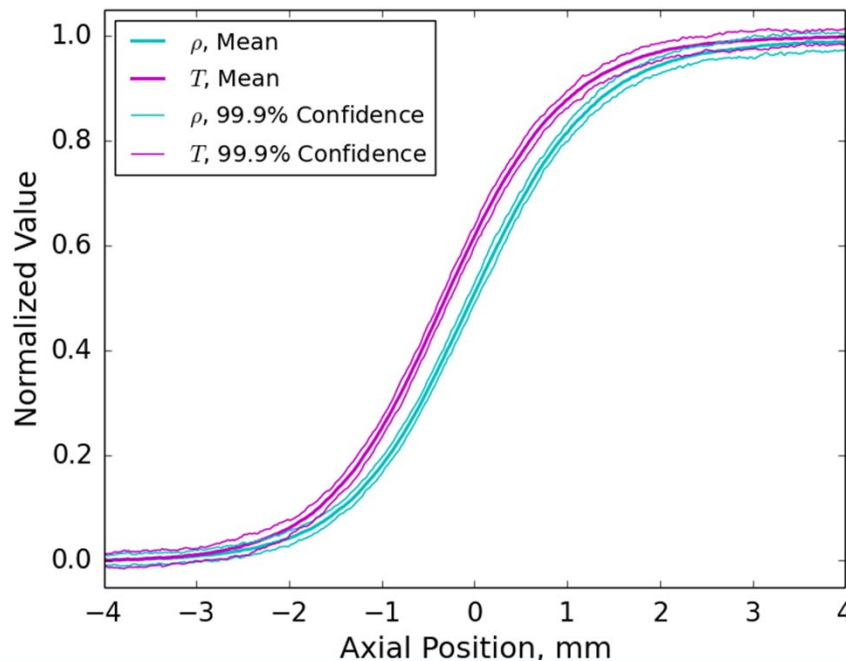


Chi-Square Test: Standard Deviation



- Determine point-wise expected value (μ) and standard deviation (σ) for N cells

$$\mu_n = \frac{1}{M} \sum_{m=1}^M x_{n,m}, \quad \sigma_n = \frac{1}{M-1} \sum_{m=1}^M (x_{n,m} - \mu_n)^2$$



% Confidence Level	# of σ s from Mean
99.9	3.2905
99	2.5758
95	1.9600
90	1.6449
80	1.2816
70	1.0364
50	0.6745



Chi-Square Test



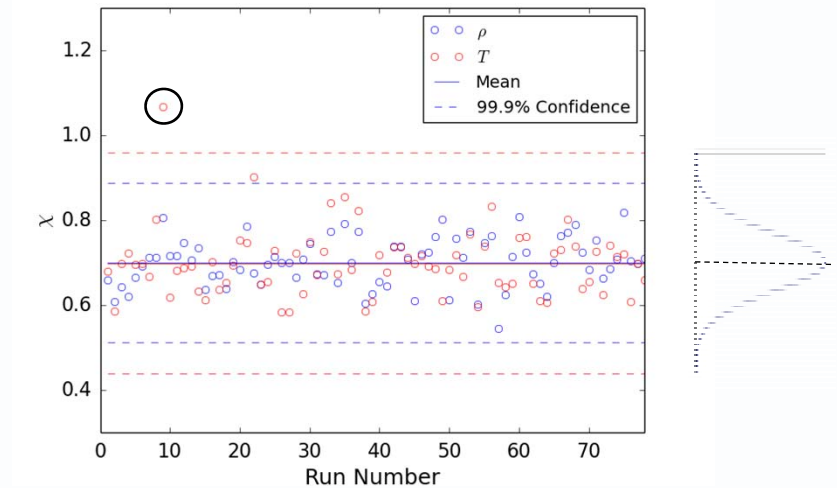
4. For a given run, deduce a global parameter (χ) using μ and σ

$$P = \left[\prod_{n=1}^N f_n \sigma_n \sqrt{2\pi} \right]^{1/N} = \prod_{n=1}^N \exp\left(-\frac{(x_n - \mu_n)^2}{2N\sigma_n^2} \right)$$

$$\Rightarrow -\log P = \frac{1}{2N} \sum_{n=1}^N \left(-\frac{(x_n - \mu_n)^2}{\sigma_n^2} \right) = \chi^2 < \chi_{\text{ref}}^2$$

VSS Diameter (Angstrom)	χ	
	ρ	T
4.11	0.753	1.02
4.00	1.10	1.06
3.90	1.33	1.31
3.80	2.79	2.64

↓
Generally increasing



* All runs performed with the same RNG seed



Chi-Square Test: Result



- Plots of two normal distributions for different VSS diameter
 - The mean of one distribution is larger than the other with larger cross-section, but some portion of it should still overlap

Distribution overlaps...

Could we effectively identify the distribution given a value in the overlapping region?



Remove/reduce statistical noise

- **Run more particles and time-steps?**

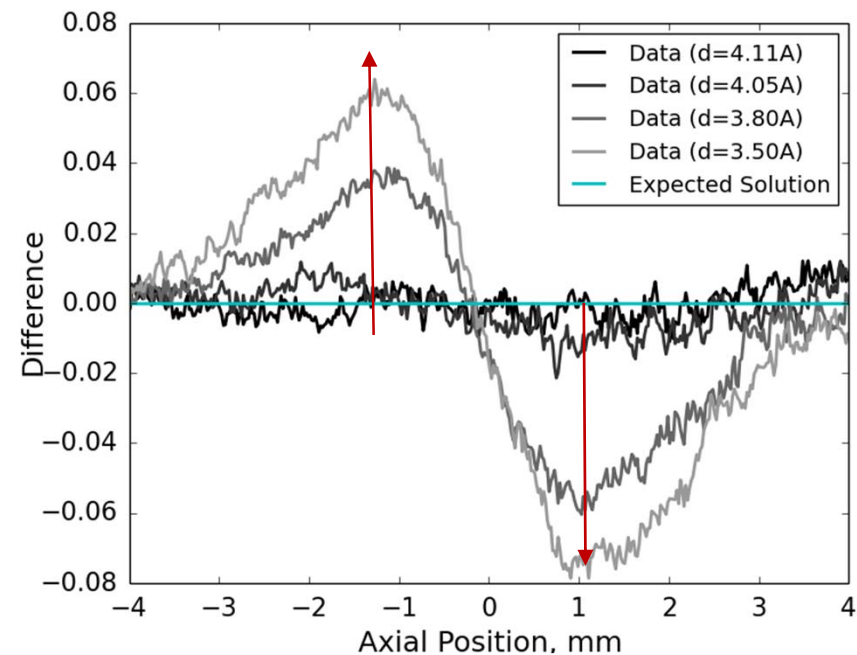
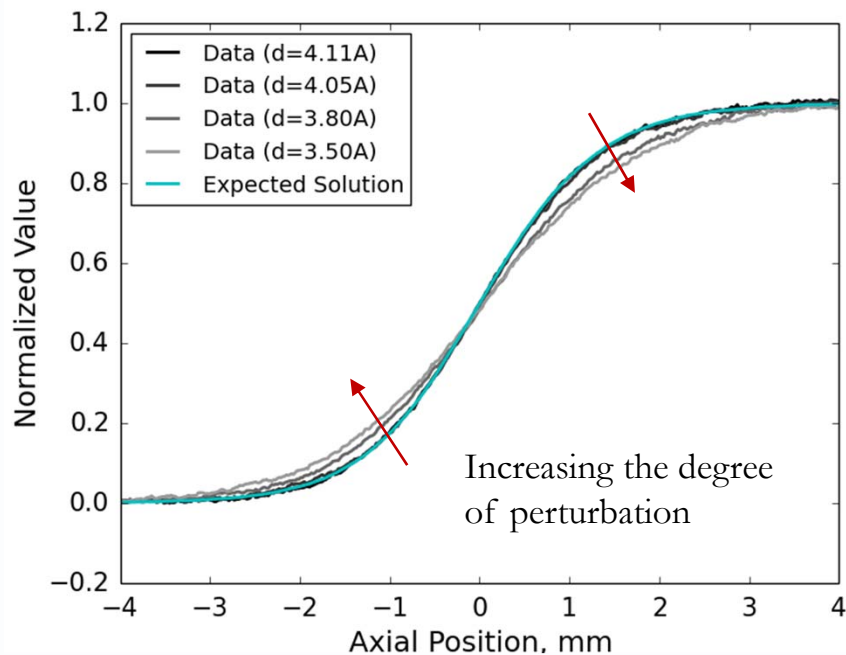


Spectral Analysis: Difference Profiles



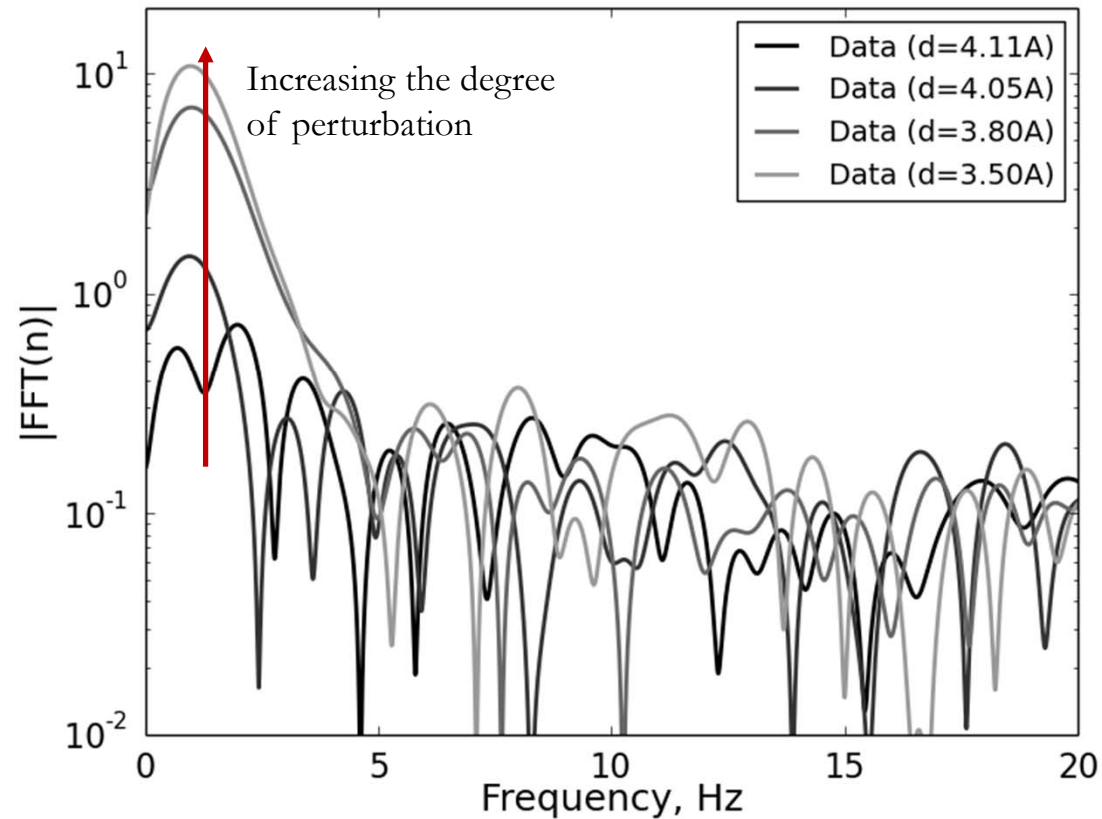
Perform analysis in frequency space

- High frequency mode – Purely statistical
- Low frequency mode – Comes from perturbed input





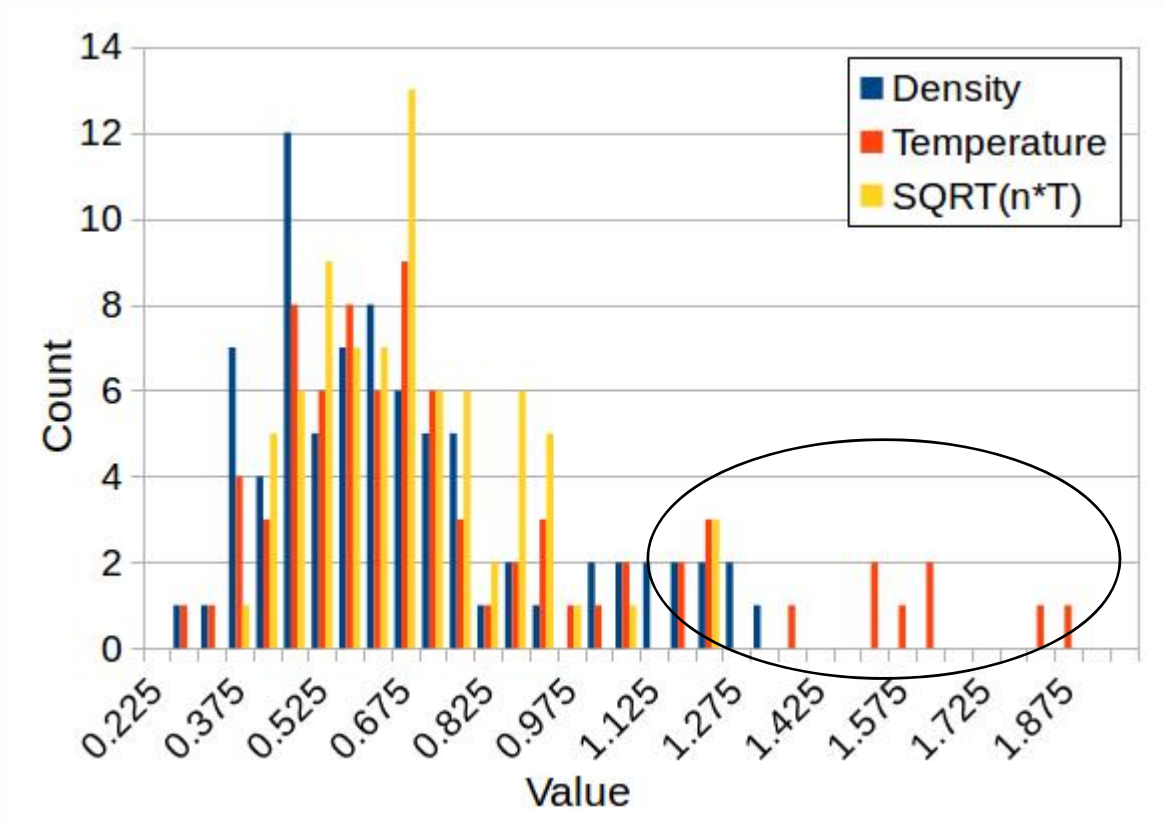
Spectral Analysis: FFT on Difference Profile



Smaller low mode amplitude as approaches the true input solution



Spectral Analysis: Distribution of Low-Mode Amplitude



How do we deal with outliers...?



Spectral Analysis: Boosting

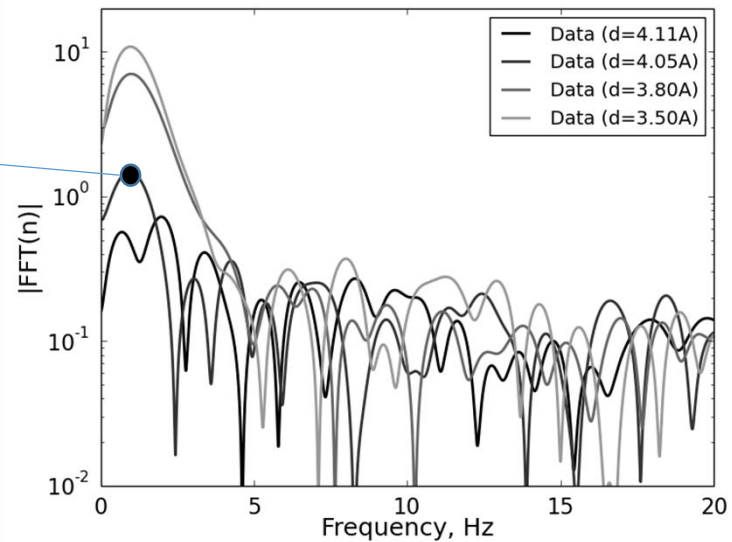


- Need to pass the runs with outliers
 - What is the probability of outliers occurring multiple times on the roll?
 - Probability of one outlier: 1%
 - Probability of outliers three times on the roll: $(1\%)^3$
- Use geometric mean to obtain the global spectral amplitude

$$\tilde{\rho} = \max |\text{FFT}(\rho)|,$$

$$\tilde{T} = \max |\text{FFT}(T)|,$$

$$\Rightarrow \max_{m=1, M} \left[\underbrace{\prod_{i=m, m+N} \sqrt{\tilde{\rho}_i \tilde{T}_i}}_{\text{Boosting}} \right]^{1/N}$$





Conclusions

- Chi-Square test
 - Width of distribution is determined by the statistical noise inherent to particle simulations
- Spectral analysis
 - Strongly effective in the test problem
 - Essentially removes the effect of statistical noise in the test

Future Work

- Use the methodology in other DSMC problems to study the strength/weakness of the procedure
- Apply the knowledge in smoothing of flow properties



Thank you



Spectral Analysis



1. Perturbing the VSS diameter narrows/widens the shock width
2. Difference profile contains
 1. Low frequency mode from wrong input
 2. High frequency mode from statistical noise
3. Perform Fast Fourier Transformation (FFT) on difference profile
4. Observe the amplitude of low modes
5. Perform boosting