REPORT DOCUMENTATION PAGE	*Form Approved* *OMB No. 0704-0188*

1. REPORT DATE	**2. REPORT TYPE**	**3. DATES COVERED** *(From - To)*
28 August 2017	Briefing Charts	01 August 2017 - 31 August 2017

4. TITLE AND SUBTITLE Variable Weight Fractional Collisions for Multiple Species Mixtures	**5a. CONTRACT NUMBER** **5b. GRANT NUMBER** **5c. PROGRAM ELEMENT NUMBER**
6. AUTHOR(S) Robert Martin	**5d. PROJECT NUMBER** **5e. TASK NUMBER** **5f. WORK UNIT NUMBER** Q1AM
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 NUMBER**
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-2017-205

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for Public Release; Distribution Unlimited. PA Clearance Number: 17517 Clearance Date: 22 August 2017

13. SUPPLEMENTARY NOTES
For presentation at Direct Simulation Monte Carlo 2017; Santa Fe, NM, USA; 28 August 2017
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14. ABSTRACT
Viewgraph/Briefing Charts

15. SUBJECT TERMS
N/A

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**			Robert Martin
					19b. TELEPHONE NUMBER *(Include area code)*
Unclassified	Unclassified	Unclassified	SAR	86	N/A

Standard Form 298 (Rev. 8/98)
Prescribed by ANSI Std. Z39.18

Variable Weight Fractional Collisions for Multiple Species Mixtures

Robert Martin

In-Space Propulsion Branch,
Air Force Research Laboratory,
Edwards Air Force Base, CA USA

Direct Simulation Monte Carlo, 2017

Distribution Statement A: Approved for public release;
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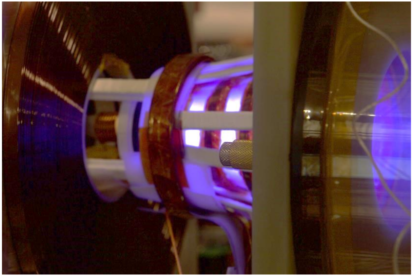
Field-Reversed Configuration:

- Concept from Fusion Energy
  - Scaled Down for Propulsion

RP3X FRC Thruster



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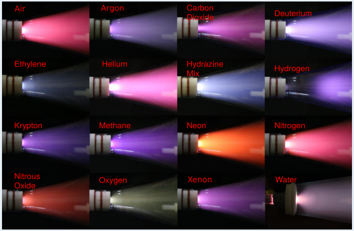
- Electrodeless
  - Limits Erosion
  - Enables Flexible Fuels



Pancotti, et al, "Adaptive Electric Propulsion for ISRU Missions", 20th Adv. Space Prop., 11/2014

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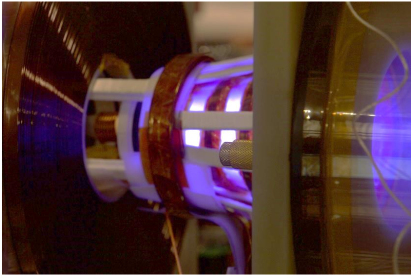

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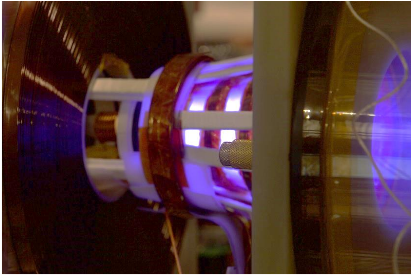

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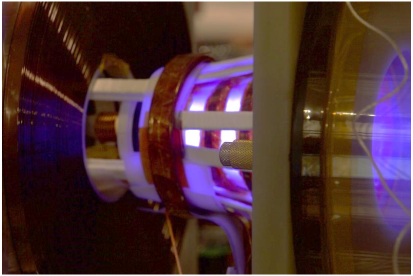

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Complex to Design

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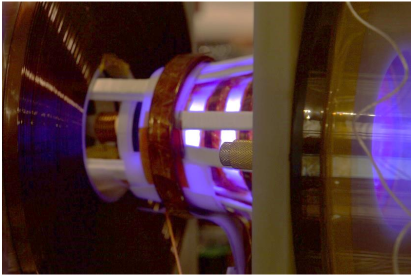

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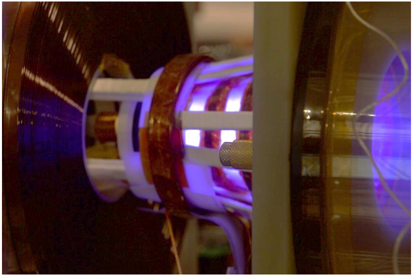
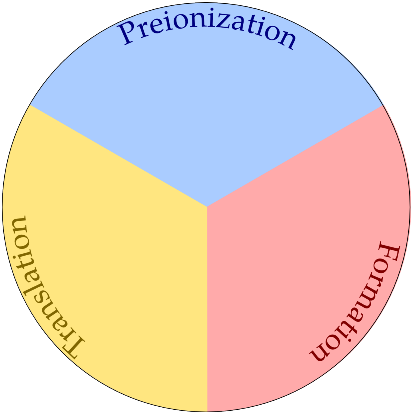
Complex to Design
Significant Modeling Challenge

RP3X FRC Thruster



Dominant Physics Varies with Cycle:



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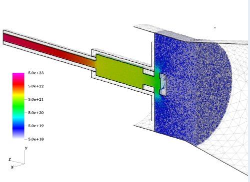

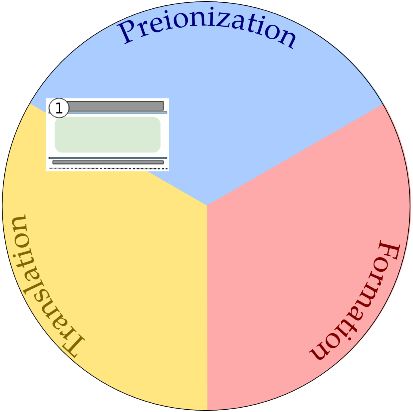

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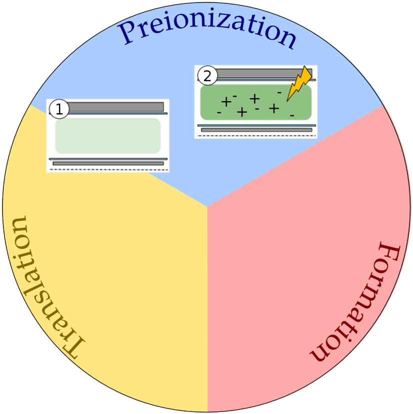

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Phases of FRC Operation

Dominant Physics Varies with Cycle:

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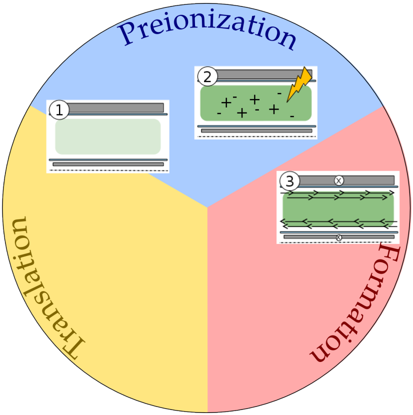
3. Driver Pulse
   - Ionization+Electromagnetics



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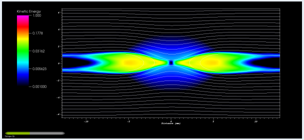
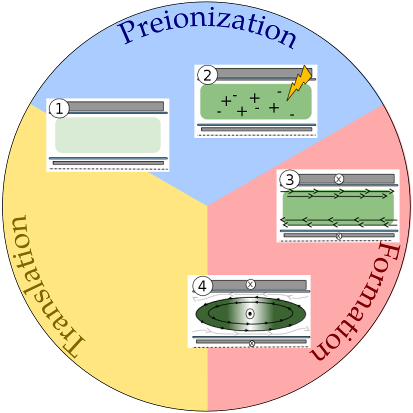


https://astrobear.pas.rochester.edu/trac/wiki/AstroBearProjects/resistiveMHD



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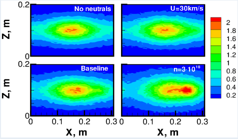

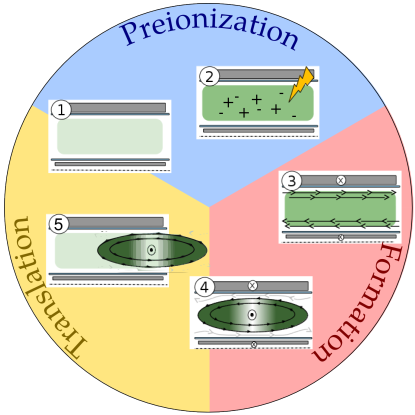

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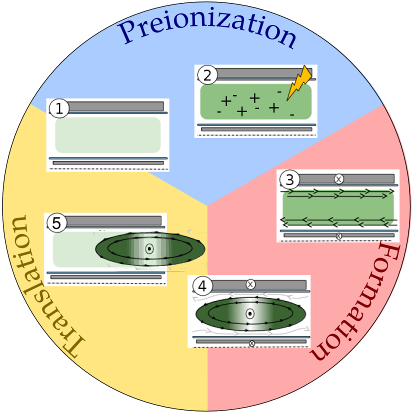
Continuous Cycle: 5 impacts 1



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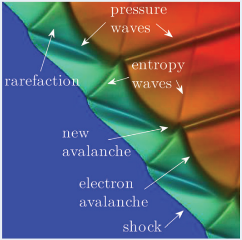
Important Collisions in Spacecraft Propulsion:

- Discharge and Breakdown in FRC
- Collisional Radiative Cooling/Ionization
- Combustion Chemistry

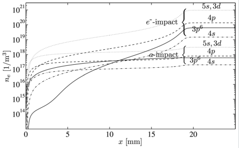
Common Features in Spacecraft Collisions:

- Relevant Densities Spanning Many Orders of Magnitude — 6+
- Transitions from Collisional to Collisionless
- Tiny Early e^- or Radical Populations Critical to Induction Delay
- Many types of Inelastic Collisions with Unknown Effects on Distribution Shapes

Shock Ionization



Kapper & Cambier, J. Appl. Phys. 109, (2011)



Importance of Collision Physics

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Need Low Noise & High Dynamic Range Collision Algorithms

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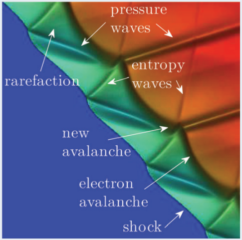

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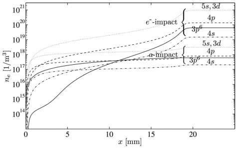


Standard Collision Models

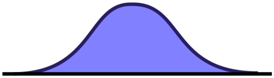
<u>Previous Collision Methods:</u>

- Monte Carlo Collisions (MCC)
  - Particles Collide with Background “Fluid”
  - Often Used in Plasma/PIC Simulation
  - Ion-e^- Collisions Assume Stationary Ions
  - No Conservation/Detailed Balance
- Direct Simulation Monte Carlo Collisions (DSMC)
  - Most Modern Versions use No-Time Counter (NTC) Method
  - Conservative/Reversible Collision
  - Satisfies Detailed Balance
  - Subset of Possible Collisions Sampled
  - Random Selection vs Z_{ij} for All/Nothing Collision

 All Random Flip vs Number of Collisions: $Z_{ij} = \frac{n_i n_j}{2} \langle \sigma v \rangle \, \mathrm{dt}$

Continuum to Discrete Representation:

- Many Particles $\xrightarrow{\sim}$ Continuous Distribution



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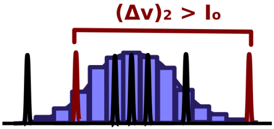

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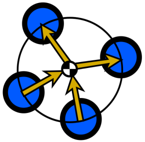
Variable Weight "All-or-Nothing" Collisions?



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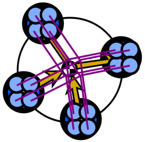

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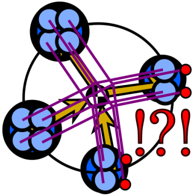
Variable Weight "All-or-Nothing" Collisions?

Physically Inconsistent!

(Mixing Violates Momentum/Energy Conservation)



Stochastic Weighted Particle Method:

- Developed by Rjasanow & Wagner

Attempted Collisions/Cell:

$$\nu = f(2\bar{w} - w_{min}) N_p (N_p - 1) \langle \sigma v \rangle^{max} dt$$

Select Pair (i,j) if:

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-or-

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Perform Standard VHS Collisions

Generate/Modify Particles with:

$$\pm \Delta w / f = \pm \texttt{min}(w_i, w_j) / f$$

Update $\langle \sigma v \rangle^{max}$

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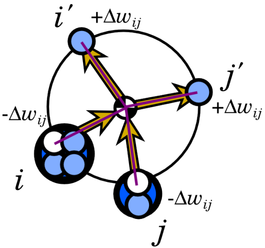

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- Still Requires Merge $w_i \neq$ `const`

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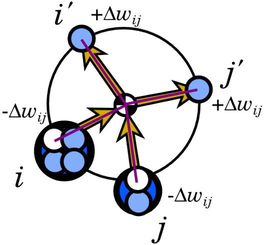

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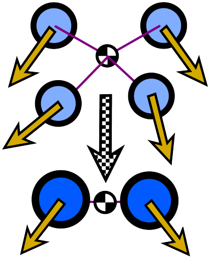
Update $\langle \sigma v \rangle^{max}$

Merge to Pair → DOF for Conservation:

- (n+2):2 yields Exact Mass, Momentum, and Kinetic Energy Conservation
- Applied Spatially also Shown to Conserve Electrostatic Energy
- Though Energy Conserving, Still Thermalizes VDF



$$w_{cell} = \sum_i^{(n+2)} w_i$$
$$\overline{\vec{v}} = \frac{1}{w_{cell}} \sum_i^{(n+2)} w_i \vec{v}_i$$
$$\overline{V^2} = \frac{1}{w_{cell}} \sum_i^{(n+2)} w_i \left(\vec{v}_i - \overline{\vec{v}}\right)^2$$

$$w_{(a/b)} = w_m/2$$
$$\vec{v}_{(a/b)} = \overline{\vec{v}} \pm \hat{\mathcal{R}}\sqrt{\overline{V^2}}$$

Similarly: $\vec{x}_{(a/b)} = \overline{\vec{x}} \pm \hat{\mathcal{R}}\sqrt{\overline{x^2}}$

Merge to Pair → DOF for Conservation:

- (n+2):2 yields Exact Mass, Momentum, and Kinetic Energy Conservation
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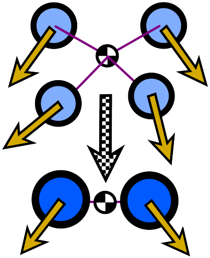
Selection of Near Neighbors in VDF Limits Thermalization



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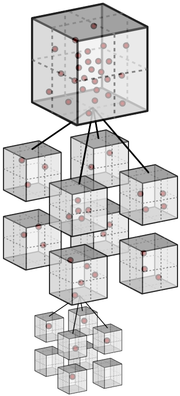
Selection of Near Neighbors in VDF Limits Thermalization

Merge via Separate Octree/Species
Only Change for Mixtures!

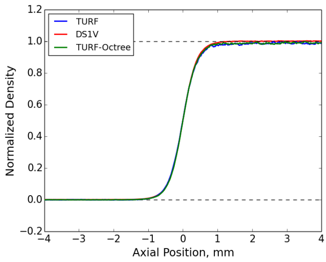
Octree Velocity Bins



Efficient Neighbor Selection

1D Normal Argon Shock Test

- Simple Verification vs. DS1V
- Initial Conditions:
  $T_0 = 293\text{K}$, $n_0 = 1\text{E}22/\text{m}^3$, $v_0 = 637.4(\text{m/s})$
- Initial Jump to Post-Shock at 1cm
- VHS Collisions:
  T_{ref}=273K, d_{ref}=4.17Å, ω_{VHS}=0.81



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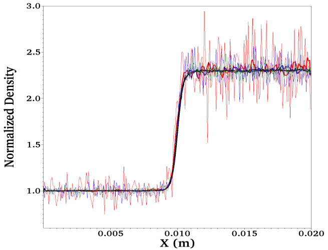
TURF - SWPM+Octree



Target N/Cell Quadrupled per Line

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- Initial Conditions:
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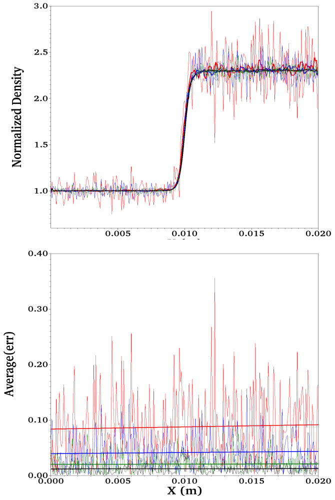
- VHS Collisions:
  T_{ref}=273K, d_{ref}=4.17Å, ω_{VHS}=0.81
- Time Average:
  $\bar{n}$ from t$\in [80, 100)\mu$s
- Error (Normalized L_1):
  err=$|n - \bar{n}|/\bar{n}$
- Error Controlled: $err \propto \sqrt{N/cell}$

TURF - SWPM+Octree

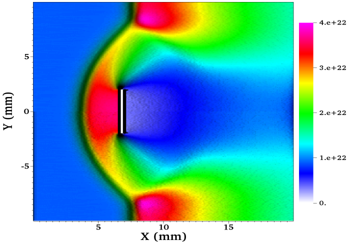


Target N/Cell Quadrupled per Line

2D Argon Shock Test

- Initial Conditions like M=2 Except: $v_0 = 2550\text{m/s}$
- Specular: x=5 − 5.04mm with y=±2mm
- Half Domain Modeled: $80\mu\text{m} \times 80\mu\text{m}$ Cells

TURF: n - Standard DSMC



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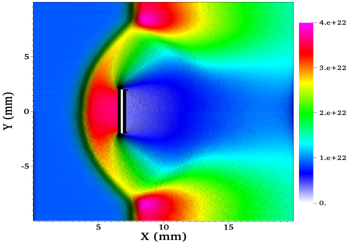
- SWPM Similar to Standard DSMC

TURF: n - Standard DSMC

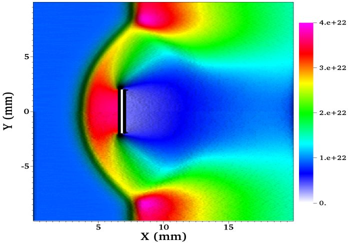


TURF: n - SWPM+Octree

2D Argon Shock Test

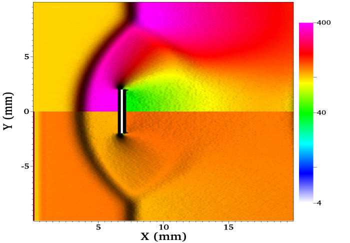
- Initial Conditions like M=2 Except: $v_0 = 2550$m/s
- Specular: x=5 − 5.04mm with y=±2mm
- Half Domain Modeled: 80μm × 80μm Cells
- Time Average: $\bar{n}$ from t∈ [80, 100)μs
- SWPM Similar to Standard DSMC
- Despite Different $Np/Cell$

TURF: n - Standard DSMC



TURF: n - SWPM+Octree

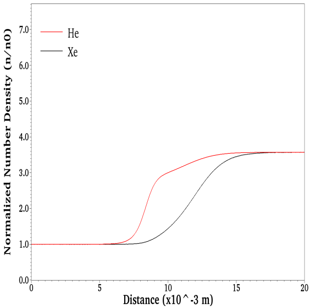
TURF Np/Cell - Standard DSMC



TURF Np/Cell - SWPM+Octree

1D Normal He:Xe Shock Test

- Mach 3.89 with He:Xe of 97:3 (i.e. Bird '94 Fig 12.35)



Converged 100x Baseline

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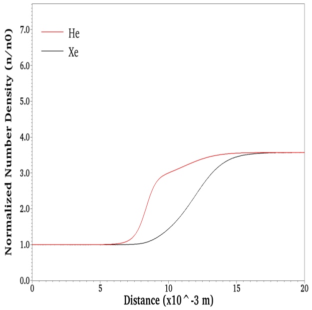

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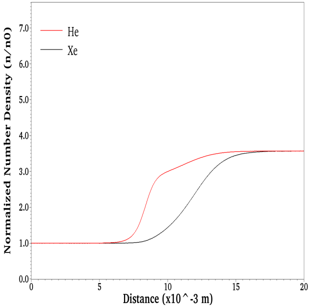

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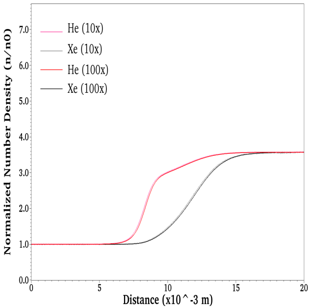
- Separation Peak at $\rho_{He} \approx \rho_{Xe}$
- DSMC needs 33x He:Xe Macroparticles (From m_{Xe}/m_{He})
- Reduced Particle Count Introduces Error



Comparison 10x vs. 100x

1D Normal He:Xe Shock Test

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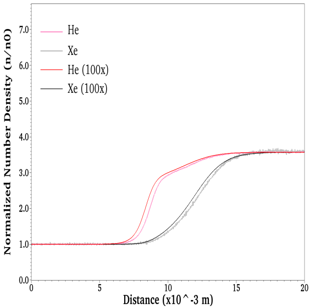

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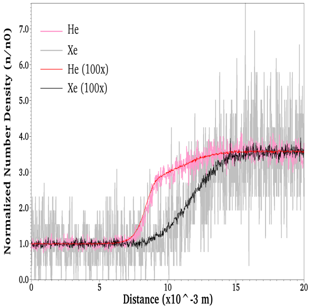
- Instantaneous: Dramatic Noise in Xe



Instantaneous Baseline vs. 100x

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- Highlights Species Separation
- Separation Peak at $\rho_{He} \approx \rho_{Xe}$
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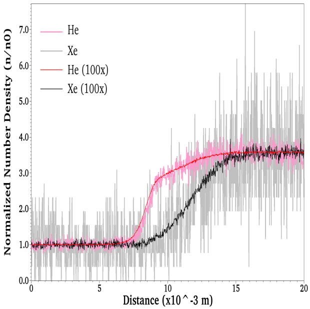
- Reduced Particle Count Introduces Error
- Error in Time Average at Baseline
- Instantaneous: Dramatic Noise in Xe

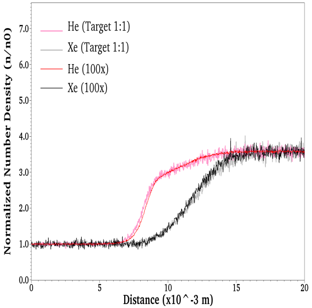
Noise Reduction via Variable Weights?



Instantaneous Baseline vs. 100x

1D He:Xe Shock with SWPM+Octrees

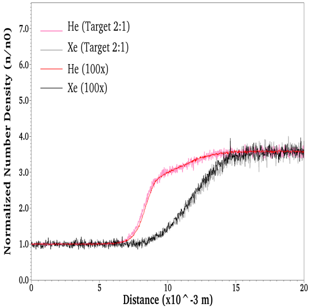
- Xe Noise Controlled by 1:1 Target
- He:Xe Noise Comparable



100x vs. FDSMC 1:1

1D He:Xe Shock with SWPM+Octrees

- Xe Noise Controlled by 1:1 Target
- He:Xe Noise Comparable
- Direct Noise Control by Target Ratio



100x vs. FDSMC 2:1

1D He:Xe Shock with SWPM+Octrees

- Xe Noise Controlled by 1:1 Target
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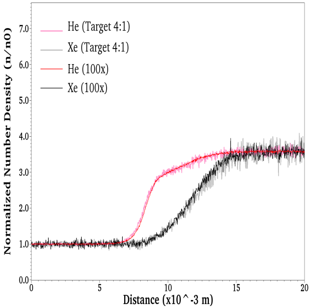
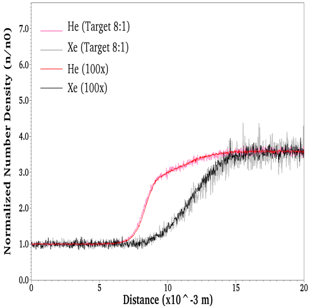


100x vs. FDSMC 4:1

1D He:Xe Shock with SWPM+Octrees

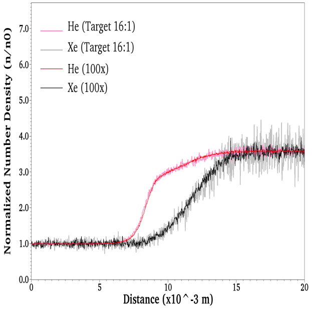
- Xe Noise Controlled by 1:1 Target
- He:Xe Noise Comparable
- Direct Noise Control by Target Ratio



100x vs. FDSMC 8:1

1D He:Xe Shock with SWPM+Octrees

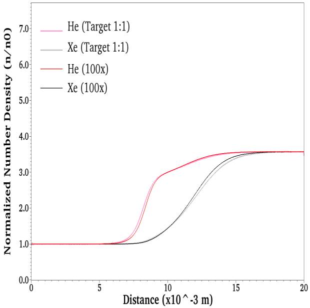
- Xe Noise Controlled by 1:1 Target
- He:Xe Noise Comparable
- Direct Noise Control by Target Ratio



100x vs. FDSMC 16:1

1D He:Xe Shock with SWPM+Octrees

- Xe Noise Controlled by 1:1 Target
- He:Xe Noise Comparable
- Direct Noise Control by Target Ratio
- Converged Error Finite! (1:1 Target)
- Error Source Still Unidentified...



Averaged 100x vs. FDSMC 1:1

1D He:Xe Shock with SWPM+Octrees

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- He:Xe Noise Comparable
- Direct Noise Control by Target Ratio
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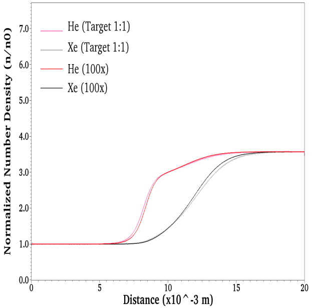
- Potentially Sensitivity to He Tails?
  - -Merge Impacts Higher Moments
  - -TBD Error vs. He-Noise Level
  - -Improvement Merge to Preserve Tails
- Adaptation of SWMP Incorrect?
  - -# of Collisions Sampled as WDF Varies?
  - -Collision Pair Rule Wrong, $w_i \ll w_j$?



Averaged 100x vs. FDSMC 1:1

HE:XE MIXTURE SHOCK - FRACTIONAL DSMC

1D He:Xe Shock with SWPM+Octrees

- Xe Noise Controlled by 1:1 Target
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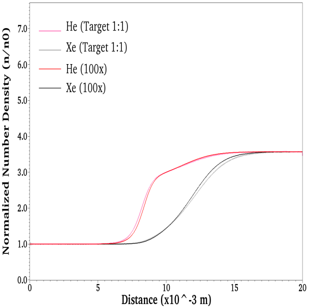
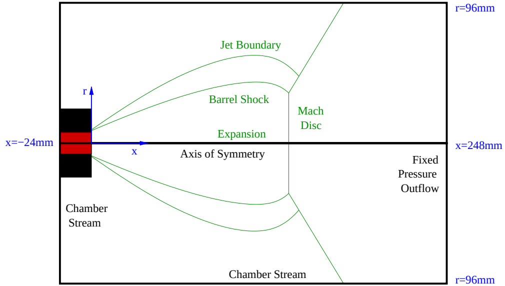
Error Identification in Future Work



Averaged 100x vs. FDSMC 1:1

- Helium-Argon Mixture
- Expanded through Nozzle to Vacuum
- *e*-Beam Concentration Measurements

Jet Flow Layout



Re=533

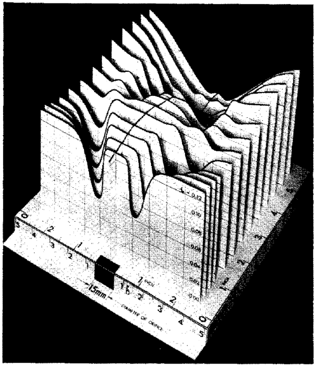
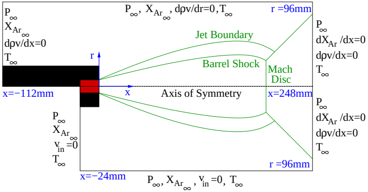


FIG. 11. Mole fraction of argon throughout the flow field of a free jet.

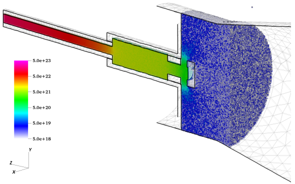
Case Tested in PhD & RGD27:

Continuum Boundary Conditions



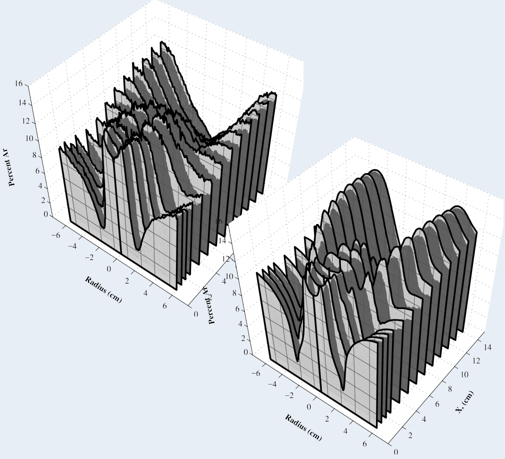
Monte Carlo Boundary Conditions

Surrogate for FRC Injection



Dynamic Range $\gg$ Shocks

Solution from DS2V



Solution from SPARTAN
(Navier-Stokes + Diffusion Velocity)

Features Found via Simulations

1. Wing Increases near Nozzle Edge

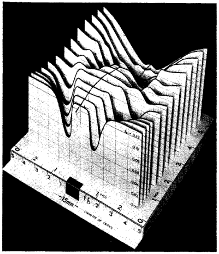
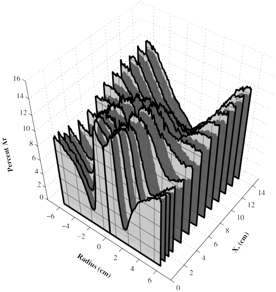
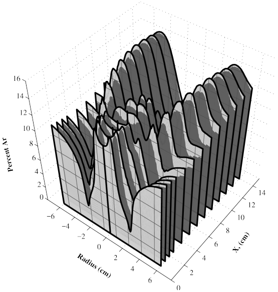


Fig. 11. Mole fraction of argon throughout the flow field of a free jet.

Experimental



DS2V



SPARTAN

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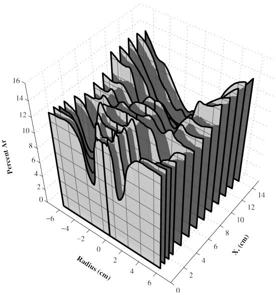

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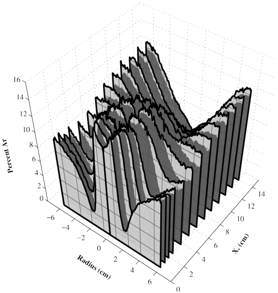
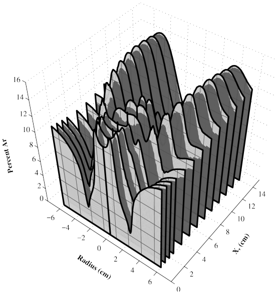
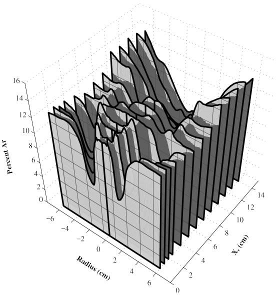


DS2V

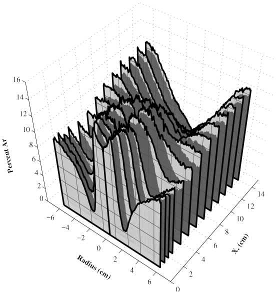


SPARTAN

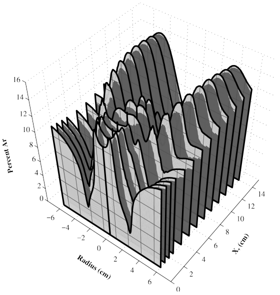
1. Wing Increases near Nozzle Edge
2. Lower Radial Boundary Edge Concentration



Experimental

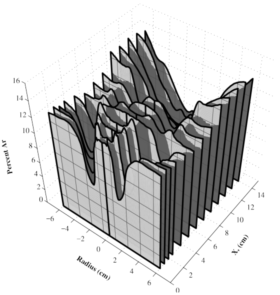


DS2V

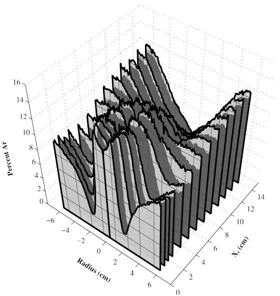


SPARTAN

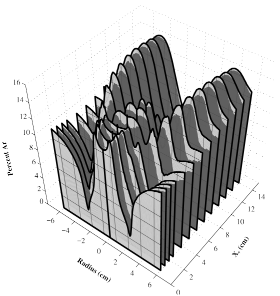
1. Wing Increases near Nozzle Edge
2. Lower Radial Boundary Edge Concentration
3. Deeper Jet Edge Concentration Drop



Experimental



DS2V



SPARTAN

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- Considered 2D-Axisymmetric TURF
- Simple DSMC but Merge Complex (Conservation on $v_{\|} v_{\perp}$-Quadtrees?)

Standard 3D DSMC

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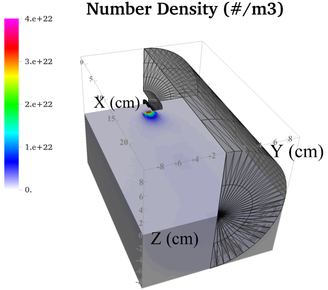
- 3D Expensive at Tractable Resolution
- Added Collision Sub-Cells to TURF

Standard 3D DSMC



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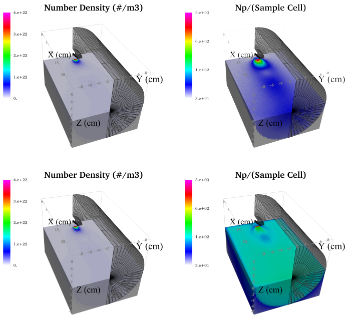
- Fractional DSMC Controls Np/Cell

Standard 3D DSMC



Multi-Species Fractional DSMC

- TURF Naturally 3D Cartesian
- Considered 2D-Axisymmetric TURF
- Simple DSMC but Merge Complex (Conservation on $v_{\|} v_{\perp}$-Quadtrees?)
- Opted to Run Coarse Full 3D (Simplified Boundary Conditions)
- 3D Expensive at Tractable Resolution
- Added Collision Sub-Cells to TURF
- Fractional DSMC Controls Np/Cell
- Linear Density Obscures Results

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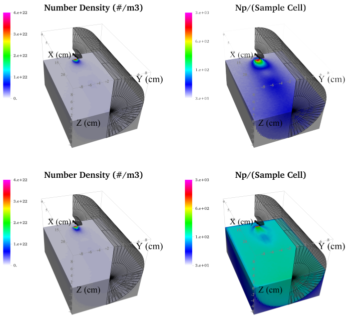

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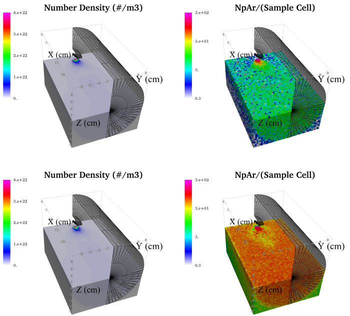

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X_{Ar} to RX-Plane $\rightarrow$ for Detailed Results...

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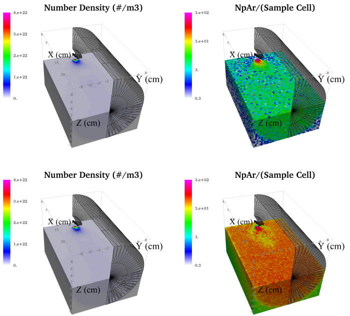

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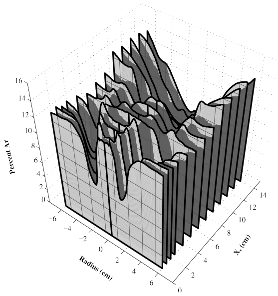
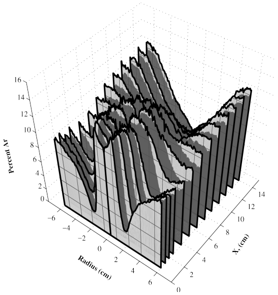
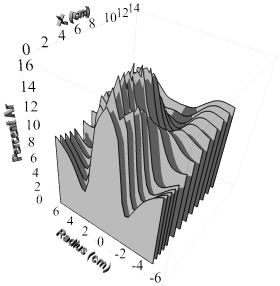


Experimental



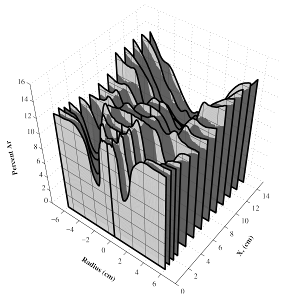
DS2V



TURF

1:1 - Collision:Sample

1. Standard DSMC Poor Results
2. 2x2x2 Collision Cell Improves Standard DSMC



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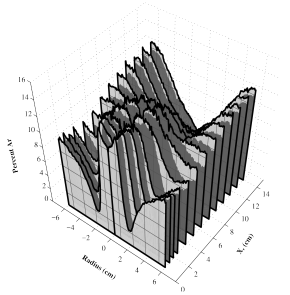

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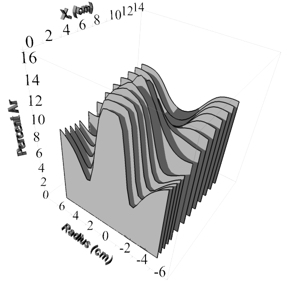
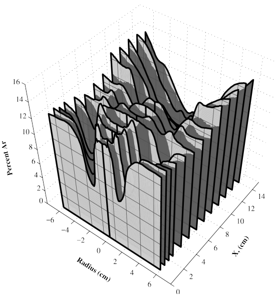


TURF

2x2x2:1 - Collision:Sample

1. Standard DSMC Poor Results
2. 2x2x2 Collision Cell Improves Standard DSMC
3. SWPM+Octree Significantly Better (2x2x2 Collision Cell)



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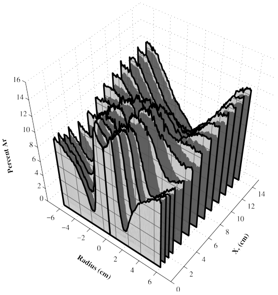

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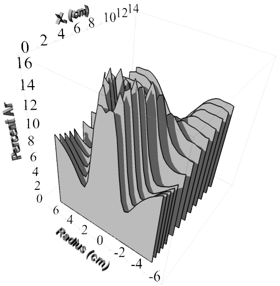

TURF

SWPM+Octree (2x2x2 Collision Cells)

The ∂f-Boltzmann for $f = f^{eq} + f^{dev}$

- ∂f - Concept Old
- How to make ∂f cheaper than full-f (Must adapt DOF Usage..?)

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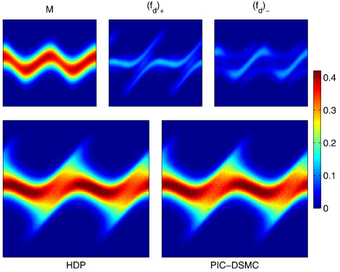
Strong Landau Damping



P-P:	v+,w+	$\rightarrow$	v'+,w'+
P-N:	v+,w-	$\rightarrow$	2v+,v'-,w'-
N-N:	v-,w-	$\rightarrow$	2v-,2w-,v'+,w'+
P-M:	M,v+	$\rightarrow$	M,w-,v'+,w'+
N-M:	M,v-	$\rightarrow$	M,w+,v'-,w'-
M-M:		$\emptyset$	

Yan, JCP 309 (2016) 18-36

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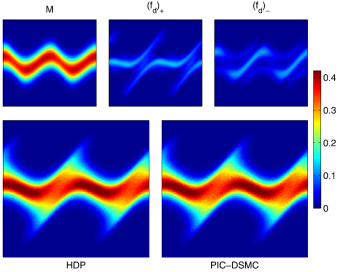

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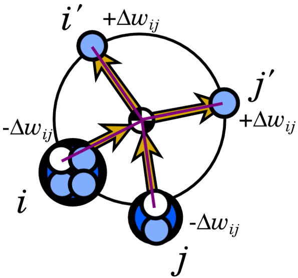
Stochastic Weight Particle Method (SWPM)



$w_i = w_i - \Delta w_{ij}$ & $w_j = w_j - \Delta w_{ij}$

$w_{(N_p+1)} = \Delta w_{ij}$ & $w_{(N_p+2)} = \Delta w_{ij}$

+2 Particles/Collision

RGD30

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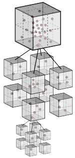
Octree ∂f-Boltzmann
Bin-to-Bin Collisions



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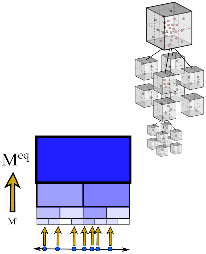

FUTURE DIRECTIONS: HYBRID ∂f

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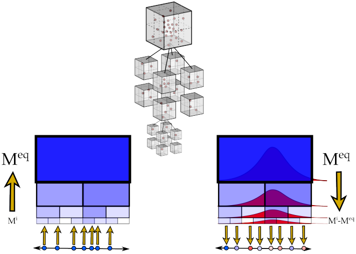

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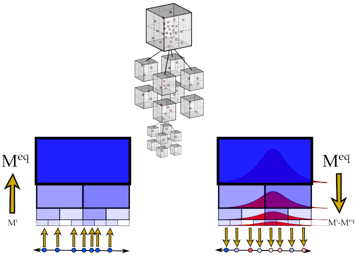

Sample Collisions using
Δw: for P-P, P-N, N-N, P-M, N-M
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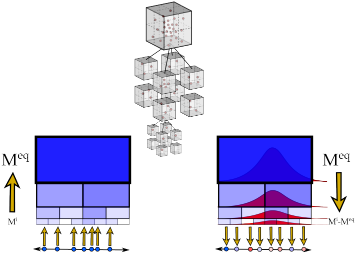

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- Valid at Adaptive Tree Depths
- Entropy Estimate for DOF Distribution

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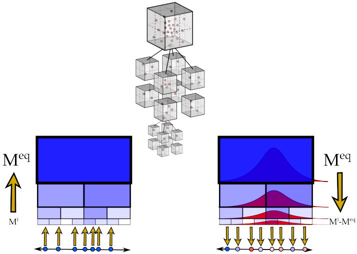
Bin-to-Bin Collisions



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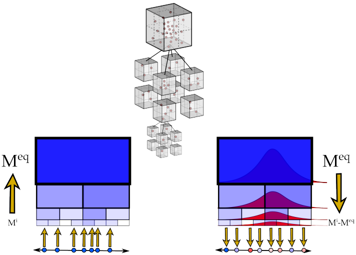

Sample Collisions using
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M-M:$\emptyset$
Combine with 2^6-Tree
XV $\rightarrow$ Multigrid Solves?

Current Results:

- SWPM+Octree Option for Variable Weight Mixture Collisions
- Multiple Octree Merge only Modification for Multi-Species
- Initial Verification vs. Standard Shock Cases
- Merge/Target Enables Direct Control of Noise
- Unidentified Systematic Error with 1:1 Target
- Initial Testing on 3D Mixture Expansion Better with SWPM+Octree

Future Efforts:

- Additional Investigation of Error Source for Disparate Weights
- Improved Merge/Control of Tails
- Apply to Reacting Flow
- Adaptation for δf

Thank You

This material is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-17RQCOR465.

Any opinions, finding, and conclusion or recommendations expressed in this material are those of the author and do not necessarily reflect the views of the United States Air Force.

Questions?