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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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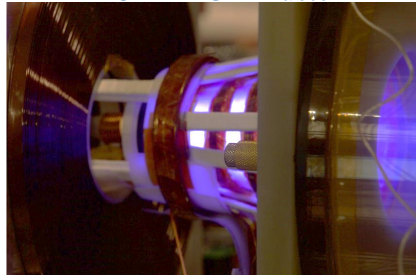
- 1 BACKGROUND & REVIEW OF METHOD
- 2 MULTI-SPECIES TEST CASES
- 3 FUTURE WORK
- 4 CONCLUSION



Field-Reversed Configuration:

- Concept from Fusion Energy
 - Scaled Down for Propulsion

RP3X FRC Thruster

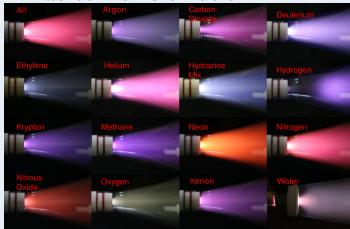




FRC THRUSTER OVERVIEW

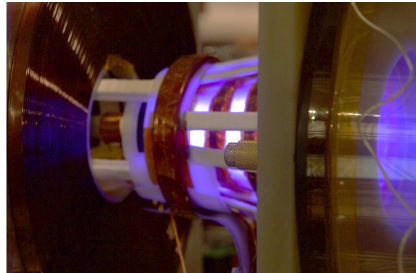
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- Concept from Fusion Energy
 - Scaled Down for Propulsion
- Electrodeless
 - Limits Erosion
 - Enables Flexible Fuels



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

RP3X FRC Thruster

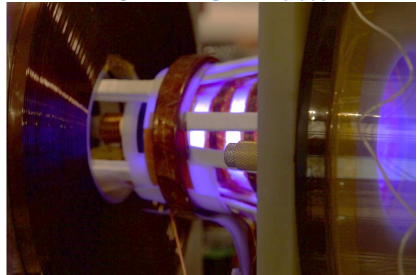




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 - Tunable Thrust/ISP
 - Coupled Dynamics

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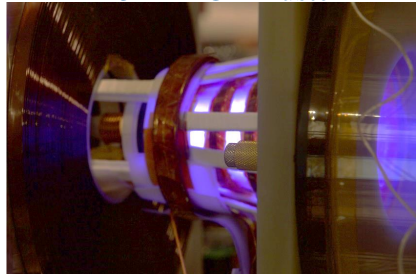




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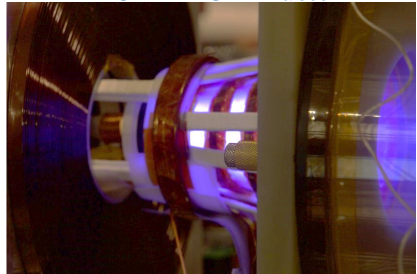


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Complex to Design

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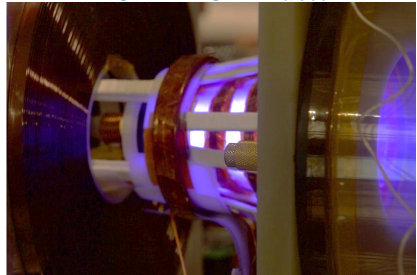


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Complex to Design
Significant Modeling Challenge

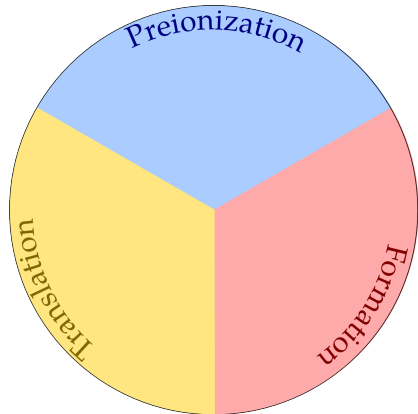
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PHASES OF FRC OPERATION

Dominant Physics Varies with Cycle:



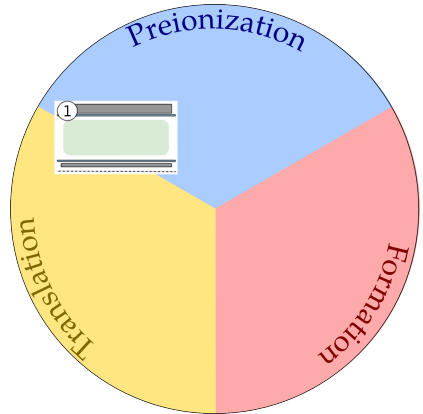
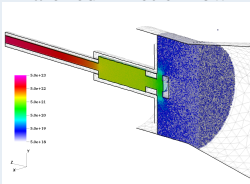
Adapted from "Annular FRC" PhD Proposal, C. (Niemela) Hill



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Dominant Physics Varies with Cycle:

- 1 Neutral Fill
- Rarefied Kinetic Flow



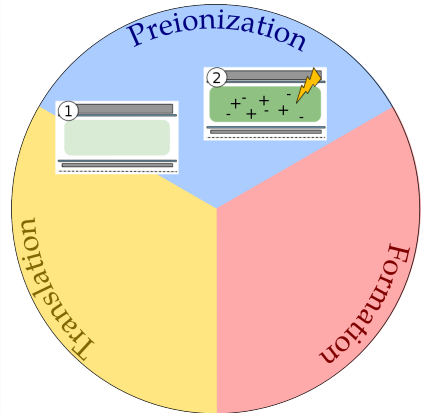
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PHASES OF FRC OPERATION

Dominant Physics Varies with Cycle:

- ① Neutral Fill
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- ② Preionization Chemistry
 - CR-Excitation/Ionization



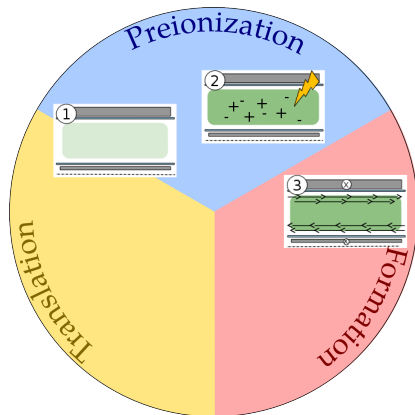
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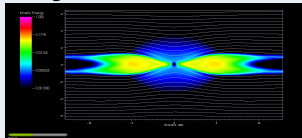
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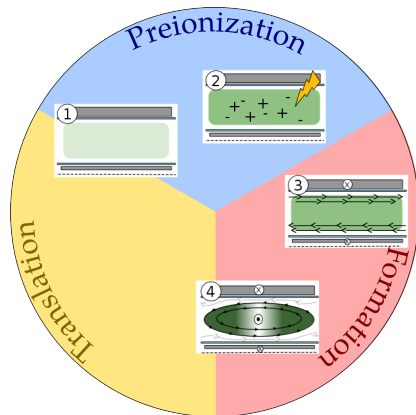
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- 4 Field Reversal
- Magnetic Reconnection



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



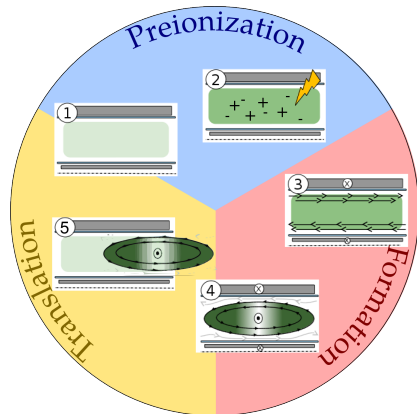
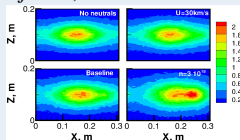
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 - $\vec{j} \times \vec{B}$, Neutral Entrainment



Adapted from "Annular FRC" PhD Proposal, C. (Niemela) Hill

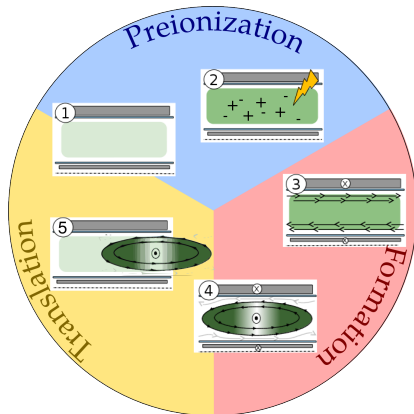


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Continuous Cycle: ⑤ impacts ①



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IMPORTANCE OF COLLISION PHYSICS

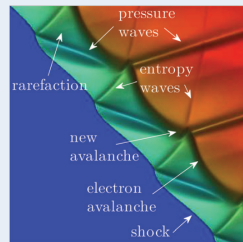
Important Collisions in Spacecraft Propulsion:

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

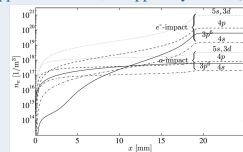
Common Features in Spacecraft Collisions:

- 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)





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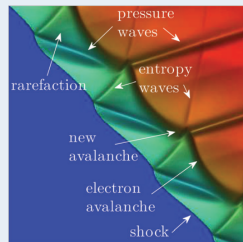
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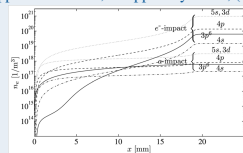
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Need Low Noise & High Dynamic Range
Collision Algorithms

Shock Ionization



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





Previous Collision Methods:

- 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: $Z_{ij} = \frac{n_i n_j}{2} \langle \sigma v \rangle dt$



VARIABLE WEIGHTS FOR DYNAMIC RANGE

Continuum to Discrete Representation:

- Many Particles $\rightsquigarrow$ Continuous Distribution





VARIABLE WEIGHTS FOR DYNAMIC RANGE

Continuum to Discrete Representation:

- Many Particles $\leadsto$ Continuous Distribution
- Discretized VDF Yields Vlasov
But Collision Integral Still a Problem





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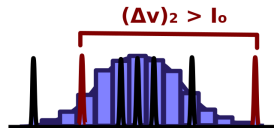
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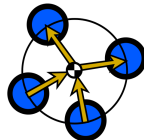




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Variable Weight “All-or-Nothing” Collisions?



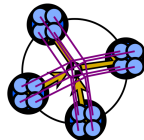


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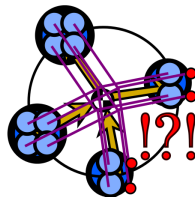
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Variable Weight “All-or-Nothing” Collisions?

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:

$$\text{Rand} < \frac{w_i + w_j - w_{min}}{N_p(N_p - 1)(2\bar{w} - w_{min})}$$

-or-

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Collide If:

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Perform Standard VHS Collisions

Generate/Modify Particles with:

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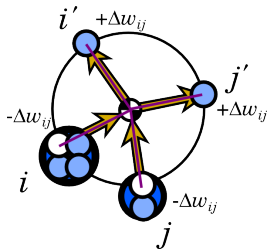


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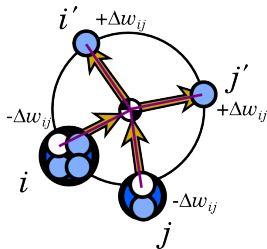


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- **Still Requires Merge $w_i \neq \text{const}$**

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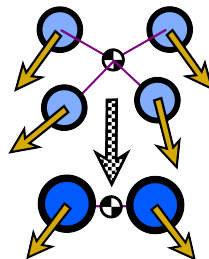
Update $\langle \sigma v \rangle^{\max}$



REVIEW OF CONSERVATIVE MERGE

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



$$w_{cell} = \sum_i^{(n+2)} w_i$$

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

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

$$w_{(a/b)} = w_m/2$$

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

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

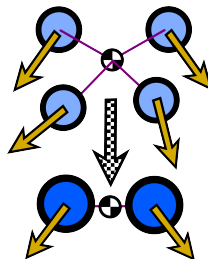


REVIEW OF CONSERVATIVE MERGE

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

Selection of Near Neighbors in VDF Limits Thermalization



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

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

$$w_{(a/b)} = w_m/2$$

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

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



REVIEW OF CONSERVATIVE MERGE

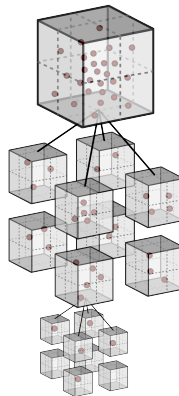
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Selection of Near Neighbors in VDF Limits Thermalization

Merge via Separate Octree/Species
Only Change for Mixtures!

Octree Velocity Bins



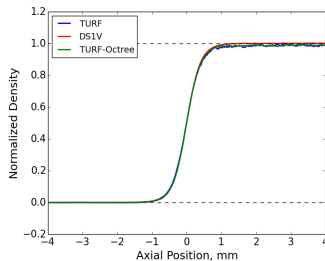
Efficient Neighbor Selection



FROM RGD30: MACH 2 ARGON SHOCK

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:
 $T_{ref}=273\text{K}$, $d_{ref}=4.17\text{\AA}$, $\omega_{VHS}=0.81$



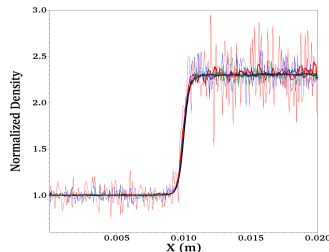


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 $T_{ref}=273\text{K}$, $d_{ref}=4.17\text{\AA}$, $\omega_{VHS}=0.81$
- Time Average:
 $\bar{n}$ from $t \in [80, 100)\mu\text{s}$

TURF - SWPM+Octree



Target N/Cell Quadrupled per Line

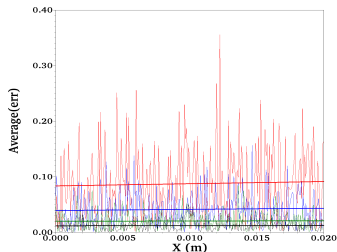
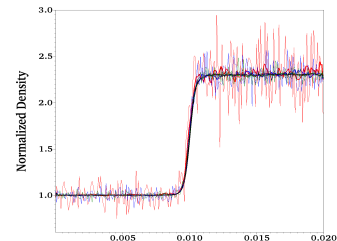


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- Time Average:
 $\bar{n}$ from $t \in [80, 100)\mu\text{s}$
- Error (Normalized L_1):
 $err = |n - \bar{n}|/\bar{n}$
- Error Controlled: $err \propto \sqrt{N/cell}$

TURF - SWPM+Octree



Target N/Cell Quadrupled per Line

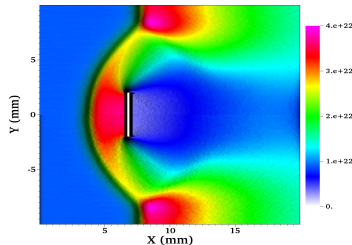


FROM RGD30: MACH 8 ARGON BOW SHOCK

2D Argon Shock Test

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

TURF: n - Standard DSMC



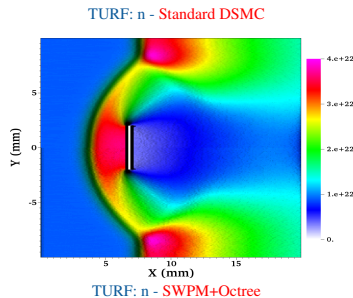
TURF: n - SWPM+Octree



FROM RGD30: MACH 8 ARGON BOW SHOCK

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- Half Domain Modeled:
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- Time Average:
 $\bar{n}$ from $t \in [80, 100)\mu\text{s}$
- SWPM Similar to Standard DSMC



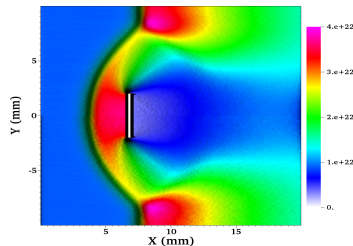


FROM RGD30: MACH 8 ARGON BOW SHOCK

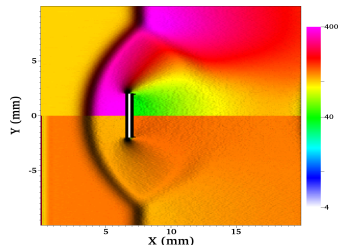
2D Argon Shock Test

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- Specular: $x=5 - 5.04\text{mm}$ with $y=\pm 2\text{mm}$
- Half Domain Modeled:
 $80\mu\text{m} \times 80\mu\text{m}$ Cells
- Time Average:
 $\bar{n}$ from $t \in [80, 100)\mu\text{s}$
- SWPM Similar to Standard DSMC
- Despite Different N_p/Cell

TURF: n - Standard DSMC



TURF: n - SWPM+Octree
TURF N_p/Cell - Standard DSMC



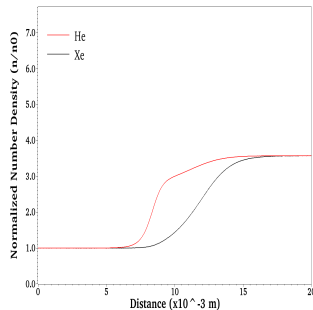
TURF N_p/Cell - SWPM+Octree



HE:XE MIXTURE SHOCK

1D Normal He:Xe Shock Test

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



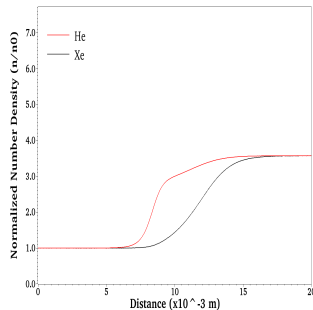
Converged 100x Baseline



HE:XE MIXTURE SHOCK

1D Normal He:Xe Shock Test

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



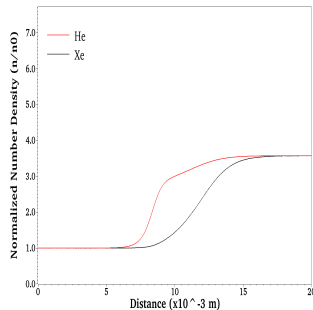
Converged 100x Baseline



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- Separation Peak at $\rho_{He} \approx \rho_{Xe}$



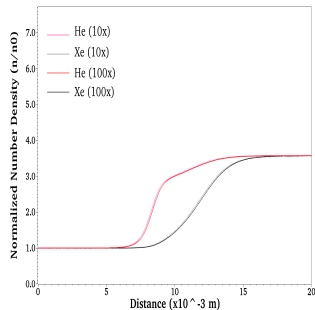
Converged 100x Baseline



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- DSMC needs 33x He:Xe Macroparticles (From m_{Xe}/m_{He})
- Reduced Particle Count Introduces Error



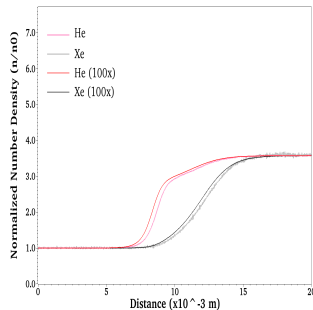
Comparison 10x vs. 100x



HE:Xe MIXTURE SHOCK

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- Error in Time Average at Baseline



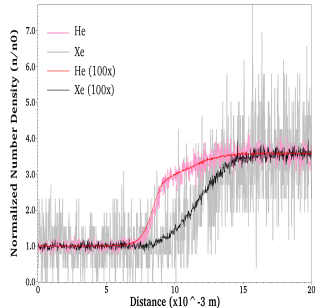
Comparison Baseline vs. 100x



HE:Xe MIXTURE SHOCK

1D Normal He:Xe Shock Test

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- Reduced Particle Count Introduces Error
- Error in Time Average at Baseline
- Instantaneous: Dramatic Noise in Xe



Instantaneous Baseline vs. 100x

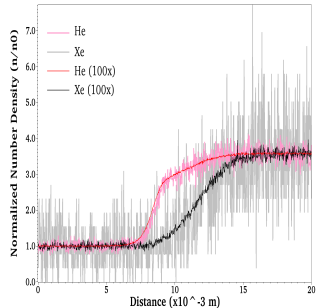


HE:Xe MIXTURE SHOCK

1D Normal He:Xe Shock Test

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



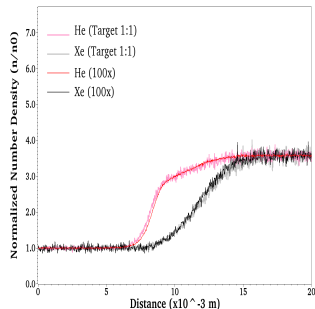
Instantaneous Baseline vs. 100x



He:Xe MIXTURE SHOCK - FRACTIONAL DSMC

1D He:Xe Shock with SWPM+Octrees

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

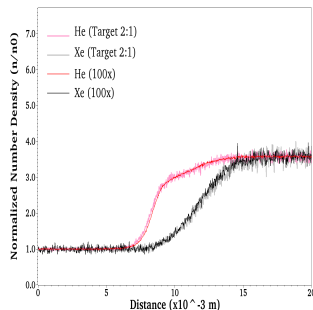


100x vs. FDSMC 1:1



1D He:Xe Shock with SWPM+Octrees

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

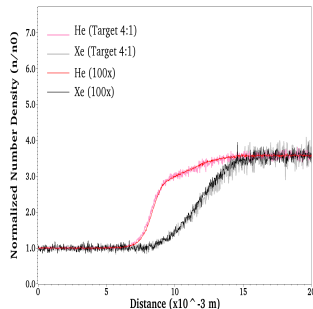


100x vs. FDSMC 2:1



1D He:Xe Shock with SWPM+Octrees

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



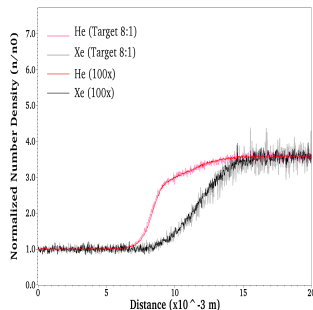
100x vs. FDSMC 4:1



HE:Xe MIXTURE SHOCK - FRACTIONAL DSMC

1D He:Xe Shock with SWPM+Octrees

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

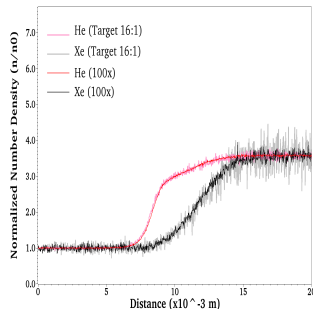


100x vs. FDSMC 8:1



1D He:Xe Shock with SWPM+Octrees

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



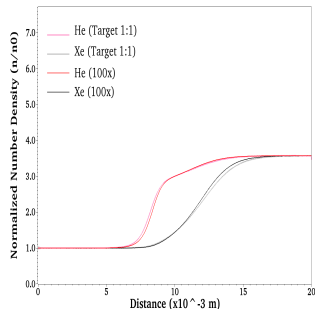
100x vs. FDSMC 16:1



HE:Xe MIXTURE SHOCK - FRACTIONAL DSMC

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...

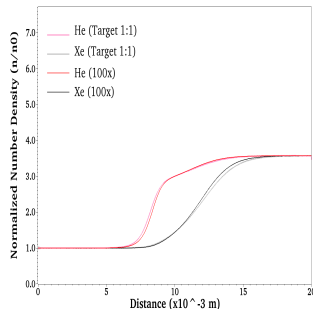


Averaged 100x vs. FDSMC 1:1



1D He:Xe Shock with SWPM+Octrees

- 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...
- 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, $w_i \ll w_j$?



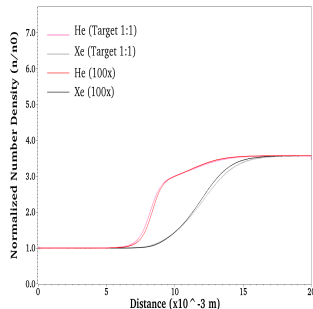
Averaged 100x vs. FDSMC 1:1



1D He:Xe Shock with SWPM+Octrees

- Xe Noise Controlled by 1:1 Target
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 - Improvement Merge to Preserve Tails
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Error Identification in Future Work



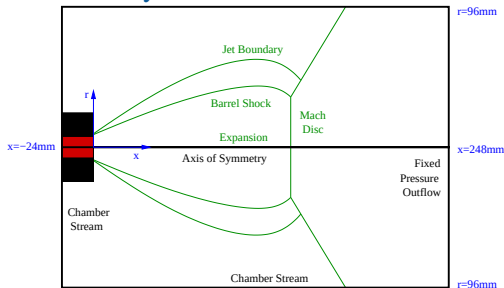
Averaged 100x vs. FDSMC 1:1



ROTHE'S HE:AR FREE-JET EXPERIMENT

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

Jet Flow Layout



$Re = 533$

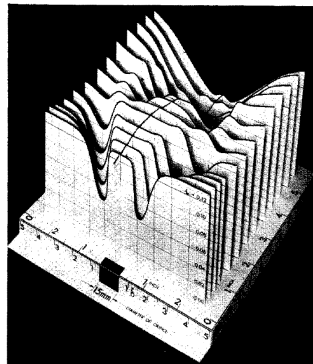
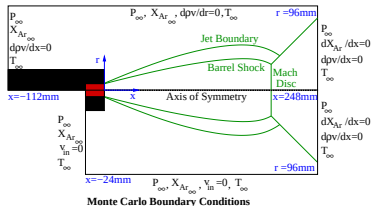


FIG. 11. Mole fraction of argon throughout the flow field of a free jet.

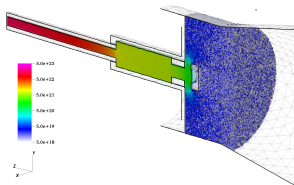


Case Tested in PhD & RGD27:

Continuum Boundary Conditions

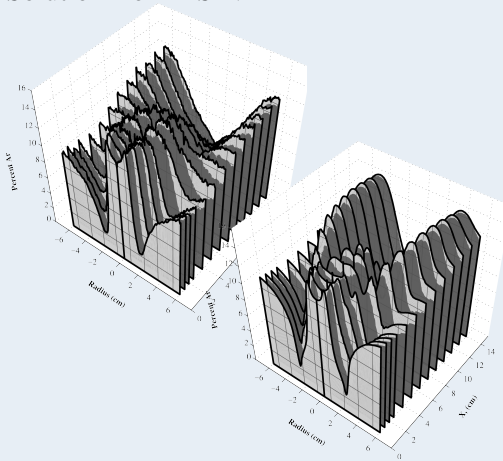


Surrogate for FRC Injection



Dynamic Range $\gg$ Shocks

Solution from DS2V



Solution from SPARTAN
(Navier-Stokes + Diffusion Velocity)



FEATURES FOUND VIA SIMULATIONS

1 Wing Increases near Nozzle Edge

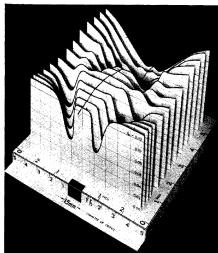
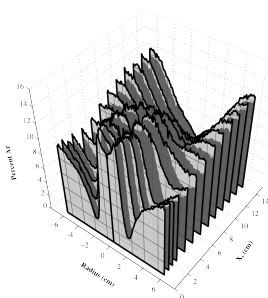
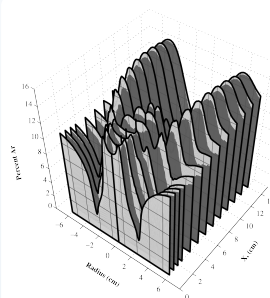


FIG. 11. Mole fraction of argon throughout the flow field of a free jet.

Experimental



DS2V

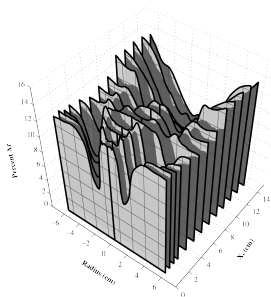


SPARTAN

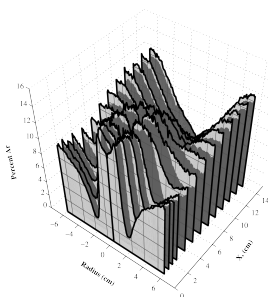


FEATURES FOUND VIA SIMULATIONS

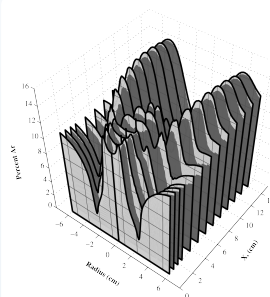
1 Wing Increases near Nozzle Edge



Experimental



DS2V

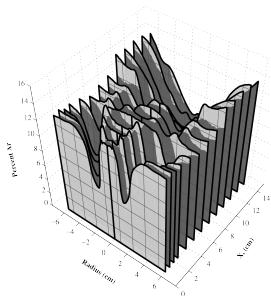


SPARTAN

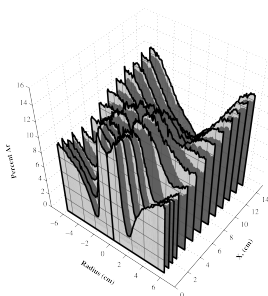


FEATURES FOUND VIA SIMULATIONS

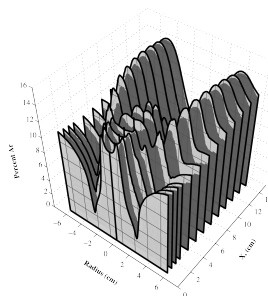
- 1 Wing Increases near Nozzle Edge
- 2 Lower Radial Boundary Edge Concentration



Experimental



DS2V



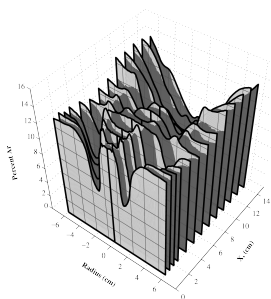
SPARTAN



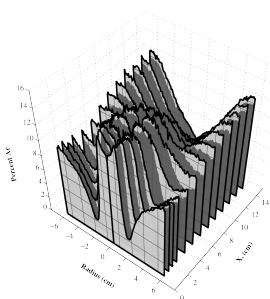
FEATURES FOUND VIA SIMULATIONS



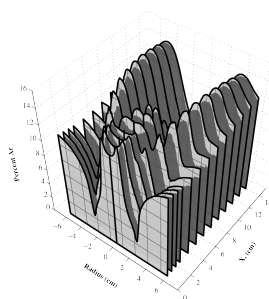
- 1 Wing Increases near Nozzle Edge
- 2 Lower Radial Boundary Edge Concentration
- 3 Deeper Jet Edge Concentration Drop



Experimental



DS2V



SPARTAN



CHALLENGES FOR JET IN TURF

- TURF Naturally 3D Cartesian
- Considered 2D-Axisymmetric TURF
- Simple DSMC but Merge Complex
(Conservation on $v_{\parallel} v_{\perp}$ -Quadrees?)

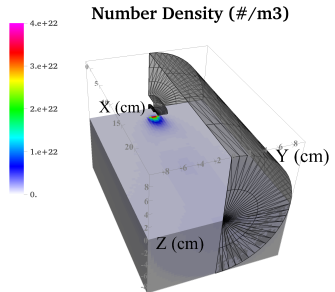
Standard 3D DSMC



CHALLENGES FOR JET IN TURF

- TURF Naturally 3D Cartesian
- Considered 2D-Axisymmetric TURF
- Simple DSMC but Merge Complex (Conservation on $v_{\parallel} v_{\perp}$ -Quadtrees?)
- Opted to Run Coarse Full 3D (Simplified Boundary Conditions)
- 3D Expensive at Tractable Resolution
- Added Collision Sub-Cells to TURF

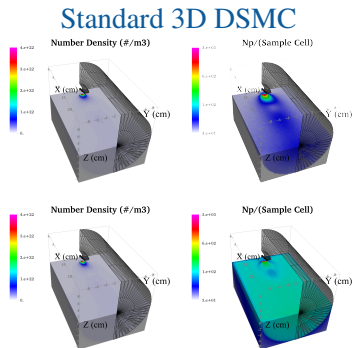
Standard 3D DSMC





CHALLENGES FOR JET IN TURF

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- Considered 2D-Axisymmetric TURF
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- 3D Expensive at Tractable Resolution
- Added Collision Sub-Cells to TURF
- Fractional DSMC Controls Np/Cell

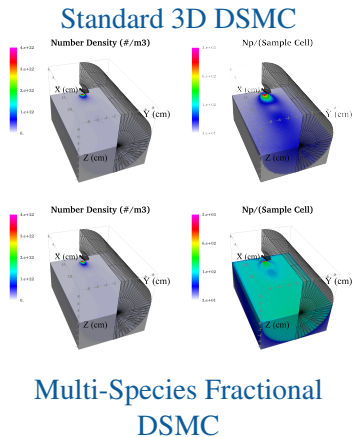


Multi-Species Fractional DSMC



CHALLENGES FOR JET IN TURF

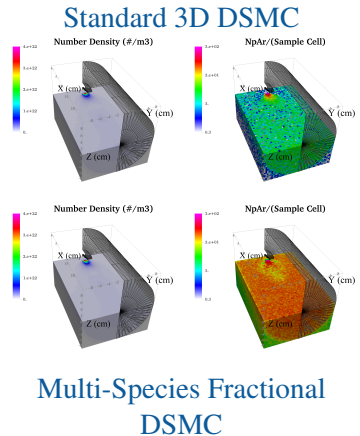
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- Considered 2D-Axisymmetric TURF
- Simple DSMC but Merge Complex (Conservation on $v_{||}v_{\perp}$ -Quadtrees?)
- Opted to Run Coarse Full 3D (Simplified Boundary Conditions)
- 3D Expensive at Tractable Resolution
- Added Collision Sub-Cells to TURF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





CHALLENGES FOR JET IN TURF

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- Considered 2D-Axisymmetric TURF
- Simple DSMC but Merge Complex (Conservation on $v_{||}v_{\perp}$ -Quadrees?)
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- Added Collision Sub-Cells to TURF
- Fractional DSMC Controls Np/Cell
- Linear Density Obscures Results
- Issue Clearer with NpAr/Cell

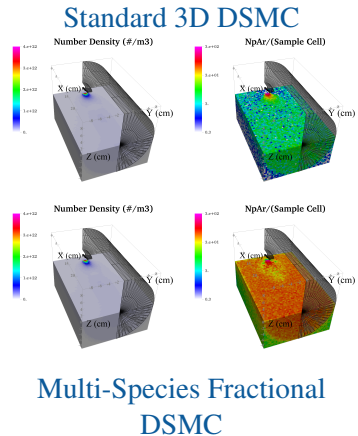




CHALLENGES FOR JET IN TURF

- TURF Naturally 3D Cartesian
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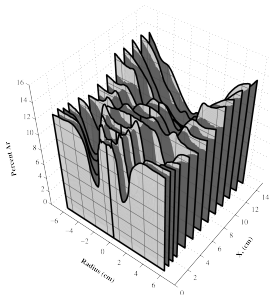
X_{Ar} to RX-Plane $\rightarrow$ for Detailed Results...



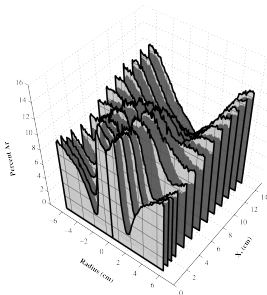


PRELIMINARY TURF RESULTS: HE:AR JET

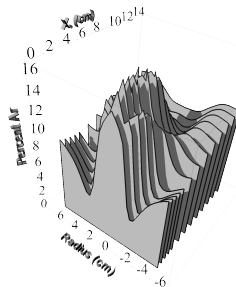
1 Standard DSMC Poor Results



Experimental



DS2V



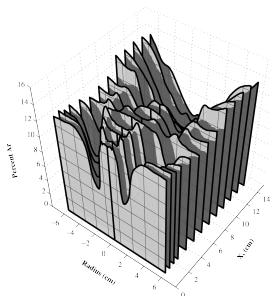
TURF

1:1 - Collision:Sample

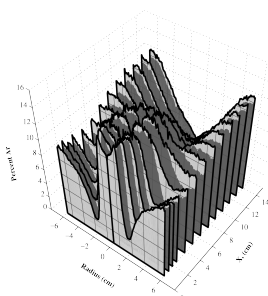


PRELIMINARY TURF RESULTS: HE:AR JET

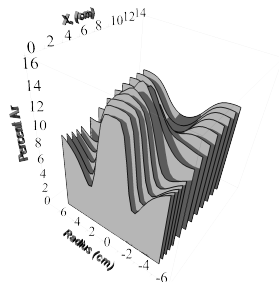
- 1 Standard DSMC Poor Results
- 2 2x2x2 Collision Cell Improves Standard DSMC



Experimental



DS2V



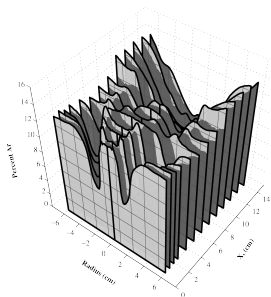
TURF

2x2x2:1 - Collision:Sample

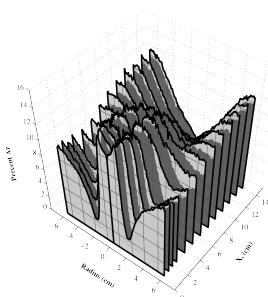


PRELIMINARY TURF RESULTS: HE:AR JET

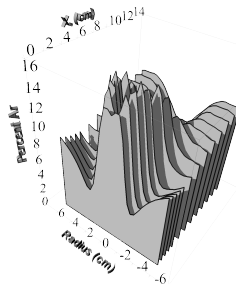
- 1 Standard DSMC Poor Results
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Experimental



DS2V



TURF

SWPM+Octree (2x2x2 Collision Cells)



FUTURE DIRECTIONS: HYBRID ∂f

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

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

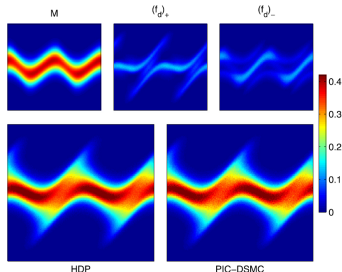


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Strong Landau Damping



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:		$\rightarrow$	$\emptyset$

Yan, JCP 309 (2016) 18-36

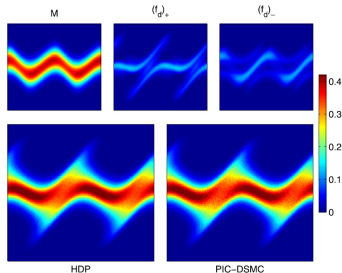


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Yan, JCP 309 (2016) 18-36

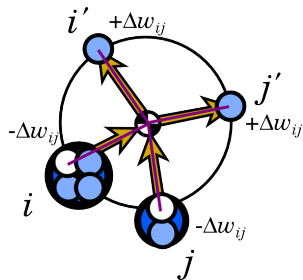


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Stochastic Weight Particle Method (SWPM)



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

+2 Particles/Collision

RGD30



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Octree ∂f -Boltzmann Bin-to-Bin Collisions



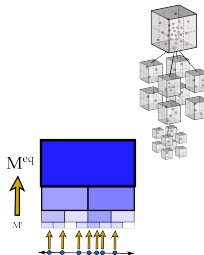


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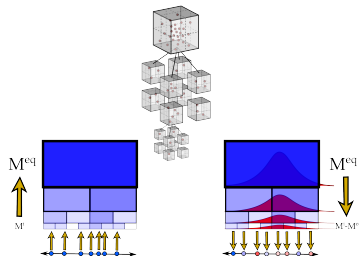


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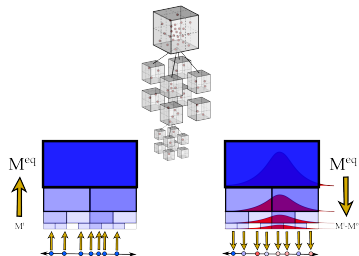


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- B2B Collision Recast with δw Particles

Octree ∂f -Boltzmann Bin-to-Bin Collisions



Sample Collisions using
 Δw : for P-P, P-N, N-N, P-M, N-M
M-M: $\emptyset$

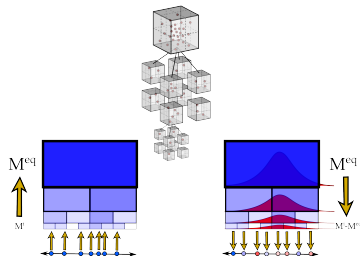


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- Collision Work $\propto \partial f$, not f

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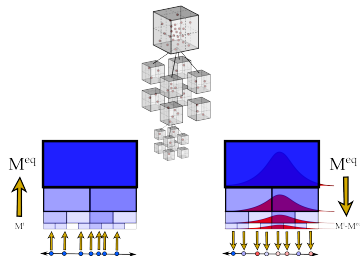


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- Valid at Adaptive Tree Depths
- Entropy Estimate for DOF Distribution

Octree ∂f -Boltzmann Bin-to-Bin Collisions



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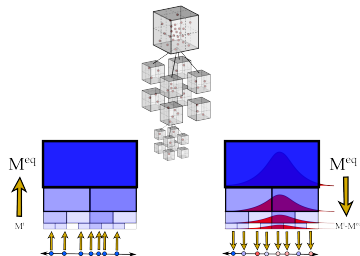


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Combine with 2^6 -Tree
XV $\rightarrow$ Multigrid Solves?



CONCLUSION

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



END



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?