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CONSERVATIVE BIN-TO-BIN FRACTIONAL COLLISIONS

Robert Martin

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SPACECRAFT PROPULSION BRANCH
AIR FORCE RESEARCH LABORATORY
EDWARDS AIR FORCE BASE, CA USA



30th International Symposium on Rarefied Gas Dynamics
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- 1 BACKGROUND
- 2 FRACTIONAL COLLISIONS
- 3 BIN-TO-BIN FRACTIONAL COLLISIONS
- 4 CONCLUSION



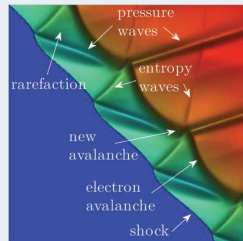
Important Collisions in Spacecraft Propulsion:

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

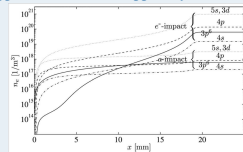
Common Features in Spacecraft Collisions:

- 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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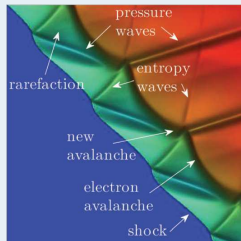
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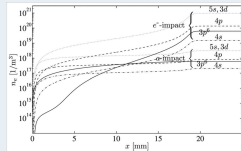
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Need Low Noise & High Dynamic Range
Collision Algorithms

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



Continuum to Discrete Representation:

- Many Particles \rightsquigarrow Continuous Distribution



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- Discretized VDF Yields Vlasov
But Collision Integral Still a Problem



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- Collisions between Discrete Velocities



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(Tail Critical to Inelastic Collisions)



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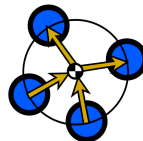
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Variable Weight “All-or-Nothing” Collisions?

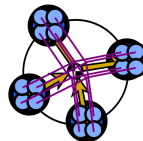




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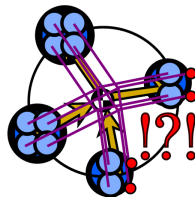
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Variable Weight “All-or-Nothing” Collisions?

Physically Inconsistent!

(Mixing Violates Momentum/Energy Conservation)





NTC Collisions:

- (Collision Rate Volume):(Cell Volume)

Fractional-NTC Collisions:

$$Z_{ij} = \frac{n_i n_j}{2} \langle \sigma v \rangle_{ij} dt = \frac{w_i w_j}{2V_{cell}^2} \langle \sigma v \rangle_{ij} dt$$



NTC Collisions:

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- Select Fraction of $\frac{1}{2}N^2$ Possible

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$$P_{max} = w \langle \sigma v \rangle_{ij}^{max} dt / V_{cell}$$

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Collide if:

$$\text{Rand}(1) < \frac{N_{collide}}{N_{select}} = \frac{P_{ij}}{P_{max}} = \frac{\langle \sigma v \rangle_{ij}}{\langle \sigma v \rangle_{ij}^{max}}$$



NTC Collisions:

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Fractional-NTC Collisions:

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Fractional-NTC Collisions:

- Select f by Cost/Accuracy Tradeoff
- Collision Δw Scaled for Skipped
- Add Particles & Original Reduced

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

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



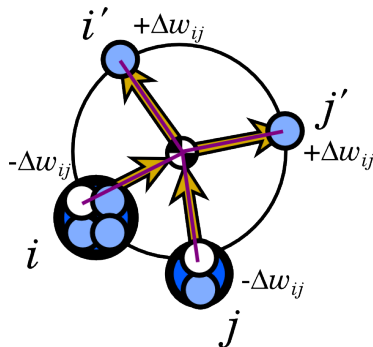
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Fractional-NTC Collisions:

- Select f by Cost/Accuracy Tradeoff
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- Add Particles & Original Reduced
- **+2 Particles/Collision!** → **Must Merge**

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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-

$$\text{Rand} < \frac{w_i + w_j - w_{min}}{(2w_{max} - w_{min})}$$

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Perform Standard VHS Collisions

Generate/Modify Particles with:

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

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



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

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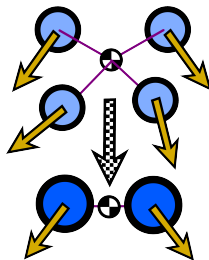
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Update $\langle \sigma v \rangle^{max}$



Merge to Pair \rightarrow 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



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

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

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

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

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

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

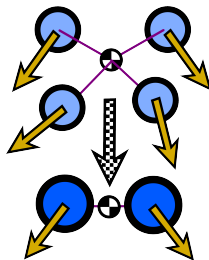


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Selection of Near Neighbors in VDF Limits Thermalization

(\approx Near Neighbor Pairs in 2:1 Merges that Limit Numerical Cooling)



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

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



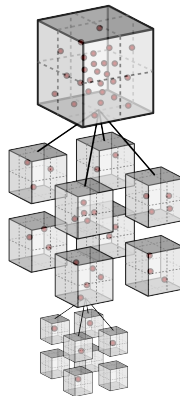
Merge to Pair → DOF for Conservation:

- $(n+2):2$ 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

(\approx Near Neighbor Pairs in 2:1 Merges that Limit Numerical Cooling)

Octree Velocity Bins

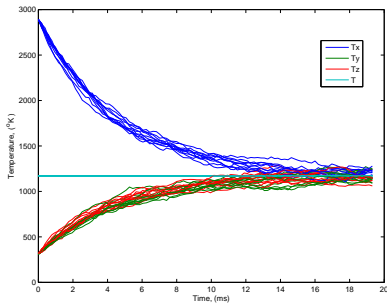


Efficient Neighbor Selection

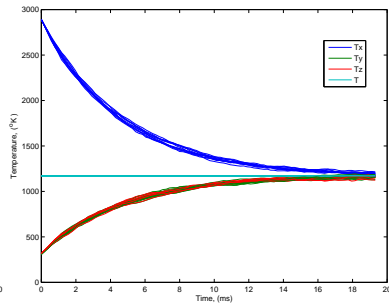


Bi-Maxwellian Thermalization Results

Original-NTC



Fractional-NTC

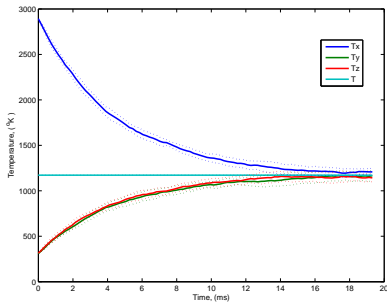


Comparison of 10x Runs from Same Initial Distribution

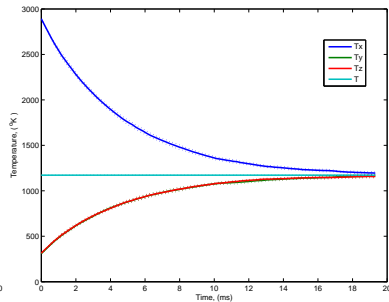


Bi-Maxwellian Thermalization Results

Original-NTC



Fractional-NTC

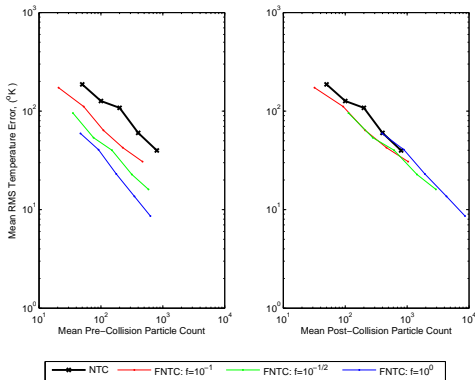


Mean and RMS Fluctuation of Sample Runs

Fluctuations Level Tuneable with f Independent of Particles Count



Bi-Maxwellian Thermalization Results



Fluctuations Level Tuneable with f Independent of Particles Count

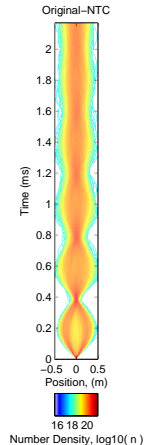


- Initial Bi-Maxwellian Distribution in Potential Well



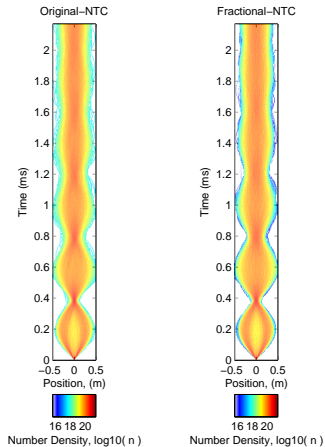


- Initial Bi-Maxwellian Distribution in Potential Well
- NTC Collisions Results in Beam Thermalization



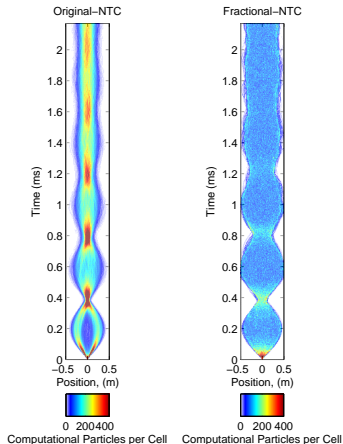


- Initial Bi-Maxwellian Distribution in Potential Well
- NTC Collisions Results in Beam Thermalization
- Fractional-NTC Collisions Produce Same Behavior



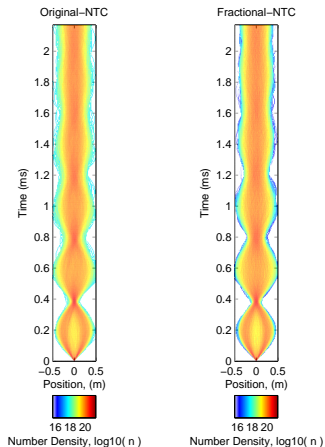


- Initial Bi-Maxwellian Distribution in Potential Well
- NTC Collisions Results in Beam Thermalization
- Fractional-NTC Collisions Produce Same Behavior
- Particles/Cell Dramatically Different



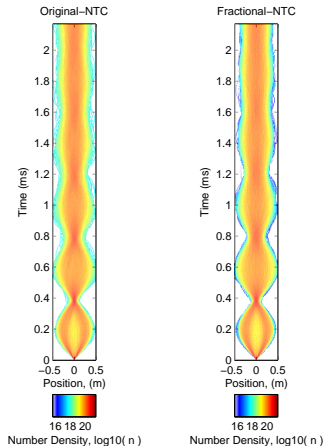


- Initial Bi-Maxwellian Distribution in Potential Well
- NTC Collisions Results in Beam Thermalization
- Fractional-NTC Collisions Produce Same Behavior
- Particles/Cell Dramatically Different
- Fringe Extends to Lower Densities with Variable Weights





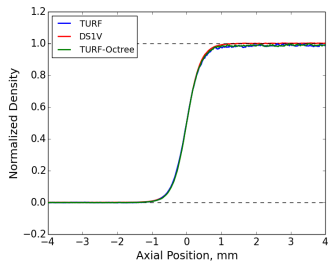
- Initial Bi-Maxwellian Distribution in Potential Well
- NTC Collisions Results in Beam Thermalization
- Fractional-NTC Collisions Produce Same Behavior
- Particles/Cell Dramatically Different
- Fringe Extends to Lower Densities with Variable Weights
- Relative 'Error' Unknown without Analytical Solution or High Fidelity Simulation





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

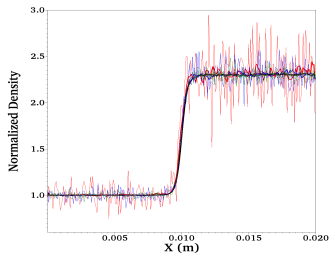




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 $T_{ref}=273\text{K}$, $d_{ref}=4.17\text{\AA}$, $\omega_{VHS}=0.81$
- Time Average:
 \bar{n} from $t \in [80, 100)\mu\text{s}$

TURF - SWPM+Octree



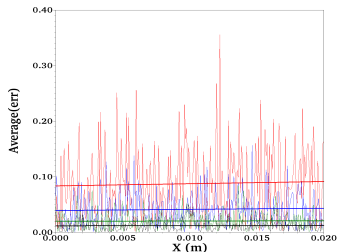
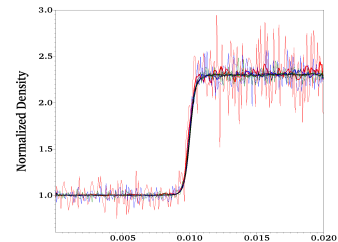
Target N/Cell Quadrupled per Line



1D Normal Argon Shock Test

- Simple Verification vs. DS1V
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 $T_0 = 293\text{K}$, $n_0 = 1\text{E}22/\text{m}^3$, $v_0 = 637.4(\text{m/s})$
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 $T_{ref}=273\text{K}$, $d_{ref}=4.17\text{\AA}$, $\omega_{VHS}=0.81$
- Time Average:
 \bar{n} from $t \in [80, 100)\mu\text{s}$
- Error (Normalized L_1):
 $err = |n - \bar{n}| / \bar{n}$
- Error Controlled: $err \propto \sqrt{N/cell}$

TURF - SWPM+Octree



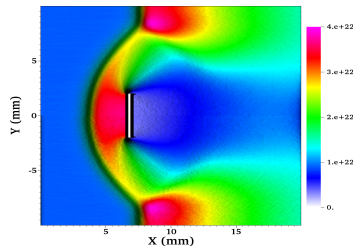
Target N/Cell Quadrupled per Line



2D Argon Shock Test

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

TURF: n - Standard DSMC



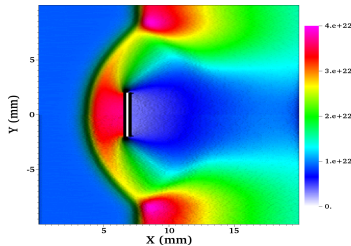
TURF: n - SWPM+Otree



2D Argon Shock Test

- Initial Conditions like M=2 Except:
 $v_0 = 2550\text{m/s}$
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- 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

TURF: n - Standard DSMC



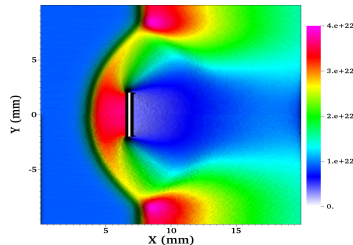
TURF: n - SWPM+Octree



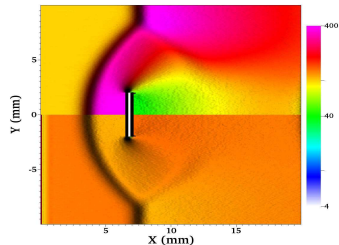
2D Argon Shock Test

- 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
- 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



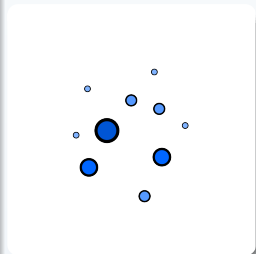
TURF: n - SWPM+Octree
TURF N_p/Cell - Standard DSMC



TURF N_p/Cell - SWPM+Octree

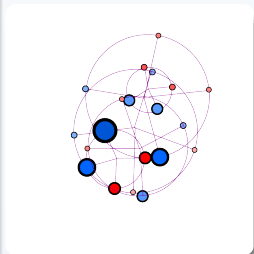


- Larger N_{select} \rightarrow Better Approx. of Collision Integral



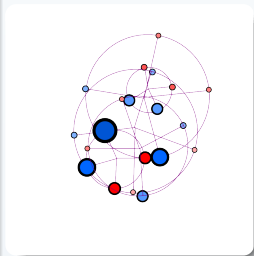


- Larger N_{select} \rightarrow Better Approx. of Collision Integral
- f-NTC Produces 2x-Particles per $N_{select} = f N_p$
- Particle Memory Requires $\propto N_{max} \rightarrow (1 + 2f)N_{max}$



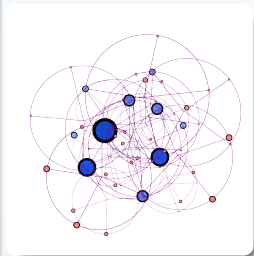


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- For DSMC-like Results, $f \approx O(1)$



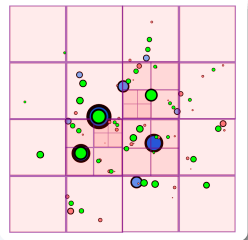


- Larger N_{select} \rightarrow Better Approx. of Collision Integral
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- For DSMC-like Results, $f \approx O(1)$
- Time Accurate or Dense Simulations, $f \approx O(10)+?$



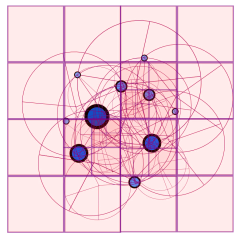


- Larger $N_{select} \rightarrow$ Better Approx. of Collision Integral
- f-NTC Produces 2x-Particles per $N_{select} = f N_p$
- Particle Memory Requires $\propto N_{max} \rightarrow (1 + 2f)N_{max}$
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- Merge Contracts back to $O(N_{max})$ Particles
- Merge Immediately after Collide per Spatial Cell?..
- Sort for Merge still $\propto (1 + 2f) \log(1 + 2f)?$





- Larger N_{select} \rightarrow Better Approx. of Collision Integral
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- Time Accurate or Dense Simulations, $f \approx O(10)+?$
- Merge Contracts back to $O(N_{max})$ Particles
- Merge Immediately after Collide per Spatial Cell?..
- Sort for Merge still $\propto (1 + 2f) \log(1 + 2f)?$
- Combine Collision and Merge in Single Step?





- Fractional Collision as Rate Equation

$$\begin{bmatrix} \vdots \\ \dot{w}_i \\ \vdots \\ \dot{w}_j \\ \vdots \\ \dot{w}_{i'} \\ \vdots \\ \dot{w}_{j'} \\ \vdots \end{bmatrix} = \sum_{k=1}^{N_{select}} \begin{bmatrix} \vdots \\ -w_i \langle \sigma v \rangle_{ij}^k w_j \\ \vdots \\ -w_i \langle \sigma v \rangle_{ij}^k w_j \\ \vdots \\ w_i \langle \sigma v \rangle_{ij}^k w_j \\ \vdots \\ w_i \langle \sigma v \rangle_{ij}^k w_j \\ \vdots \end{bmatrix}$$



- Fractional Collision as Rate Equation
- Bin Moments needed for Particle Pairs

$$\begin{bmatrix} \dot{w}_i \\ \dot{w}_j \\ \dot{w}_{i'} \\ \dot{w}_{j'} \\ - \\ \dot{(wv)}_i \\ \dot{(wv)}_j \\ \dot{(wv)}_{i'} \\ \dot{(wv)}_{j'} \\ - \\ \dot{(wv^2)}_i \\ \dot{(wv^2)}_j \\ \dot{(wv^2)}_{i'} \\ \dot{(wv^2)}_{j'} \end{bmatrix} = \sum_{k=1}^{N_{select}} \begin{bmatrix} -\Delta w_{ij} \\ -\Delta w_{ij} \\ \Delta w_{ij} \\ \Delta w_{ij} \\ - \\ -\Delta w_{ij}v_i \\ -\Delta w_{ij}v_j \\ \Delta w_{ij}v_{i'} \\ \Delta w_{ij}v_{j'} \\ - \\ -\Delta w_{ij}v_i^2 \\ -\Delta w_{ij}v_j^2 \\ \Delta w_{ij}v_{i'}^2 \\ \Delta w_{ij}v_{j'}^2 \end{bmatrix}$$



COLLIDE TO BINS

- Fractional Collision as Rate Equation
- Bin Moments needed for Particle Pairs
- Particle Pairs (i,j) Picked Randomly
- DSMC-like Collision (VHS,VSS,etc.)
Random $\chi, \theta \rightarrow (v_{i'}, v_{j'})$

$$\begin{bmatrix} \dot{w}_i \\ \dot{w}_j \\ \dot{w}_{i'} \\ \dot{w}_{j'} \\ - \\ (\dot{wv})_i \\ (\dot{wv})_j \\ (\dot{wv})_{i'} \\ (\dot{wv})_{j'} \\ - \\ (\dot{wv^2})_i \\ (\dot{wv^2})_j \\ (\dot{wv^2})_{i'} \\ (\dot{wv^2})_{j'} \end{bmatrix} = \sum_{k=1}^{N_{select}} \begin{bmatrix} -\Delta w_{ij} \\ -\Delta w_{ij} \\ \Delta w_{ij} \\ \Delta w_{ij} \\ - \\ -\Delta w_{ij}v_i \\ -\Delta w_{ij}v_j \\ \Delta w_{ij}v_{i'} \\ \Delta w_{ij}v_{j'} \\ - \\ -\Delta w_{ij}v_i^2 \\ -\Delta w_{ij}v_j^2 \\ \Delta w_{ij}v_{i'}^2 \\ \Delta w_{ij}v_{j'}^2 \end{bmatrix}$$



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- Bin Moments needed for Particle Pairs
- Particle Pairs (i,j) Picked Randomly
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Random $\chi, \theta \rightarrow (v_{i'}, v_{j'})$
- Octree to Find i' and j' Bins
 $8^L \rightarrow$ Few Levels to Search

$$\begin{bmatrix} \dot{w}_i \\ \dot{w}_j \\ \dot{w}_{i'} \\ \dot{w}_{j'} \\ - \\ (\dot{wv})_i \\ (\dot{wv})_j \\ (\dot{wv})_{i'} \\ (\dot{wv})_{j'} \\ - \\ (\dot{wv}^2)_i \\ (\dot{wv}^2)_j \\ (\dot{wv}^2)_{i'} \\ (\dot{wv}^2)_{j'} \end{bmatrix} = \sum_{k=1}^{N_{select}} \begin{bmatrix} -\Delta w_{ij} \\ -\Delta w_{ij} \\ \Delta w_{ij} \\ \Delta w_{ij} \\ - \\ -\Delta w_{ij}v_i \\ -\Delta w_{ij}v_j \\ \Delta w_{ij}v_{i'} \\ \Delta w_{ij}v_{j'} \\ - \\ -\Delta w_{ij}v_i^2 \\ -\Delta w_{ij}v_j^2 \\ \Delta w_{ij}v_{i'}^2 \\ \Delta w_{ij}v_{j'}^2 \end{bmatrix}$$



COLLIDE TO BINS

- Fractional Collision as Rate Equation
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Random $\chi, \theta \rightarrow (v_{i'}, v_{j'})$
- Octree to Find i' and j' Bins
 $8^L \rightarrow$ Few Levels to Search

Conserve Mass, Momentum, and Energy

Memory Constant Independent of N^{select}

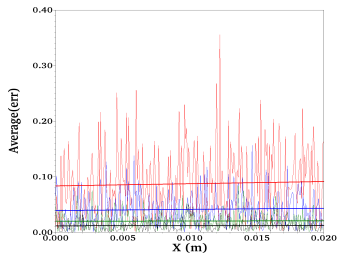
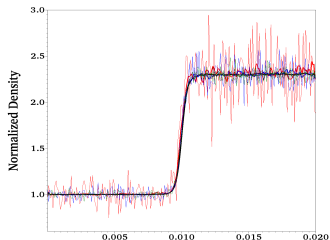
$$\begin{bmatrix} \dot{w}_i \\ \dot{w}_j \\ \dot{w}_{i'} \\ \dot{w}_{j'} \\ - \\ (\dot{wv})_i \\ (\dot{wv})_j \\ (\dot{wv})_{i'} \\ (\dot{wv})_{j'} \\ - \\ (\dot{wv^2})_i \\ (\dot{wv^2})_j \\ (\dot{wv^2})_{i'} \\ (\dot{wv^2})_{j'} \end{bmatrix} = \sum_{k=1}^{N^{select}} \begin{bmatrix} -\Delta w_{ij} \\ -\Delta w_{ij} \\ \Delta w_{ij} \\ \Delta w_{ij} \\ - \\ -\Delta w_{ij}v_i \\ -\Delta w_{ij}v_j \\ \Delta w_{ij}v_{i'} \\ \Delta w_{ij}v_{j'} \\ - \\ -\Delta w_{ij}v_i^2 \\ -\Delta w_{ij}v_j^2 \\ \Delta w_{ij}v_{i'}^2 \\ \Delta w_{ij}v_{j'}^2 \end{bmatrix}$$



1D Normal Argon Shock Test

- Mach 2 Case Repeated

TURF - SWPM+Octree

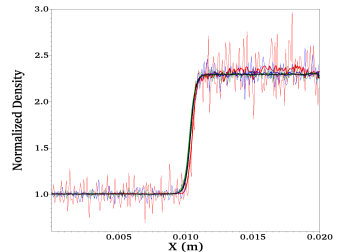
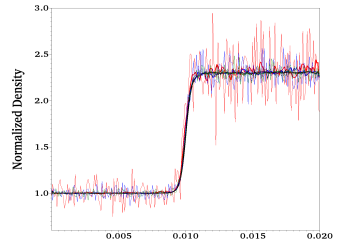




1D Normal Argon Shock Test

- Mach 2 Case Repeated
- Bin-to-Bin Collisions Results Similar

TURF - SWPM+Octree



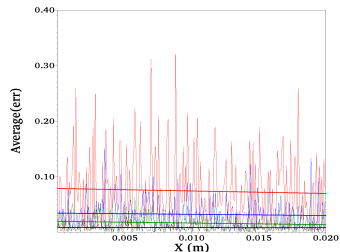
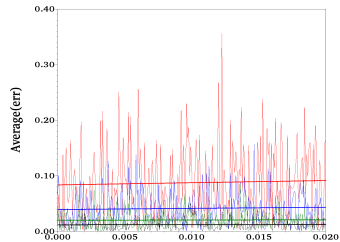
TURF - Bin to Bin



1D Normal Argon Shock Test

- Mach 2 Case Repeated
- Bin-to-Bin Collisions Results Similar
- Target $N_p/Cell$ Still Error Control
(Target N/Cell Quadrupled per Line)

TURF - Octree



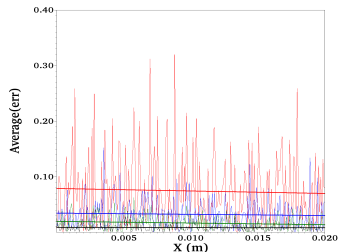
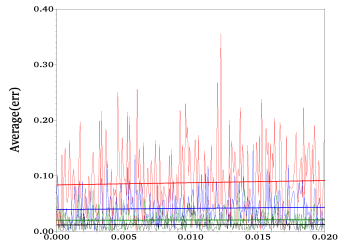
TURF - Bin to Bin



1D Normal Argon Shock Test

- Mach 2 Case Repeated
- Bin-to-Bin Collisions Results Similar
- Target $N_p/Cell$ Still Error Control (Target N/Cell Quadrupled per Line)
- Collision Core $\approx 3x$ Slower
- Non-Ideal: Dynamic Range Low

TURF - Octree



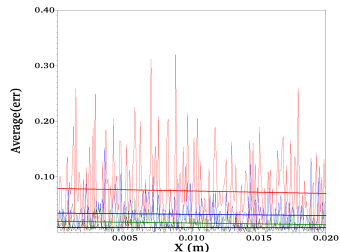
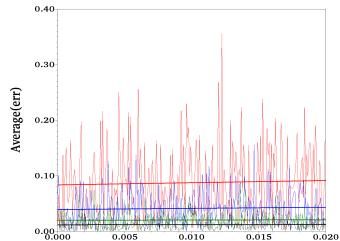
TURF - Bin to Bin



1D Normal Argon Shock Test

- Mach 2 Case Repeated
- Bin-to-Bin Collisions Results Similar
- Target $N_p/Cell$ Still Error Control (Target N/Cell Quadrupled per Line)
- Collision Core $\approx 3x$ Slower
- Non-Ideal: Dynamic Range Low
- Proof-of-Concept with Real X-Section
- Expansion/Plume will be Better Case

TURF - Octree



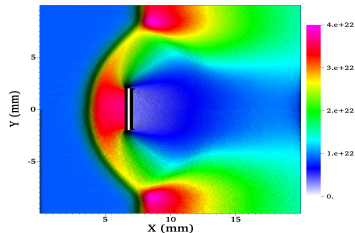
TURF - Bin to Bin



2D Argon Shock Test

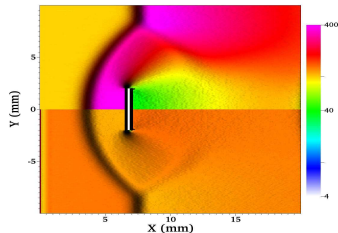
- Mach 8 Case Also Repeated

TURF: n - Standard DSMC



TURF: (n) SWPM+Octree

TURF: Np/Cell - Standard DSMC



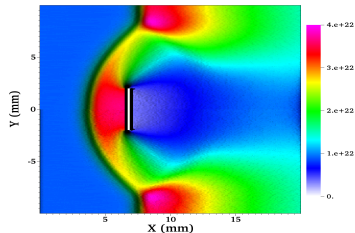
TURF: (Np/Cell) SWPM+Octree



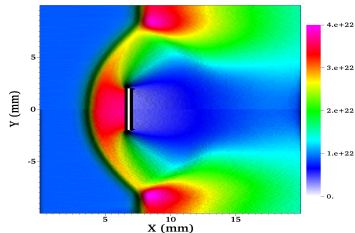
2D Argon Shock Test

- Mach 8 Case Also Repeated
- Bin-to-Bin Collisions Results Similar

TURF: n - Standard DSMC



TURF: (n) SWPM+Octree
TURF: n - Standard DSMC



TURF: (n) Bin-to-Bin

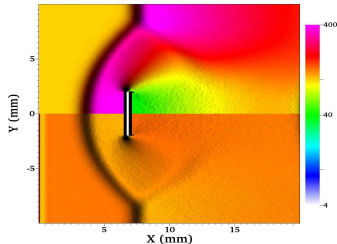


MACH 8 ARGON BOW SHOCK

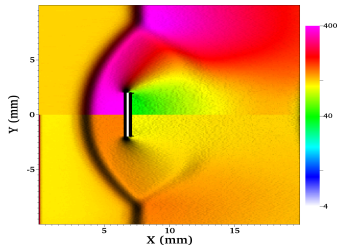
2D Argon Shock Test

- Mach 8 Case Also Repeated
- Bin-to-Bin Collisions Results Similar
- Target $Np/Cell$ Still Error Control

TURF: Np/Cell - Standard DSMC



TURF: (Np/Cell) SWPM+Octree
TURF: Np/Cell - Standard DSMC



TURF: (Np/Cell) Bin-to-Bin



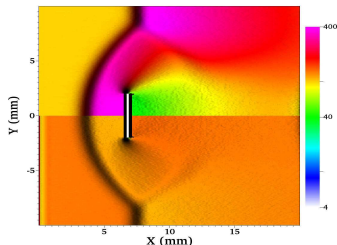
MACH 8 ARGON BOW SHOCK

2D Argon Shock Test

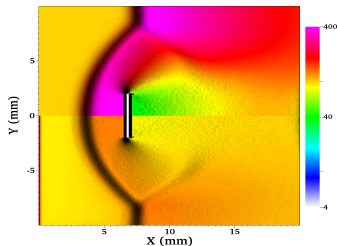
- Mach 8 Case Also Repeated
- Bin-to-Bin Collisions Results Similar
- Target $Np/Cell$ Still Error Control
- B2B Run with $f=4x$ Collisions
(Note: SWPM+Octree $f=1x$)

Standard - Collisions	548.9s	1x
Standard - Total Run	7945.3s	100%
SWPM+Octree - Collisions	2719.6s	4.95x
SWPM+Octree - Total Run	9542.4s	120%
Bin-to-Bin - Collisions	13163.6s	24.0x
Bin-to-Bin - Total Run	18860.5s	237%

TURF: Np/Cell - Standard DSMC



TURF: (Np/Cell) SWPM+Octree
 TURF: Np/Cell - Standard DSMC



TURF: (Np/Cell) Bin-to-Bin



MACH 8 ARGON BOW SHOCK

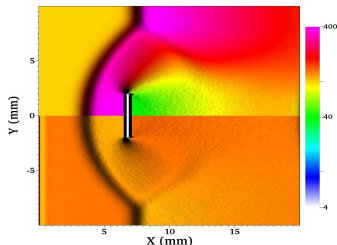
2D Argon Shock Test

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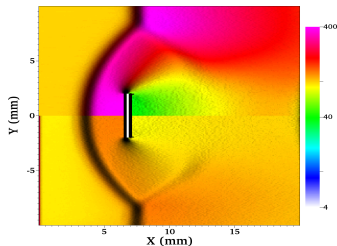
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- Some Cost Compensated by Lower Np
- Too much Fill for Better Wake
- Significant Optimizations Still Needed
(i.e. Data Structures, Sort->Sums, v-Bounds, Morton curve)

TURF: Np/Cell - Standard DSMC



TURF: (Np/Cell) SWPM+Octree
 TURF: Np/Cell - Standard DSMC



TURF: (Np/Cell) Bin-to-Bin



- Standard Collision Incompatible with Variable Weight
- SWPM+Octree Option for Variable Weight Collision
- Bin-To-Bin Potentially Alleviates Memory Constraints
- Initial Verification vs. Standard Shock Cases Positive
- Limited Utility in Standard Shock Cases
- Performance with Strong Expansion/Plume Needed
- SWPM/Bin-to-Bin more Useful for Trace Species?



END



Thank You
Questions?