Modeling and Testing Flowing Gas in Eunomia

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Introduction

Background/Purpose:

- B2.5-Eunomia is a kinetic neutral and multifluid plasma code
- Eunomia replaces Eirene for linear geometries
- Good for modeling experiments using a linear plasma generator

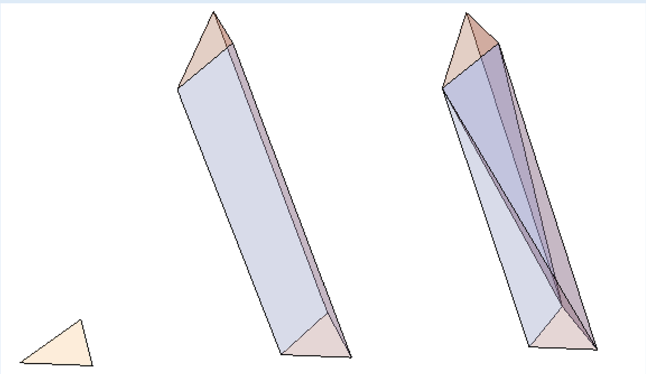
Goals:

- Develop integrated test cases
- Model a uniform gas flowing through a surface
- Test Galilean invariance of collisions

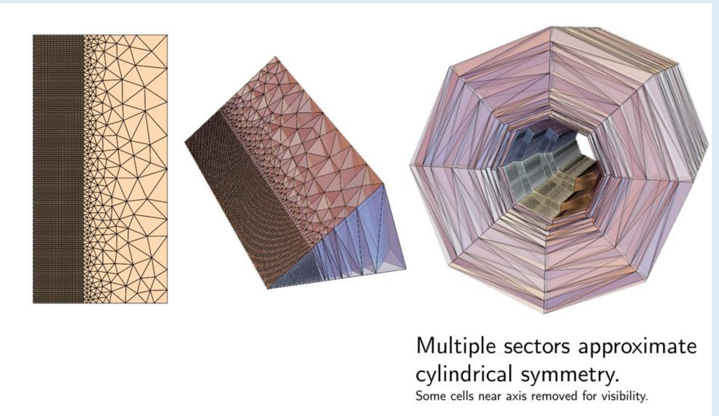
Eunomia Background Info

Geometry

Triangular grid unit → Extruded prism → Tetrahedron cells

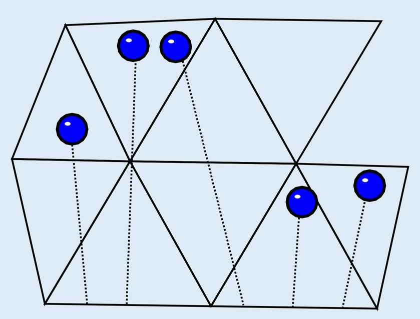


Triangular grid → Extruded sector → full volume

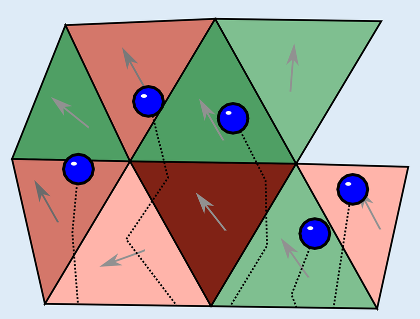


Simulated Particles Move through Background

Initial paths set background



Background affects collisions



References:

[1] Wieggers, Rob. "B2.5-Eunomia simulations of Pilot-PSI." PhD Thesis, Dutch Institute for Fundamental Energy Research, 2012.
[2] Bird, G.A. *Molecular Gas Dynamics and the Direct Simulation of Gas Flow*. 2013.
[3] Chapman, S. & Cowling, T.G. *The Mathematical Theory of Non-Uniform Gases*. 1958.

Boundary Condition: Flowing Gas

Source Strength:

from [2]

$$\dot{N} = n\frac{e^{-u_0^2\beta^2} + \sqrt{\pi}u_0\beta(1+\mathrm{erf}(u_0\beta))}{2\beta\sqrt{\pi}}$$

where $\beta = \sqrt{\frac{m}{2kT}}$

$\dot{N}$ # particles s^{-1} m^{-2}

u_0 Component of flow velocity perpendicular to the surface

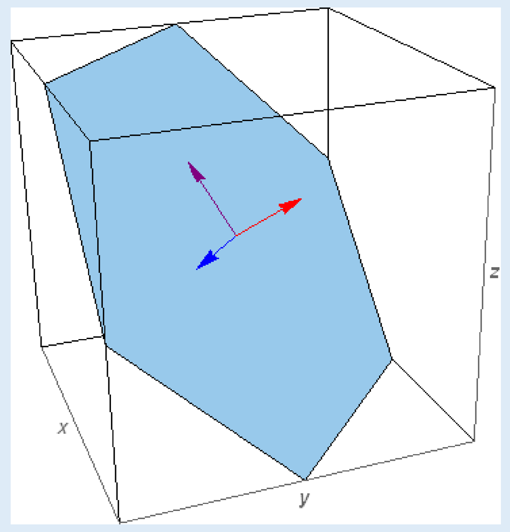
Velocity Distribution:

Normal Basis

Basis for non-horizontal walls: $\{\boldsymbol{\Phi Wall}, \boldsymbol{\Psi Wall}, \hat{\boldsymbol{n}}\}$

$\boldsymbol{\Phi Wall}$, $\boldsymbol{\Psi Wall}$ in plane of wall

$\boldsymbol{\Phi Wall} = \hat{\boldsymbol{n}} \times \hat{\boldsymbol{z}}$ $\quad$ $\boldsymbol{\Psi Wall} = \boldsymbol{\Phi Wall} \times \hat{\boldsymbol{n}}$



Velocity Vector Generation

Normal component

chosen through **rejection sampling** from Maxwellian distribution of flowing gas through surface

Wall **parallel** components

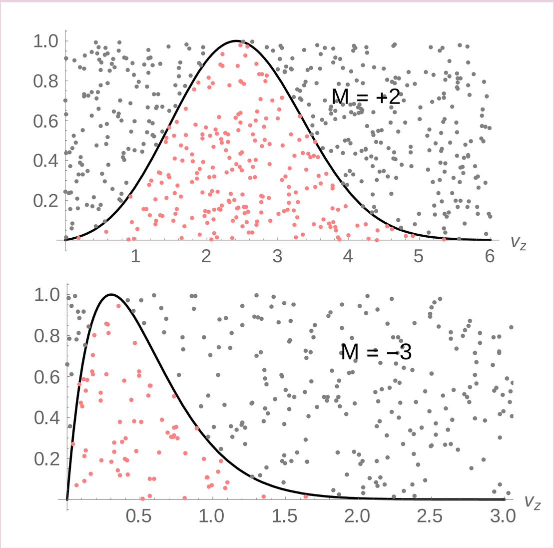
chosen from a shifted Gaussian around respective flow velocity components

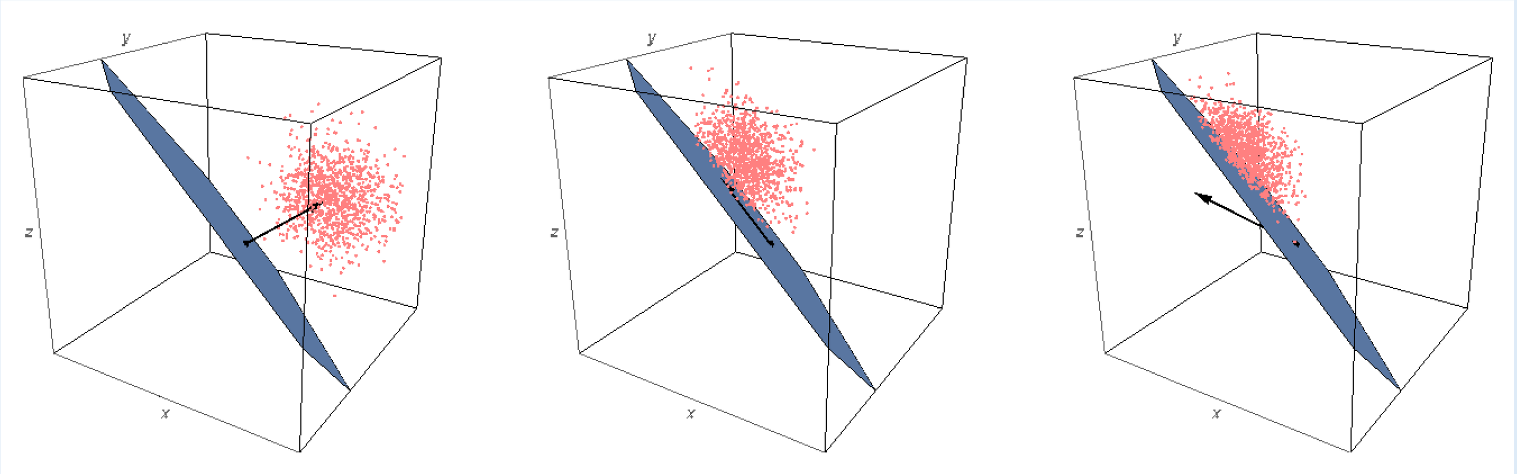
Steps to rejection sampling process:

- $M = u_0/v_{th}$ where $v_{th} = \sqrt{\frac{2kT}{m}}$
- New value (M') chosen from uniform distribution between +/-3 of M
- Value of Maxwellian distribution is calculated

$$p = \frac{2(M'+M)}{M+\sqrt{M^2+2}}\ e^{\frac{1}{2}+\frac{M}{2}\left(M-\sqrt{M^2+2}\right)-M'^2}$$

- Sample $R \in (0,1)$; accept if $R < p$, else restart with new M'





Testing the Boundary Condition:

Test	Result
Uniform gas flowing through system; M = 0, 1000	✓ Uniform density, temperature, and velocity
Vertical uniform gas flow from vertical side wall; M = 1000	✓ Uniform density, temperature, and velocity
Phi-velocity flow from side wall	✓ Solid body rotation

Issue in Collision Operation

Summary of Tests for Velocity Invariance:

- uniform vertical gas flow
- different M
- different # of particles
- Eunomia's **Leonard-Jones** type cross section
- **hard sphere** gas

Parameters of Tests:	
Particle Type	Lithium
n (particles/m^3)	1.0E20
d (m)	2.8517E-10
T (eV)	0.0431
m (amu)	6.941

Results/Analysis:

Calculation of collision frequency in collisions s^{-1} m^{-3} from Eunomia output:

$$\nu_{coll} = \frac{C\,\Gamma_{real}}{N_{sim}V}$$

Γ_{real} Flux (real particles/s) from source

C # collisions simulated

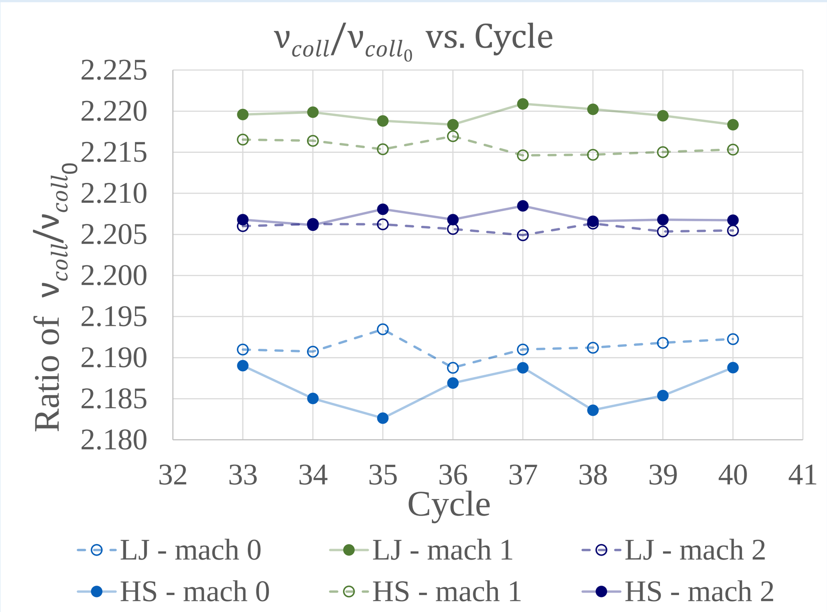
N_{sim} # particles simulated

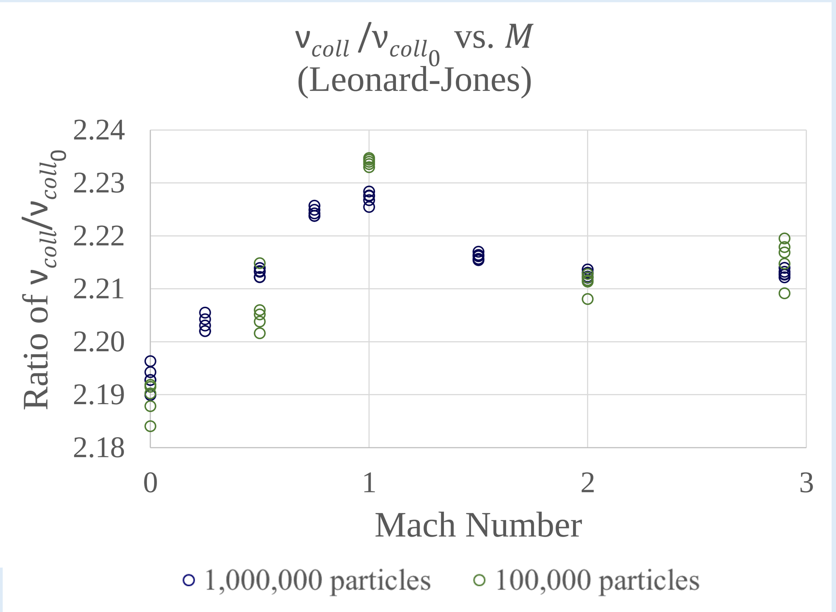
V Volume of container

Analytical collision frequency for hard sphere gas [3]:

$$\nu_{coll_0} = 4n^2d^2\sqrt{\frac{\pi kT}{m}}$$

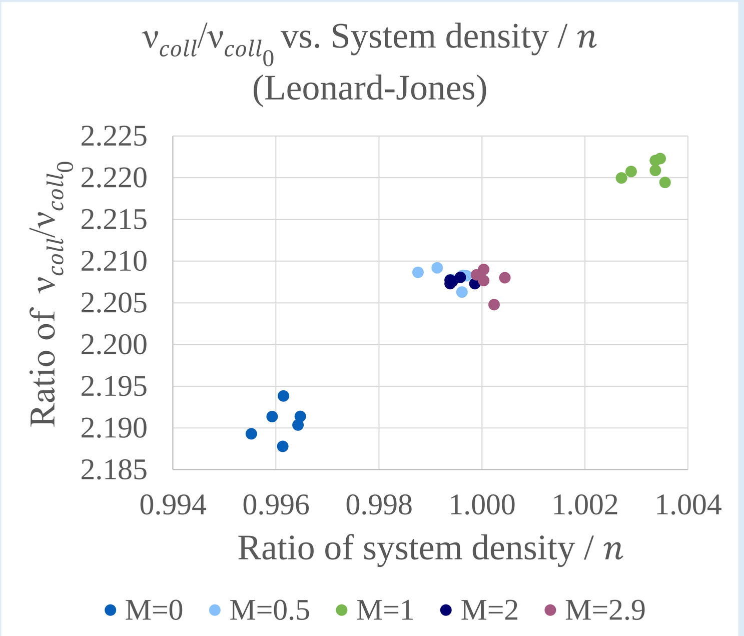
Expected Value: 4.46E24 collisions s^{-1} m^{-3}





Results and Conclusions:

- **Output collision frequencies off by factor of 2.2 from analytical**
- Variation in collision frequency for different M by 1%
  - Attributed to a difference in the number of particles in the system
    - → **Passes test for Galilean invariance**
- Leonard-Jones and hard sphere models give similar collision frequencies
- Eunomia is not self-consistent



Investigation of the effect of other variables:

- Density fluctuations between cycles → no clear relationship
- Number of processors → no uniform effect
- Half density → mimics analytical behavior
- Maxwellian distribution spread for velocity → no uniform effect
- Source type → uniform source gives same frequency

Recommendations for Further Investigation:

- Determine why M affects density
- Test case for time before a particle's collision
- Investigate calculation of outputted collision frequency