A generalized reduction scheme for the Stochastic Weighted Particle Method

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SIAM NNP 2025, Nov 2, 2025

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Our paper is on arxiv

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Motivation for Plasma

- A Plasma is a macroscopically neutral substance containing many interacting free electrons and ionized atoms/molecules.
- It is estimated that 99% of the known universe is plasma including: stars, the ionosphere (aurora), interstellar space, lightning, fire, ...
- Applications in the semiconductor industry such as
  - Etching silicon for integrated circuit
  - Growing layered semiconductor material
- Medical applications such as
  - Sterilization of medical equipment
  - Wound healing

Spatially homogeneous Boltzmann equation

- System of plasma particles can be modeled by velocity pdfs
- The spatially homogeneous Boltzmann equation for the velocity pdf, $f(\mathbf{v}, t)$, of a single species is

$$\frac{\partial f}{\partial t}(\mathbf{v}, t) = Q(f, f)(\mathbf{v}, t),$$

  where $Q(f, f)$ gives the rate of change of f due to collisions.

- Analytical solutions
  - Maxwellian
  - BKW
- Two approaches for numerical solutions
  - Stochastic
  - Deterministic

Accurate computation of low probability tails of velocity pdf is important as high energy electrons drive chemical reactions.

Collision operator

- The rate of change of f due to Maxwell type binary collisions

$$Q(\mathbf{v}, t) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \int_{S^2} \left[f(\widetilde{\mathbf{v}}, t) f(\widetilde{\mathbf{u}}, t) - f(\mathbf{v}, t) f(\mathbf{u}, t) \right] d\mathbf{\Theta}\, d\mathbf{w}.$$

- Post collisional velocities

$$\begin{aligned} \widetilde{\mathbf{v}}(\mathbf{v}, \mathbf{u}, \mathbf{\Theta}) &= \frac{1}{2} \Big[(\mathbf{v} + \mathbf{u}) + \mathbf{\Theta} |\mathbf{v} - \mathbf{u}| \Big], \\ \widetilde{\mathbf{u}}(\mathbf{v}, \mathbf{u}, \mathbf{\Theta}) &= \frac{1}{2} \Big[(\mathbf{v} + \mathbf{u}) - \mathbf{\Theta} |\mathbf{v} - \mathbf{u}| \Big], \end{aligned}$$

- The total collision frequency ν is given by

$$\nu(t) = \frac{1}{4\pi} \int_{\mathbf{u} \in \mathbb{R}^3} \int_{\mathbf{v} \in \mathbb{R}^3} \int_{\mathbf{\Theta} \in S^2} f(\mathbf{v}, t)\; f(\mathbf{u}, t)\, d\mathbf{\Theta}\, d\mathbf{v}\, d\mathbf{u}.$$

Bird: Direct Simulation Monte Carlo (DSMC)

- Allows for particle collisions, transport, chemistry, surface interactions, ...
- A set of n physical particles is represented by a set of m stochastic particles, each with weight

$$w = \frac{n}{m}.$$

- Bird's algorithm [collisions only for today]
  - Choose a Poisson distributed random jump time Δt_k
  - Choose 2 particles i and j at random from m particles
  - Choose a direction vector, $\boldsymbol{\Theta}$, for the relative post collisional velocity, $\widetilde{\mathbf{v}}_i - \widetilde{\mathbf{v}}_j$
  - Update the velocities and the velocity pdf
  - Update the time: $t_{k+1} \,=\, t_k + \Delta t_k$
  - Repeat the process

Rjasanow & Wagner: Stochastic Weighted Particle Method

- Variable weights to allow for more stochastic particles & accuracy in tails.
- State of the system:
  - $z(t) = \{(\mathbf{v}_1(t), w_1(t)), (\mathbf{v}_2(t), w_2(t)), \ldots, (\mathbf{v}_m(t), w_m(t))\}$,
  - $\mathbf{v}_i$ is velocity and w_i is weight of the i-th stochastic particle.
  - **Need** $m = m(t)$
- The empirical measure (histogram) of the system is:

$$\mu_m(t, dv) = \sum_{i=1}^{m(t)} w_i(t) \delta_{\mathbf{v}_i(t)}(dv)$$

Wagner's convergence theorem:

$\mu_m \to f$ **as** $m(0) \to \infty$ **under certain conditions on simulation set up**

Bird's Model vs Rjasanow and Wagner's model

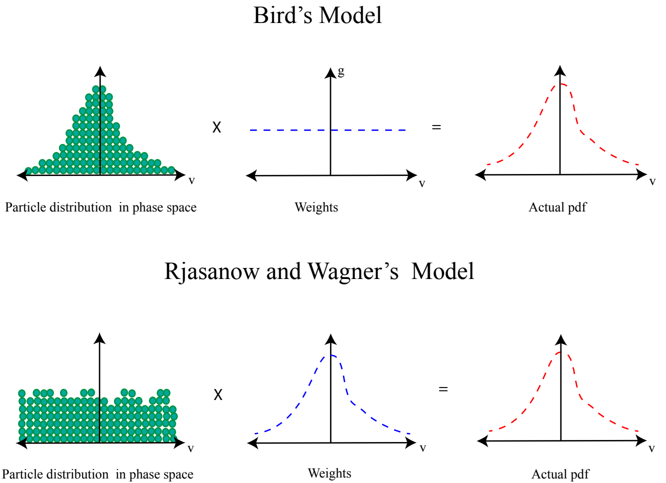


Fig: Schematic diagram of stochastic models

A stochastic collision

- During a collision between the stochastic particles only a portion, $\gamma_{\mathrm{coll}}(z; i, j, \boldsymbol{\Theta})$, of physical particles undergo collisions.
- Remaining particles continue with the pre-collision velocities.
- The state, $[J_{\mathrm{coll}}(z, i, j, \boldsymbol{\Theta})]_k$, of the k-th stochastic particle after a collision between particles i and j is given by

$$[J_{\mathrm{coll}}(z; i, j, \boldsymbol{\Theta})]_k \;=\; \begin{cases} (\mathbf{v}_k, w_k), & \text{if } k \le m, \;\; k \notin \{i, j\}, \\ (\mathbf{v}_i, w_i - \gamma_{\mathrm{coll}}(z; i, j, \boldsymbol{\Theta})), & \text{if } k \;=\; i, \\ (\mathbf{v}_j, w_j - \gamma_{\mathrm{coll}}(z; i, j, \boldsymbol{\Theta})), & \text{if } k \;=\; j, \\ (\widetilde{\mathbf{v}}_i, \gamma_{\mathrm{coll}}(z; i, j, \boldsymbol{\Theta})), & \text{if } k \;=\; m+1, \\ (\widetilde{\mathbf{v}}_j, \gamma_{\mathrm{coll}}(z; i, j, \boldsymbol{\Theta})), & \text{if } k \;=\; m+2, \end{cases}$$

resulting in a new system state with **two additional particles**,

$$z \;=\; \{(\mathbf{v}_1, w_1), (\mathbf{v}_2, w_2), \ldots, (\mathbf{v}_{m+1}, w_{m+1}), (\mathbf{v}_{m+2}, w_{m+2},)\}.$$

Reduction process

- SWPM has time complexity of $O(m)$.
- Each collision increases the number of stochastic particles by one or two.
- Must periodically reduce the number of particles.
- Reduction Process:
  1. Cluster the stochastic particle into groups.
  2. Reduction scheme: Replace each group with a smaller group.

Goal:

Reduction should preserve physically important statistical quantities:

Moments of the pdf &Tail functionals.

$$\mathrm{Tail}(R) = \iiint_{|\mathbf{v}|\geq R} f(\mathbf{v})\, d\mathbf{v}$$

Grouping and Reduction Methods

- For today's results, group based on rectangular boxes in velocity space
  - Probably not best choice!

- Within each group we select velocities of reduced particles so to preserve:

  - **K1:** Total mass and average velocity of group[1]
    - 1 particle per group
  - **K2: K1** + full pressure tensor[2]
    - 7 particles per group
  - **K2.5: K2** + M_{300}, M_{030} & M_{003}
    - 10 particles per group
  - **K3:** All moments of order less than or equal to three
    - 27 particles per group

To what degree are
even higher order moments and tail functionals preserved?

[1] Rjasanow&Wagner,2005
[2] Lama, Zweck & Goeckner, 2020

Moment Preservation as a Linear System

Given original group of $N_{\rm orig}$ particles, compute $N_{\rm mom}$ moments

$$M_{k_x k_y k_z} = \sum_{j=1}^{N_{\rm orig}} w_j \, v_{x,j}^{k_x} \, v_{y,j}^{k_y} \, v_{z,j}^{k_z}, \qquad \text{of order } k_x + k_y + k_z = K \tag{1}$$

Form $N_{\rm mom} \times 1$-moment vector $\boldsymbol{\mu}$ whose i-th entry is $M_{k_x k_y k_z}$.
Goal: Find reduced group of $N_{\rm red}$ particles with velocities, $\mathbf{v}_j = (v_{x,j}, v_{y,j}, v_{z,j})$, and weights, w_j so that for all k_x, k_y, k_z,

$$M_{k_x k_y k_z} = \sum_{j=1}^{N_{\rm red}} w_j \, v_{x,j}^{k_x} \, v_{y,j}^{k_y} \, v_{z,j}^{k_z}. \tag{2}$$

Recast (2) as $N_{\rm mom} \times N_{\rm red}$ linear system

$$\mathbf{P}\mathbf{w} \;=\; \boldsymbol{\mu} \tag{3}$$

where $\mathbf{w}$ is $N_{\rm red} \times 1$ weight vector and $\mathbf{P}$ is $N_{\rm mom} \times N_{\rm red}$ progenitor matrix

$$P_{ij} = v_{x,j}^{k_x} \, v_{y,j}^{k_y} \, v_{z,j}^{k_z}. \tag{4}$$

Preservation of all 1st-order moments, $K = 1$

Given

$$\boldsymbol{\mu} = \begin{bmatrix} M_{000} & M_{100} & M_{010} & M_{001} \end{bmatrix}^T$$

need at least 4 reduced particles (for square system):

$$M_{000} = w_0 + w_x + w_y + w_z,$$

$$\begin{bmatrix} M_{100} \\ M_{010} \\ M_{001} \end{bmatrix} = w_0 \mathbf{v}_0 + w_x \mathbf{v}_x + w_y \mathbf{v}_y + w_z \mathbf{v}_z,$$

For $\mathbf{P}$ to be **upper triangular**, choose $\mathbf{v}_0 = \mathbf{0}$ and

$$\mathbf{v}_x = \begin{bmatrix} v_x & 0 & 0 \end{bmatrix}^T, \qquad \mathbf{v}_y = \begin{bmatrix} 0 & v_y & 0 \end{bmatrix}^T, \qquad \mathbf{v}_z = \begin{bmatrix} 0 & 0 & v_z \end{bmatrix}^T,$$

$$\mathbf{P} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & v_x & 0 & 0 \\ 0 & 0 & v_y & 0 \\ 0 & 0 & 0 & v_z \end{bmatrix}, \qquad \text{which is } \textbf{invertible} \text{ if } v_{x/y/z} \neq 0.$$

Preservation of all 1st-order moments, $K = 1$

Weight positivity

- To ensure that the weights are positive, choose signs of velocities to match those of moments:

$$\text{sign}\,(v_x) = \text{sign}\,(M_{100})\,, \quad \text{sign}\,(v_y) = \text{sign}\,(M_{010})\,, \quad \text{sign}\,(v_y) = \text{sign}\,(M_{001})\,.$$

- Finally, the velocities can be scaled so that

$$w_0 \;=\; M_{000} - \left(\frac{v_x}{M_{100}} + \frac{v_y}{M_{010}} + \frac{v_z}{M_{001}} \right) \;>\; 0. \tag{5}$$

Preservation of all moments of order $K \leq 2$

Order the 10 components of the moment vector so that

$$\boldsymbol{\mu}^T = \begin{bmatrix} \mu_0 & \boldsymbol{\mu}_x^T & \boldsymbol{\mu}_y^T & \boldsymbol{\mu}_z^T & \mu_{xy} & \mu_{xz} & \mu_{yz} \end{bmatrix},$$

where $\mu_0 = M_{000}$,

$$\boldsymbol{\mu}_x = \begin{bmatrix} M_{100} \\ M_{200} \end{bmatrix}, \qquad \boldsymbol{\mu}_y = \begin{bmatrix} M_{010} \\ M_{020} \end{bmatrix}, \qquad \boldsymbol{\mu}_z = \begin{bmatrix} M_{001} \\ M_{002} \end{bmatrix},$$
$$\mu_{xy} = M_{110}, \qquad \mu_{xz} = M_{101}, \qquad \mu_{yz} = M_{011}.$$

Choose the 10 reduced particle velocities

$$\begin{bmatrix} 0 & v_{x,2} & v_{x,3} & 0 & 0 & 0 & 0 & v_{x,8} & v_{x,9} & 0 \\ 0 & 0 & 0 & v_{y,4} & v_{y,5} & 0 & 0 & v_{y,8} & 0 & v_{y,10} \\ 0 & 0 & 0 & 0 & 0 & v_{z,6} & v_{z,7} & 0 & v_{z,9} & v_{z,10} \end{bmatrix}$$

to obtain an upper trianglular P.

Preservation of all moments of order $K \leq 2$

$$
\begin{bmatrix}
1 & \mathbf{1} & \mathbf{1} & \mathbf{1} & 1 & 1 & 1 \\
\mathbf{0} & \mathbf{P}_{x,x} & \mathbf{0} & \mathbf{0} & \mathbf{P}_{x,xy} & \mathbf{P}_{x,xz} & 0 \\
\mathbf{0} & \mathbf{0} & \mathbf{P}_{y,y} & \mathbf{0} & \mathbf{P}_{y,xy} & 0 & \mathbf{P}_{y,yz} \\
\mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{P}_{z,z} & \mathbf{0} & \mathbf{P}_{z,xz} & \mathbf{P}_{z,yz} \\
0 & \mathbf{0} & \mathbf{0} & \mathbf{0} & P_{xy,xy} & 0 & 0 \\
0 & \mathbf{0} & \mathbf{0} & \mathbf{0} & 0 & P_{xz,xz} & 0 \\
0 & \mathbf{0} & \mathbf{0} & \mathbf{0} & 0 & 0 & P_{yz,yz}
\end{bmatrix}
\begin{bmatrix} w_0 \\ \mathbf{w}_x \\ \mathbf{w}_y \\ \mathbf{w}_z \\ w_{xy} \\ w_{xz} \\ w_{yz} \end{bmatrix}
=
\begin{bmatrix} \mu_0 \\ \boldsymbol{\mu}_x \\ \boldsymbol{\mu}_y \\ \boldsymbol{\mu}_z \\ \mu_{xy} \\ \mu_{xz} \\ \mu_{yz} \end{bmatrix},
$$

where $P_{xy,xy} = v_{x,8} v_{y,8}$ and

$$
\mathbf{P}_{x,x} = \begin{bmatrix} v_{x,2} & v_{x,3} \\ v_{x,2}^2 & v_{x,3}^2 \end{bmatrix},
$$

Choosing $v_{*,j} \neq 0$ and

$$
v_{x,3} \neq v_{x,2}, \qquad v_{y,5} \neq v_{y,4}, \qquad v_{z,7} \neq v_{z,6},
$$

P is invertible.

Preservation of all moments of order $K \leq 2$: 2D Case

Weight positivity

Working in frame in which covariance matrix is identity, system reduces to

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & v_{x,1} & v_{x,2} & 0 & 0 & v_{x,5} \\ 0 & v_{x,1}^2 & v_{x,2}^2 & 0 & 0 & v_{x,5}^2 \\ 0 & 0 & 0 & v_{y,3} & v_{y,4} & v_{y,5} \\ 0 & 0 & 0 & v_{y,3}^2 & v_{y,4}^2 & v_{y,5}^2 \\ 0 & 0 & 0 & 0 & 0 & v_{x,5}v_{y,5} \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \end{bmatrix} = \begin{bmatrix} M_{000} \\ M_{100} \\ M_{200} \\ M_{010} \\ M_{020} \\ M_{110} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}. \tag{6}$$

Set $w_5 = 0$ and

$$v_{x,1} = v_{y,3} = s \qquad \text{and} \qquad v_{x,2} = v_{y,4} = -s$$

gives

$$\mathbf{w} = \begin{bmatrix} 1 - \frac{2}{s^2} & \frac{1}{2s^2} & \frac{1}{2s^2} & \frac{1}{2s^2} & \frac{1}{2s^2} \end{bmatrix}^T,$$

which has positive components, provided $s > \sqrt{2}$.

Similar approach with extra tricks solves case $K = 3$ in 3D.

Importance sampling pdf prior to reduction

Rather than simulating entire SWPM process:

- We sample from Maxwellian-like distributions, f, with skewness and kurtosis.
- Then group and reduce.
- Quantifies uncertainty due to particle grouping and reduction processes.
- DSMC-like system:
  - Sample m particle velocities via standard CDF method
  - Choose constant weights
- SWPM-like system:
  - Sample m particle velocities uniformly distributed in a ball of radius $v_R = 7$.
  - Choose weights so that $\mu_m \approx f$

To what extent is uncertainty of the reduced system on the order of the uncertainty prior to reduction?

Moments and tail functionals prior to reduction

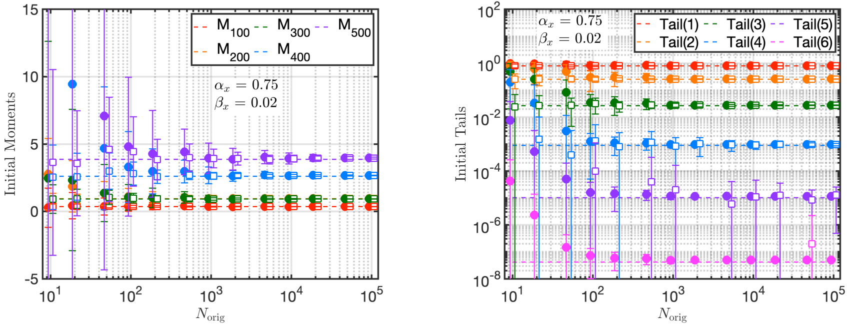
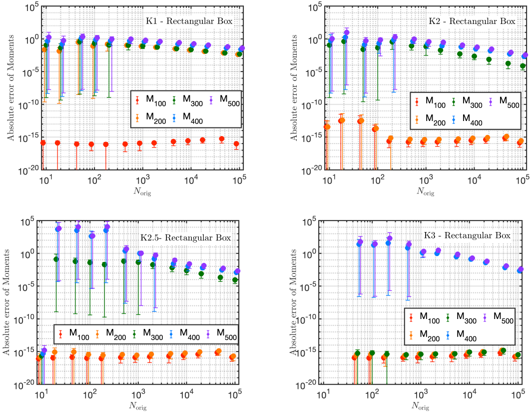


Figure: Integrate pdf (dashes), SMC-like (open squares) and SWPM-like (closed circles).

Quantifies initial uncertainty of moments and tail functionals

Absolute error in the moments for reduction schemes



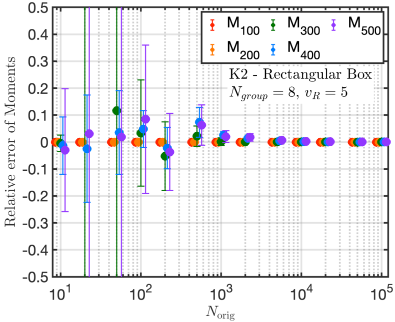
Moment to be preserved are preserved to within numerical error.

Best to preserve the full third-order tensor moment.

Errors in non-preserved moments are smaller for larger N_{orig} and n_{groups}.

Relative error in the moments with minimal group sizes

Smaller group sizes reduce group radii and increase accuracy of reduction



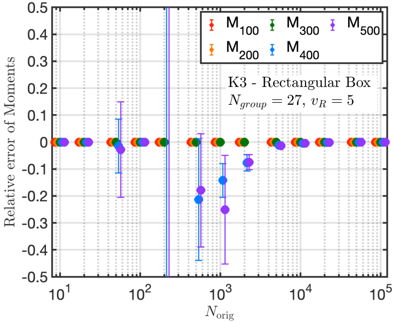
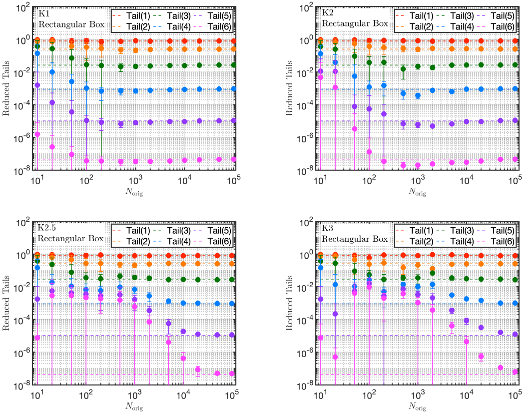


Figure: Relative error in moments for the **K2** (left panel) & **K3** (right panel) schemes when N_{group} is set to minimum values of $N_{\mathrm{group}} = N_{\mathrm{red}} + 1 = 8$ and 27, respectively.

Tail Functionals for different reduction schemes



Use K1 if goal is to simply preserve tail functionals.

Use K2 or K3 if goal is to preserve moments and tail functionals.