PhD Thesis Proposal:

An Excursion with the Boltzmann Equation at Low Speeds

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1. Problem Definition

The objective of this work is the development of efficient simulation tools for modeling gaseous flows in micro/nanoscale devices. The development of accurate engineering models of such flows is not only important for the fundamental understanding, but also in the design [2,3], and even fabrication of such devices [4,5]. It is well known[6,7] that when the mean free path becomes comparable to the flow characteristic lengthscale, the flow deviates from the Navier-Stokes (NS) description. This deviation is typically quantified by the Knudsen number $Kn = \lambda / L$, where λ is the molecular mean free path and L is the characteristic flow lengthscale. In fact, kinetic models (such as the Boltzmann Equation (BE)) are required to describe such flows completely. In the case of a hard-sphere gas the non-dimensional BE can be written as [8]:

$$\frac{\partial f}{\partial t} + \vec{C} \cdot \frac{\partial f}{\partial \vec{x}} = I(f, f)$$

$$I(f, f) = \frac{1}{Kn} \iint (f f_1' - f f_1) V \sigma \, d\Omega \, d\vec{C}_1$$

Here $f = f(\vec{x}, \vec{C}, t)$ is the single particle probability distribution function, $\vec{x}$ is position, $\vec{C}$ is the molecular velocity vector, likewise, $f_1 = f(\vec{x}, \vec{C}_1, t)$, $f' = f(\vec{x}, \vec{C}', t)$ and $f_1' = f(\vec{x}, \vec{C}_1', t)$ (where $\vec{C}'$ indicates a post-collision velocity); finally V, σ, Ω are the relative

velocity of colliding molecules, scattering angle and molecular collision cross section, respectively.

One of the most widely used methods for solving the Boltzmann Equation is the Direct Simulation Monte Carlo (DSMC) procedure, a stochastic particle based *simulation* method. In DSMC quantities of interest (eg. flow velocities) are calculated as averages over a particle population. Consequently, as the flow speed is reduced (ie. $Ma \to 0$; where *Ma* is the Mach number) more samples are needed to resolve the flow (in fact, the cost scales like $1/Ma^2$). And since gas molecules have an average speed of O(400)m/s at STP, DSMC becomes an impractical tool to use for most microfluidic applications.

There have been a number of attempts to address the issue of modeling low speed kinetic flows. In particular, the work of [9] is very promising but has a major limitation when dealing with problems that take a long time to reach steady state; an issue we address in the first part of this work. Other, particle based, methods to resolve slow flows have also been proposed [10,11] and also seem very promising (particularly for multi-dimensional situations) but are not without limitations of their own. Specifically, [10] re-formulates the BE using the deviation from equilibrium and attempts to simulate the resulting dynamics using particles in a manner analogous to DSMC. Reference [11], on the other hand, starts from a linearized BE and devises a weighted particle scheme for the low speed kinetic flows. In both cases, the particle dynamics lead to the net creation of particles that if left uncancelled make the calculation very inefficient when Kn<1.

1.1. Objective of this work

In this proposal we are interested in examining two basic questions:

I. Can we find the steady state solution of kinetic problems in a manner that is faster than direct molecular integration? This is discussed in section 2.
II. Is it possible to find an alternative method to resolve low speed flows in an exact, robust and elegant manner? This is discussed in section 3.

This document details my proposals to deal with these two questions. In Section 2, I describe the work I have done to incorporate ideas from [12-14] to accurately find steady state solutions to kinetic problems that would take a very long time to integrate. In Section 3 I describe an alternative method for reducing the variance of DSMC calculations using a particle weighting scheme.

2. Part I: Steady state solutions of multi-scale molecular problems

When trying to find steady state solutions to kinetic problems most current integration schemes (particularly [9]) have strict limits on the maximum allowed integration timesteps. This makes finding steady state solutions at lower Knudsen numbers or of problems of mixed length scales computationally expensive. In the first part of my thesis we developed a method which addresses this limitation, the approach we used was to extend the equation-free framework of Kevrekidis and coworkers[12-14] to low speed kinetic flow problems. In other words, we extract the long term/coarse-grained behavior of the system by examining the results of a series of short-term/microscopic simulations.

The iterative method proposed and used here consists of a short Boltzmann transient evolution step (using the low noise integration scheme in [9]) and a Newton-Broyden contraction mapping step; the latter step only solves for the macroscopic field of interest (e.g. flow velocity $\{u_{SS}\}$). The predicted macroscopic field is then used as an initial condition for the BE solver for the next iteration. Figure 1 illustrates the basic steps of the method.

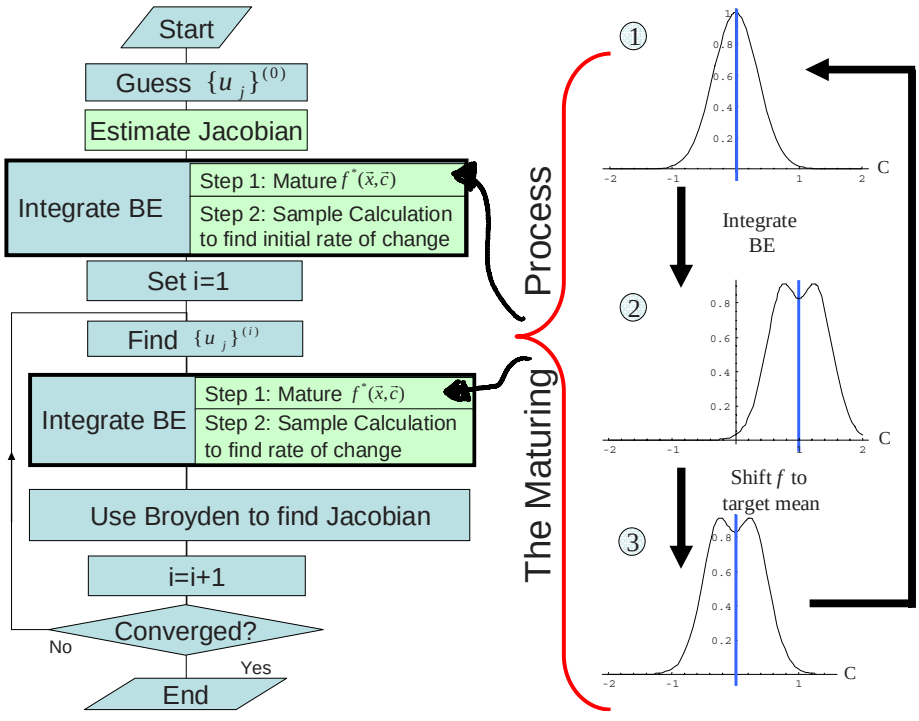

Figure 1: Schematic of this section's procedure. The left side shows a block diagram of the algorithm while the right one graphically summarizes the maturing process.

A crucial part of this procedure is the correct implementation of a maturing step as sketched on the right of the figure. The maturing step creates an "appropriate" microscopic distribution function $f^*(\vec{x},\vec{C})$ that ensures that an accurate microscopic rate of change is measured when the system is integrated for each iteration of the macroscopic field $\{u_{SS}\}^{(i)}$. Detailed of this can be found in [15].

We have validated this approach for isothermal, one-dimensional flows in a wide range of Knudsen numbers. We find that the Newton-Broyden iteration converges in O(10) iterations, starting from an arbitrary guess solution and a Navier-Stokes based initial Jacobian. When using this procedure the cost to reach steady state, to first approximation, is comparable to the time to integrate O(40) mean collision times regardless of the Knudsen number. Thus this method is preferable to explicit integration when the flow's characteristic timescale is longer than approximately 40 collision times.

3. Part II: Variance reduction using weighting factors

We will proceed in this section to propose a new methodology to reduce variance when modeling kinetic flows. The strength of the proposed methodology lies in the fact that it requires minimal modifications of the standard DSMC scheme. In what follows we will start by describing DSMC, proceed to detail the inspiration of our work, describe weighting factors and will finally discuss some initial results.

3.1. Direct Simulation Monte Carlo

The DSMC is a stochastic particle simulation technique that has been shown to solve the non-linear BE[17,8]. It works by applying a splitting approach to the motion of the particle-simulators comprising the system; the time evolution of the system is approximated by a sequence of discrete timesteps of duration *dt*, in which particles successively undergo collisionless advection and collisions. Collisions take place between partners selected randomly within cells of a maximum side length smaller than a mean free path. And as mentioned earlier, quantities of interest are calculated as averages over the sample particle simulators. The DSMC formulation eliminates the computational cost associated with calculating exact particle trajectories and leads to a simulation method that is significantly more efficient than "brute force" molecular dynamics approaches.

3.2. Basic principle of variance reduction: parallel processing of simulations

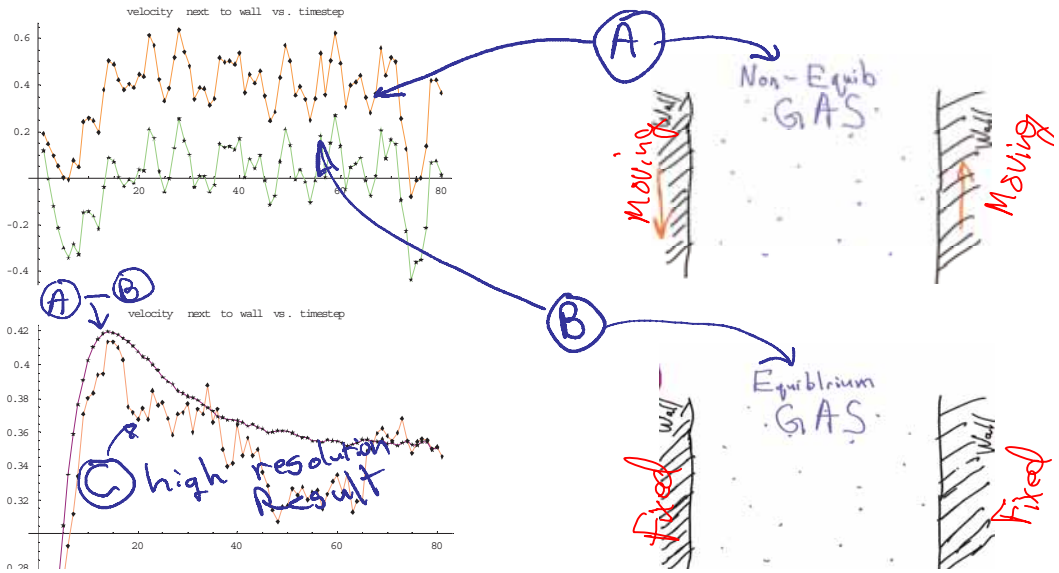

Figure 2: Schematic of two systems running in parallel with an identical sequence of random numbers used for a simple 1D kinetic Couette flow. A denotes the results of a non-equilibrium flow while B denotes those of an equilibrium flow. Finally, C denotes the results of a very high resolution calculation attempting to resolve the flow in a traditional manner.

The basic inspiration for the proposed approach can be illustrated by looking at Figure 2 for a simple low speed kinetic flow. The plot at the top shows the calculated wall speed versus time for two computations with an identical set of initial conditions and random sequences differing only in boundary conditions (A is flow of interest and B is an equilibrium flow). It is very hard to discern the behavior of the system because the flow speed is much smaller than the thermal fluctuations of the system and only a much more expensive calculation (labeled C) would be able to directly give meaningful information. On the other hand, simply subtracting the results of both systems will give a result that is essentially unaffected by the thermal fluctuations. This idea has been successfully pioneered in the field of polymer modeling by Öttinger and others and has been the basis of large body of work in variance reduction there[1]. Our work tries to apply this idea to DSMC by introducing weighting factors as a method of representing and calculating, in parallel, the equilibrium flow in addition to the normal non-equilibrium flow.

3.3. Basic building block: weighting factors

The weighing factors that are discussed here are a method of "effectively" generating very correlated sample sequences from two different distributions. While only one of the sequences is explicitly generated, weighting factors are used to extract properties of the second sequence. To illustrate the concept let us consider two random sequences S_{NE} and S_{Eq} that are generated from different PDFs, $P_{NE}(x)$ and $P_{Eq}(x)$ (elements of S_{NE} and S_{Eq} are labeled S_{NEi} and S_{Eq_i} respectively). If we want to estimate $\overline{S_{NE} - S_{Eq}}$, we can simply calculate $\frac{1}{N}\sum_{i=1}^{N}(S_{NEi} - S_{Eqi})$ which would, in general, have a variance of the order of the variance of the sequences S_{NE} and S_{Eq}. An other approach however is to generate elements of sequence S_{NE} and a conjugate sequence W_i instead of S_{Eq_i}. Here W_i is the ratio of probability of a sample in distribution Eq to the same sample in distribution NE:

$$W_i = \frac{P_{Eq}(S_{NEi})}{P_{NE}(S_{NEi})}$$

Using this, $\overline{S_{NE} - S_{Eq}}$ is estimated by calculating $\sum_{i=1}^{N}(1-W_i)S_{NEi}$ and if both $P_{NE}(x)$ and $P_{Eq}(x)$ are close to each other the values of the weights will be of O(1) and consequently $O((1-W_i)S_{Ai}) << O(S_{Ai})$. Hence, the variance of the new estimator $\overline{S_{NE} - S_{Eq}}$ (and $\overline{S_{NE}}$ since $\overline{S_{Eq}}$ =0) will be much smaller than the one generated by sampling S_{NE} or S_{Eq} directly.

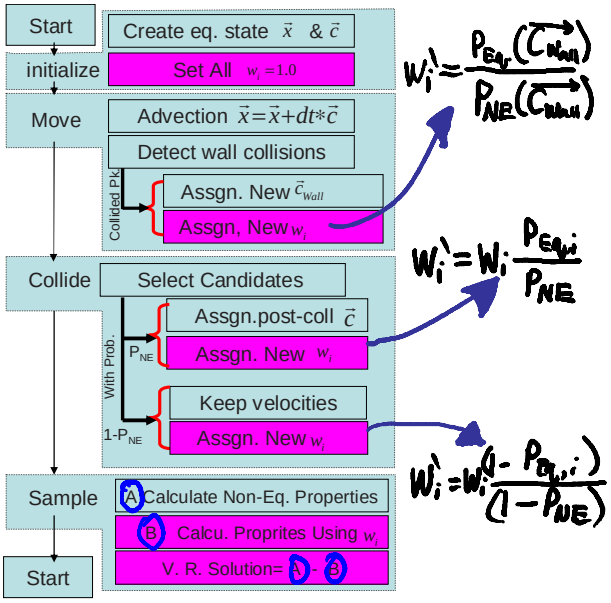

Figure 3: Flow chart of the new method. Blocks in light blue are standard DSMC steps, while purple ones are steps that are added by our VR implementation.

We have successfully applied this basic idea to DSMC and developed a method that samples the flow state with a standard deviation of the order of the flow speed (rather than the molecular thermal speed). Figure 3 shows a sketch of DSMC and the major modifications made to it (details are discussed in Appendix I). In addition, the diagram also shows the three basic rules applied to correctly derive dynamical rules for the weights in the simulation.

3.4. Numerical results and the stability issue

As we can see in Figure 4, our method is able to accurately re-produce solutions to the BE for a number of different Couette flows of varying Knudsen numbers.

Unfortunately, on close inspection we can see the major flaw of the method, namely, that after a few collision times noise starts to creep in the result and contaminates the variance reduced solution.

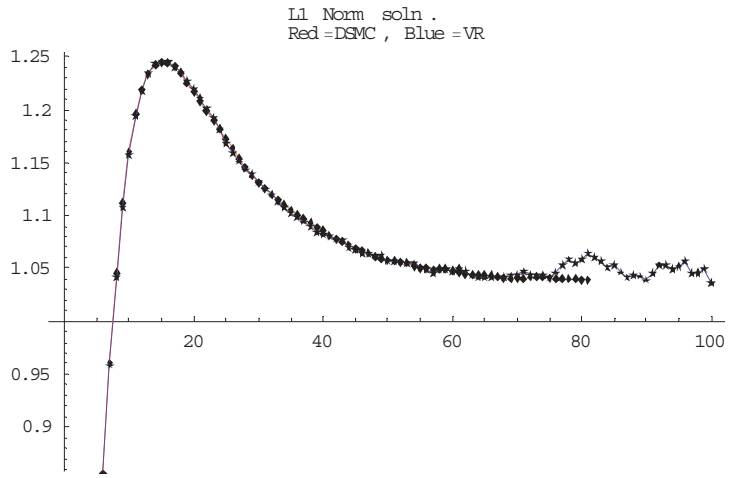

Figure 4: Plots of the solution velocity (normalized to wall speed) of a 1D Couette flow at Kn=1.0. The plot is of the L1 norm of the solution with the VR solution (blue) comparing reasonably well to the direct DSMC result show in red[1] (timesteps are on the abscissa). The error slowly grows until it overwhelms the solution but at this Kn number we reach steady state before this happens.

The noise growth is caused by an increase in the number of very heavy ($W_i \to \infty$) and very light ($W_i \to 0$) particles that represent the equilibrium distribution; the divergence seems to be exponential in nature but of a long time constant. Specifically, our suspicion is that the collision steps allow a random addition or subtraction of particles that represent equilibrium at a certain velocity class. As the simulation progresses these do not completely cancel out and we get a random drift that is somewhat analogous to a random walk. Consequently, as the weights drift away from being O(1) the variance reduction is destroyed.

4. Outlook

The approach presented in Part II seems to provide an accurate, efficient, and elegant method of modeling low speed flows. Unfortunately, due to the stability issue just described we are limited to runs shorter than 4-5 mean collision times. This is a serious limitation that practically precludes the efficient simulation of flows characterized by Kn<1. *The main objective of this thesis is to address this limitation in a satisfactory manner.*

Although it is fairly easy to see "mechanically" how the instability issue arises by looking at collision weight propagation scheme in Figure 3, it is harder to fit this issue (and indeed the whole scheme) in a more general theoretical framework. It would be of most

[1] But at a wall speed of 10m/s for DSMC vs. 1m/s for the VR result.

interest if such a framework can be found and if it would point to a robust method of controlling the divergence of the weights.

Alternatively, I can envision a number of different ways of overcoming this limitation; using mass/momentum/energy consideration to derive restrictions on weights may lead to a stable scheme. A different approach would be to reduce the noise by smoothing the "troublesome" particles either by averaging, filtering or perhaps a particle re-meshing approach similar to [16]. Finally, using the course-grained framework of Part I is also a possibility, since within this framework steady state solutions can be found using *short* transient evolution periods.

5. References

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6. Appendix: Details of variance reduction weighting scheme for DSMC

Figure 5 shows two sketches describing the concept of variance reduction in DSMC using parallel processing. Starting from identical initial conditions, equilibrium and non-equilibrium runs are represented by particles with identical positions and velocities but different weights. At a point $\vec{x}$ the average velocity is $\sum \vec{C}_i$ for the non-equilibrium flow and $\sum \vec{C}_i * W_i$ for the equilibrium flow, the difference between the two ($\sum (1-W_i)*\vec{C}_i$) is the variance reduced flow velocity. The challenge in this technique lies in developing rules for processing and assigning weights that ensure that for every particle $W_i = \frac{P_{Eq}(\vec{C}_i)}{P_{NE}(\vec{C}_i)}$ at all times.

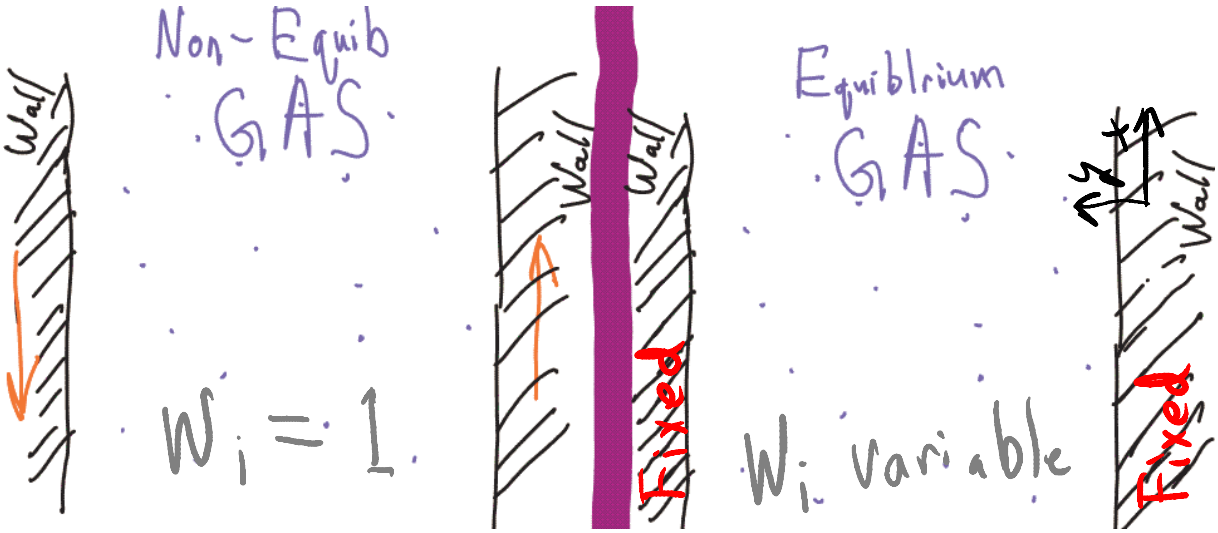

Figure 5: Sketch of two different Couette flows modeled using DSMC. The one on the left is a non-equilibrium flow with moving walls while the right sketch is of an equilibrium gas with fixed walls. Only weights distinguish one from the other.

6.1. Convection and wall collisions

The calculation is started in an equilibrium configuration with all W_i's assigned a value of 1.0. The standard DSMC convection step is used to update the positions of the particles in the domain and only particles that interact with the walls are assigned updated weights. When a particle hits a wall it is assigned a new velocity vector $\vec{C}_i$, and a weight

$$W_i = \frac{\mathrm{P}_{\mathrm{Eq},wall}(\vec{C}_i)}{\mathrm{P}_{\mathrm{NE},wall}(\vec{C}_i)} = Exp\left[\frac{-2V_{wall}C_x + {V_w}^2}{C_{mpv}}\right]$$

Here V_{wall} is the wall speed and C_x is the velocity assigned to the particle by DSMC in the direction of the wall's movement and C_{mpv} is the most probable speed of the equilibrium Maxwell-Boltzmann distribution[2].

6.2. Particle-particle collisions

The simple fact to keep in mind when designing the collision weight update formulas is that while a standard DSMC particle represents $N_{Effective}$ real molecules, a weighted particle in the equilibrium simulation represents $W_i * N_{Effective}$ molecules. When this is done, everything else follows quite naturally as is explained in the next subsections.

6.2.1. Collision candidates and probabilities

We start by devising a method of calculating collision probabilities that is common to both the equilibrium and non-equilibrium flows. We proceed in a manner that is identical to what is done in standard gas kinetic theory (ie. calculate the number of particles swept in unit time etc.) and arrive at the conclusion that in a time *dt* and volume V a particle i will have: $\frac{N_{Effective} W_j C_{ij} \sigma\, dt}{2V}$ collisions with particle j (where particles i and j have velocities $\vec{C}_i$ and $\vec{C}_j$ respectively and C_{ij} is their relative speed)[3]. Consequently, if one would select $\frac{N_{Effective} MX\, \sigma\, dt}{2V}$ collision candidates and collide them with a probability

$$P_{Eq,i} = \frac{W_j C_{ij}}{MX} \quad \text{and} \quad P_{Eq,j} = \frac{W_i C_{ij}}{MX} \qquad (\text{s.t. } MX = \max_{i \in cell}(W_i \vec{C}_i))$$

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[2] This is not the only possible procedure to assign weights and in fact this procedure assumes a fixed gas density (ie. the incoming particles on average have a known density). An alternative ($W_i' = W_i * P_{Eq}(\vec{C}_i) / P_{NE}(\vec{C}_i)$) would work but the variance reduction is reduced appreciably in a similar fashion to the collisions update formulas.

[3] NB: The collision rate (from a weighted particle's perspective) is Asymmetric! The number of collisions particle *i* faces is $\frac{N_{Effective} W_j C_{ij} \sigma\, dt}{2V}$ while particle *j* is expected to have $\frac{N_{Effective} W_i C_{ij} \sigma\, dt}{2V}$ collisions.

one would guarantee the correct collision rate in a cell for the weighted particles. The above formulae reduce to the standard DSMC ones if a unit weight is used.

6.2.2. Weight propagation scheme for collisions

To understand the basis for the collision update formula let us look at $N_{\vec{C}_i}$ particles of class $\vec{C}_i$ that have collision probabilities P_{NE} and P_{Eq} and end up in class $\vec{C}_i'$ as illustrated in Figure 6. In the non-equilibrium case (blue) we start out with $N_{\vec{C}_i}$ collision candidates of class $\vec{C}_i$ and end up with $P_{NE} * N_{\vec{C}_i}$ particles of class $\vec{C}_i'$ and $(1-P_{NE}) * N_{\vec{C}_i}$ particles that stay in class $\vec{C}_i$. Likewise, in the equilibrium case (red), when we collide $W_i * N_{\vec{C}_i}$ equilibrium candidate particles with probability P_{Eq} we would end up with $W_i * N_{\vec{C}_i} * P_{Eq}$ particles at $\vec{C}_i'$ and $W_i * N_{\vec{C}_i} * (1- P_{Eq})$ that stay at $\vec{C}_i$.

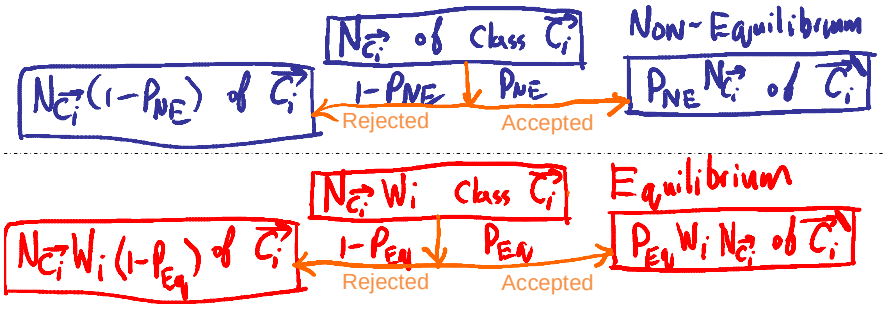

Figure 6: illustration of expected number of accepted and rejected particles for the non-equilibrium (Blue) and equilibrium (Red) if processed with probability P_{NE} and P_{Eq} respectively.

The key to this scheme is to realize that we are executing the collisions with a probability P_{NE} not P_{Eq}, to retain the equilibrium distribution we need to have the accepted and rejected particles *represent* the correct number of equilibrium particles *as if* they have been collided at the correct probability. But since there is $P_{NE} * N_{\vec{C}_i}$ particles (each with a weight W_i') that represent $W_i * N_{\vec{C}_i} * P_{Eq}$ particles the post collision weight for accepted particles should be:

$$W_i' = \frac{N_{\vec{C}_i} P_{Eq,i} W_i}{N_{\vec{C}_i} P_{NE}} = W_i \frac{P_{Eq,i}}{P_{NE}} = W_i * W_j = \frac{P_{Eq,j}}{P_{NE}} W_i = W_j'$$

Likewise, to correctly account for the difference between the equilibrium and non-equilibrium rejection rate we would need to modify the weights of the *rejected* particles so that:

$$W_i' = \frac{1-P_{Eq,i}}{1-P_{NE}} W_i \text{ and } W_j' = \frac{1-P_{Eq,j}}{1-P_{NE}} W_j .$$

One fundamental difference between our work and that of Wagner et el. [18] and Chun et el. [11] is that they account for different collision rates by introducing extra particles to represent deviation while our approach does that by modifying expected weights. Although we do not create new particles, we still have problems simulating Kn<1 flows efficiently because of the weight instability issue explained in Section 3.4.