The rim model

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In this working document we present a simulation of a hard-disk gas contained in two compartments (red and blue). The compartments have specular walls. The wall separating the two compartments has an aperture (a hole) as in Figure 1a. The aperture size is *A=0.99 D* where *D* is the diameter of the disks. A disk can protrude through the aperture but cannot pass to the opposite compartment. In this setup, the red and blue gases can exchange energy (through red-blue collisions) but they cannot exchange mass.

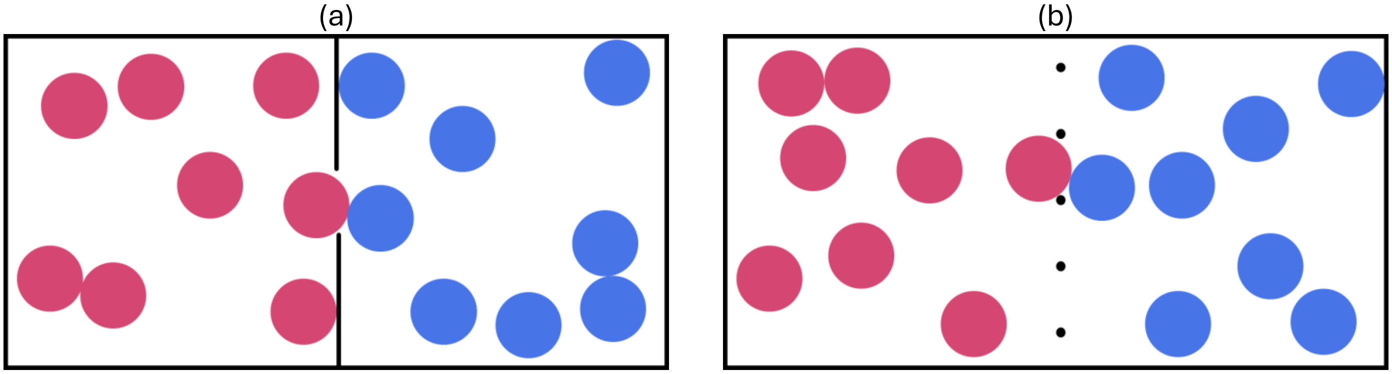


Figure 1: (a) A hard-disk gas inside two boxes with specular walls. There is an aperture in the wall separating the two compartments with size A=0.99 D where D is the diameter of the disks. Red and blue disks can protrude through the aperture but cannot pass to the opposite compartment. (b) Same setup with multiple apertures. The black dots are fixed points where disks are reflected specularly. The dots have zero area and the distance between them is 0.99 D.

In Figure 1b, we have the same setup but multiple apertures. The black dots represent fixed points in space on which the disks are reflected specularly. The distance between the dots is *A=0.99 D,* so the red-blue collisions are allowed but no disk can escape to the opposite compartment. With this setup we multiply the frequency of the red-blue collisions in the simulation.

We call these dots "*the rim"* because they resemble the rim on a basketball game (where the ball is a little larger than the rim and so nobody can score a point).

The simulation follows the principles of EDMD (Event Driven Molecular Dynamics). We have three main event types:

- Particle-to-particle collision, divided in two sub-events
    - Same color particles collision
    - Red-blue collisions
- Wall reflections, when a particle hits a specular wall
- Rim reflections, when a particle hits a rim fixed point.

A video illustrating the system can be found at the same site as this document.

In this working document we will present the results of a rim model simulation run with the following configuration:

- Number of particles *N=200,000* (100,000 in each compartment)
- Particles' diameter *D=2*
- Particles' mass *M=1*

- Boltzmann constant $k_B=1$
- Packing fraction $\phi=0.2$
- Compartment size $L=1{,}253$
- Total width $W = 2L=2{,}506$
- Number of rim fixed points $R=633$

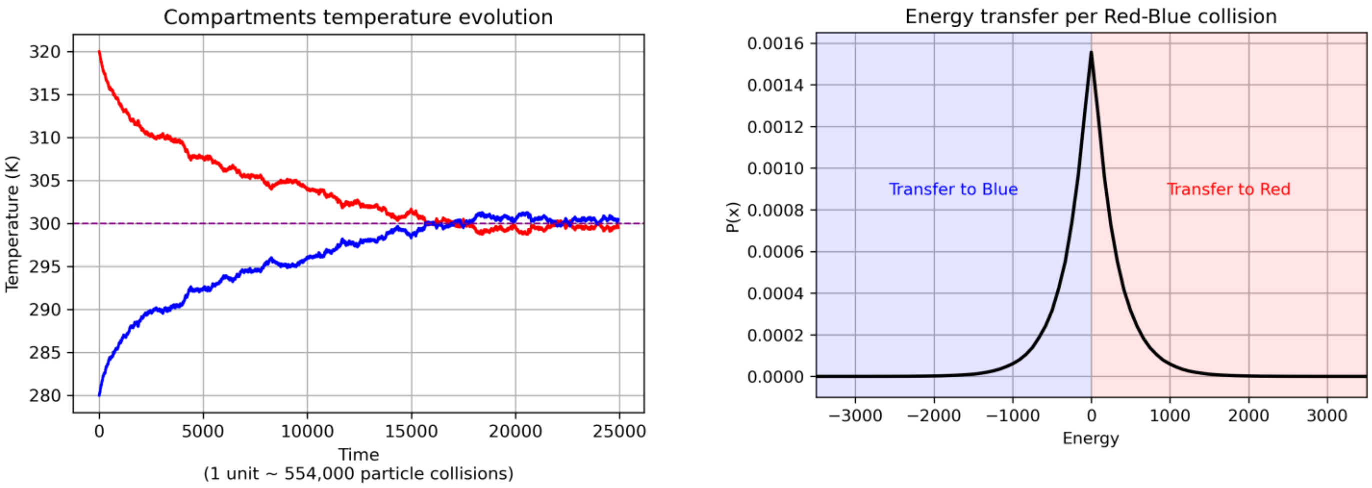
Particle positions are initialized randomly from a uniform distribution, with resampling in cases of overlap. Particles velocities are drawn from a Maxwell-Boltzmann distribution with temperature parameters $T_{red}=320$ and $T_{blue}=280$ for the particles in the red and blue compartments respectively.

We let the system evolve and we maintain two log files.

On every red-blue collision, we calculate the difference between the kinetic energy of the red particle before the collision and its kinetic energy after collision. We then log in a computer file the difference $\Delta E=E_{after} - E_{before}$. This is the energy gained (lost) by the red gas due to the red-blue collision.

In regular time intervals, corresponding to about 554,000 particle collisions (any particles, not just red-blue), we measure total kinetic temperature of the two gases and we log it in a computer file.

After a few billion collisions, the system converges to a single temperature $T_{red}=T_{blue}=300$. The convergence is shown in Figure 2a.



(a)

(b)

Figure 2: (a) Convergence of the two compartments to a single temperature. (b) PDF of the interaction channel between the two subsystems. Energy transferred to a compartment through a red-blue collision.

In Figure 2b we show the probability density function of the interaction channel between the two subsystems (between the red and the blue gas). Here the random variable is the amount of energy transferred to the red compartment during a red-blue collision. The distribution is zero-mean, symmetric, and Laplace-like, exhibiting exponential tails with small deviations attributable to geometry-constrained collision statistics. The sample used to construct this PDF was taken *after* the temperatures of the two compartments converged to the common temperature (steady state).

Before reaching this steady state and as the system evolves from $T_R > T_B$ to $T_R = T_B$, the mean of this RB energy-exchange distribution evolves as shown in Figure 3.

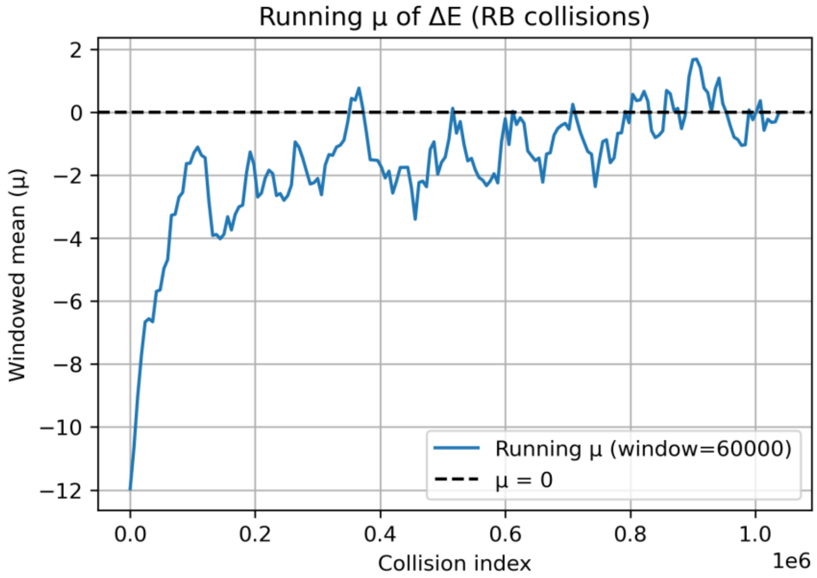


Figure 3: Evolution of the mean RB energy transfer during equilibration

The RB energy-exchange distribution may be written in the general form

$$P_{\mathrm{RB}}\left(\Delta E_R \mid T_R, T_B, \phi_R, \phi_B, m_R, m_B, d_R, d_B, \mathcal{G}_{\mathrm{rim}}^{(R)}, \mathcal{G}_{\mathrm{rim}}^{(B)}\right).$$

This notation emphasizes that the distribution is not determined solely by the instantaneous temperatures of the two compartments, but by the full collision-conditioned statistics of particles participating in RB collisions.

The dependence on the temperatures T_R and T_B arises because the pre-collisional velocity distributions determine the typical relative velocities,

$$\mathbf{g} = \mathbf{v}_R - \mathbf{v}_B,$$

and the exchanged energy depends primarily on the normal component of the relative velocity,

$$g_n = \mathbf{g} \cdot \hat{n}.$$

If $T_R \neq T_B$, the distribution acquires a drift, producing a nonzero mean energy exchange

$$\mu = \langle \Delta E_R \rangle.$$

Since ΔE_R denotes the energy gained by the red gas, the sign of the mean follows the temperature difference:

$$\mathrm{sign}(\mu) = \mathrm{sign}(T_B - T_R).$$

Thus, if the red gas is hotter than the blue gas, $T_R > T_B$, the red gas loses energy on average through RB collisions and therefore $\mu < 0$.

Conversely, if $T_B > T_R$, then $\mu > 0$.

The dependence on the packing fractions ϕ_R and ϕ_B is more subtle. The RB exchange distribution depends on the collision-conditioned pair distribution

$$f_2(\mathbf{v}_R, \mathbf{v}_B \mid \mathrm{RB}),$$

which generally does not factorize as

$$f_2 \neq f_1(\mathbf{v}_R) f_1(\mathbf{v}_B).$$

At finite density, collisions generate dynamical correlations and memory effects through ring kinetics and repeated encounters. These correlations modify the probability of specific relative velocities and collision geometries. Since the strength and persistence of such correlations increase with density, the structure of the RB exchange distribution depends on ϕ_R and ϕ_B. Moreover, near a specular boundary velocity anisotropy and density oscillation effects are developing. These effects are more pronounced in high packing fractions. Also, near the rim boundary these effects are expected to develop as well and also be more complex, due to the more complex scattering geometry. These effects can filter the velocities selected for RB collisions.

The dependence on m_R, m_B and d_R, d_B arises because masses determine the redistribution of kinetic energy during a collision, while particle diameters affect collision cross sections, excluded-volume structure, and the set of accessible protrusion geometries near the rim.

The dependence on the rim geometry,

$$\mathcal{G}_{\mathrm{rim}}^{(R)}, \mathcal{G}_{\mathrm{rim}}^{(B)},$$

arises because RB collisions may not be sampled isotropically. The fixed scatterers constrain which trajectories may protrude through the rim and therefore bias the distribution of collision normals $\hat{n}$. An asymmetric arrangement of fixed points may impose different geometric constraints on particles approaching from the two sides, thereby altering the statistics of RB collisions even when the bulk gases themselves are identical. In the sketch of Figure 4 we see an example of such an asymmetrical rim.

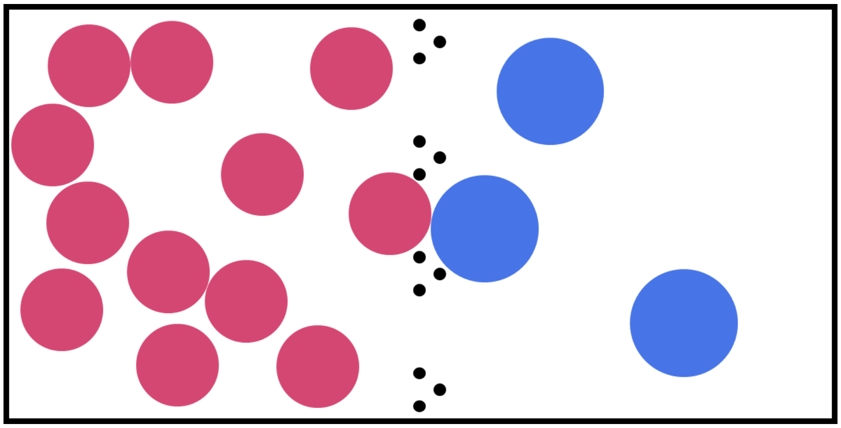


Figure 4: Illustrative example of an asymmetric system. Red compartment has higher packing fraction ϕ, blue particles have higher diameter D, rim is not left-right symmetric.

The RB energy-exchange distribution is generally not stationary when

$$\mu = \langle \Delta E_R \rangle \neq 0.$$

In that case, RB collisions produce a systematic energy transfer between the two compartments, causing the macroscopic state variables T_R and T_B to evolve in time. Since the RB energy-exchange distribution itself depends on these state variables, the distribution must also evolve in time. Consequently, the distribution becomes stationary only when its parameters satisfy

$$\langle \Delta E_R \rangle = 0.$$

Thus, the interaction channel itself possesses a nontrivial statistical structure that evolves together with the macroscopic state variables.

For each RB collision, energy conservation implies

$$\Delta E_R = -\Delta E_B.$$

In the fully symmetric equilibrium case (as in our example simulation run),

$$T_R = T_B, \phi_R = \phi_B, m_R = m_B, d_R = d_B, \mathcal{G}_{\mathrm{rim}}^{(R)} = \mathcal{G}_{\mathrm{rim}}^{(B)},$$

the red and blue compartments become *interchangeable*. The RB energy-exchange distribution must therefore remain invariant under the transformation

$$R \leftrightarrow B, \Delta E_R \leftrightarrow -\Delta E_R,$$

leading to the symmetry relation

$$P_R(\Delta E) = P_R(-\Delta E).$$

Thus, in the symmetric equilibrium case, the RB energy-exchange distribution is symmetric around zero and has vanishing mean,

$$\langle \Delta E_R \rangle = 0.$$