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Chapter 1

Theoretical Background

1.1 Collisions: MCC-Null Model

First we will go through the Monte Carlo Collisional model and then show how the Null-Collision scheme can reduce the amount of arithmetic operations. To avoid spending computational time on the neutral particles we consider them as background species. We assume for simplicity that the neutral particles are uniformly distributed, with a normal velocity distribution.

Particle species s has N type of collisions with a target species. Each particle has kinetic energy

$$\varepsilon_i = \frac{1}{2} m_s \left(v_x + v_y + v_z\right) \tag{1.1}$$

The collisional cross section σ_j for each type of collision is dependent on the kinetic energy of the particle and the total cross section is given by adding together all the types of collisions.

$$\sigma_T(\varepsilon_i) = \sum_j^N \sigma_j(\varepsilon_i) \tag{1.2}$$

The probability that a particle has a collision with a target species, in one timestep, is be dependent on the collisional cross section, distance travelled, $\Delta r_i = v_i \Delta t$, and the density of the target specie, $n_t(\mathbf{r_i})$ by the following relation.

$$P_i = 1 - \exp\{-v_i \Delta t \sigma_T(\varepsilon_i) n_t(\mathbf{r_i}\} \tag{1.3}$$

In a Monte Carlo model we say that a collision has taken place for a particle if a random number $r = [0, 1]$, is smaller than P_i. To compute P_i for each particle, we need to find ε_i, all the cross sections σ_j, and the density $n_t(\mathbf{r_i}$. This demands many floating point operations for each particle, so we will use a Null-Collisional

for Each particle **do**
  if $r \leq P_{Null}$ **then**

	r	$\leq \nu_0(\varepsilon_i)/\nu'$	Type 0
$\nu_0(\varepsilon_i)/\nu' \leq$	r	$\leq (\nu_0(\varepsilon_i) + \nu_1(\varepsilon_i))/\nu'$	Type 1
	$\vdots$		
$\sum_j(\nu_j(\varepsilon_i))/\nu' \leq$	r		Type Null

Table 1.1: Algorithm to select a particle collisions

model to only compute the collisional probability for a subset of the particles. We compute a maximal collisional frequency

$$\nu' = \max(v_i \Delta t \sigma_T(\varepsilon_i)) \max(n_t(n_t)) \tag{1.4}$$

and consider if it was a dummy or one of the proper collisions, if r is smaller than the resulting constant $P_{Null} = 1 - \exp\{\nu'\}$.

The maximum collisional frequency may need to be recomputed each timestep due to the density of the target specie, n_t, changing. The algorithm for each particle is then.