Numerical Lecture #6: Monte Carlo Implementation of Collisions

Ref: C.K. Birdsall, "Particle-in-Cell Charged-Particle Simulations, Plus Monte Carlo Collisions with Neutral Atoms, PIC-MCC," IEEE Transactions on Plasma Science 19: 65 (1991).

I. Monte Carlo Collisions

A. General Idea

1. A Monte Carlo (probabilistic) approach can be taken to model collisions in plasmas.
2. Can be used to model
   a. Coulomb collisions with ions and electrons
   b. Elastic collisions with neutrals
   c. Charge exchange collisions
   d. Ionization
3. Monte Carlo Collisions (MCC) are widely used with Particle-In-Cell (PIC) simulations (self-consistent)
4. Detailed collisional modeling is used to conserve momentum & energy while reproducing desired scaling.

B. Basic Approach

Step ①

1. Compute Probability of Collision in one timestep Δt.
   a. Collision frequency $\nu(v)$ is generally a function of v.
   b. Ex: For charged particle-neutral collisions,

$$\nu(v_j) = n_{gas}\,\sigma(E_j)\,v_j$$

where n_{gas} is neutral gas density, v_j is velocity of particle "j"
$\sigma(E_j)$ is collision cross-section (depends on particle energy E_j)

I. B. 1 (Continued)

c. For Coulomb collisions, $\nu \propto \frac{1}{v^3}$ [Spitzer (1962)]

d. Probability of collision in timestep Δt: $\boxed{P_{coll} = 1 - \exp[-\nu \Delta t]}$

i) NOTE: For weakly collisional plasmas, $\nu \Delta t \ll 1$, so

$$P_{coll} = \cancel{1} - \left[\cancel{1} - \nu\Delta t + \frac{(\nu\Delta t)^2}{2!} - \ldots\right] = \nu \Delta t + \mathcal{O}((\nu \Delta t)^2)$$

~~ii) Since $\nu\Delta t \ll 1$, $P_{coll} \approx \nu \Delta t$ is a Poisson process~~

Step ②

2. Determine if collision occurs:
   a. Choose random number $0 \le R_1 \le 1$
   b. If $P_{coll} > R_1$, then a collision occurs!

Step ③

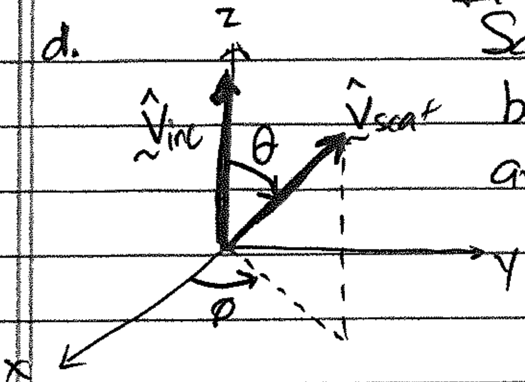
3. Determine the appropriate scattering process
   a. Only if more than one collision type is modeled.

Step ④

4. Compute the new (scattered) velocity
   a. NOTE: For self-consistent plasma simulations (PIC), collisions should conserve momentum & energy.
   b. Step ④a: Determine scattered particle energy
      i) For electron-ion collisions with $m_i \gg m_e$, no exchange of energy, so $\boxed{E_{scat,e} = E_{inc,e}}$

      ii) For like-particle collisions, colliding particle energies are constant in center-of-mass frame-of-reference.
   c. Step ④b: Compute scattering angle

I. B. 4. (Continued)

d. 

Scattering angle in 4π steradians can be described by two angles (θ, φ) away from initial velocity aligned with z-axis.

e. Transform from initial velocity $\underset{\sim}{v}_{inc}$ to scattered velocity $\underset{\sim}{v}_{scat}$.

f. Small-angle scattering: Spitzer (1962): $P(\theta)d\theta = \left(\frac{\theta\, d\theta}{\langle\theta\rangle^2}\Delta t\right)\exp\left[-\frac{\theta^2}{2\langle\theta\rangle^2}\Delta t\right]$

where $\langle\theta\rangle^2 = \frac{3a_p}{2}\frac{\ln\Lambda}{\Lambda}$, $\Lambda = \frac{6\pi n}{Z}\left[\frac{v^2}{a_p^2}\right]^{3/2}$

C. Simple Implementation

1. Consider Coulomb scattering of electrons from massive ions, $m_i \gg m_e$

a. Thus $\boxed{E_{scat,e} = E_{inc,e}}$

~~2. Simply model numerous small-angle collisions as less frequent large-angle collisions ... quantitatively accurate, but with ... qualitative ...~~

3 a. Take $\nu = \text{constant}$ s.t. $\nu\Delta t \ll 1$

$\Rightarrow$ Poisson process with $\boxed{P_{coll} = \nu\Delta t}$

4. Implement electron-ion coulomb collisions to see effect of collisions on confinement in a magnetic mirror geometry. (See HW #5a)