INSTITUTE OF PLASMA PHYSICS
OF THE CZECH ACADEMY OF SCIENCES

MC modelling used in Plasma Edge Modelling

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MINISTRY OF EDUCATION,
YOUTH AND SPORTS

Coulomb collisions in PIC codes

Motivation

1. Classical PIC simulates only macro fields and neglects particle collisions.

2. Inside grid cells the interaction between particles deviates from the Coulomb law

PIC

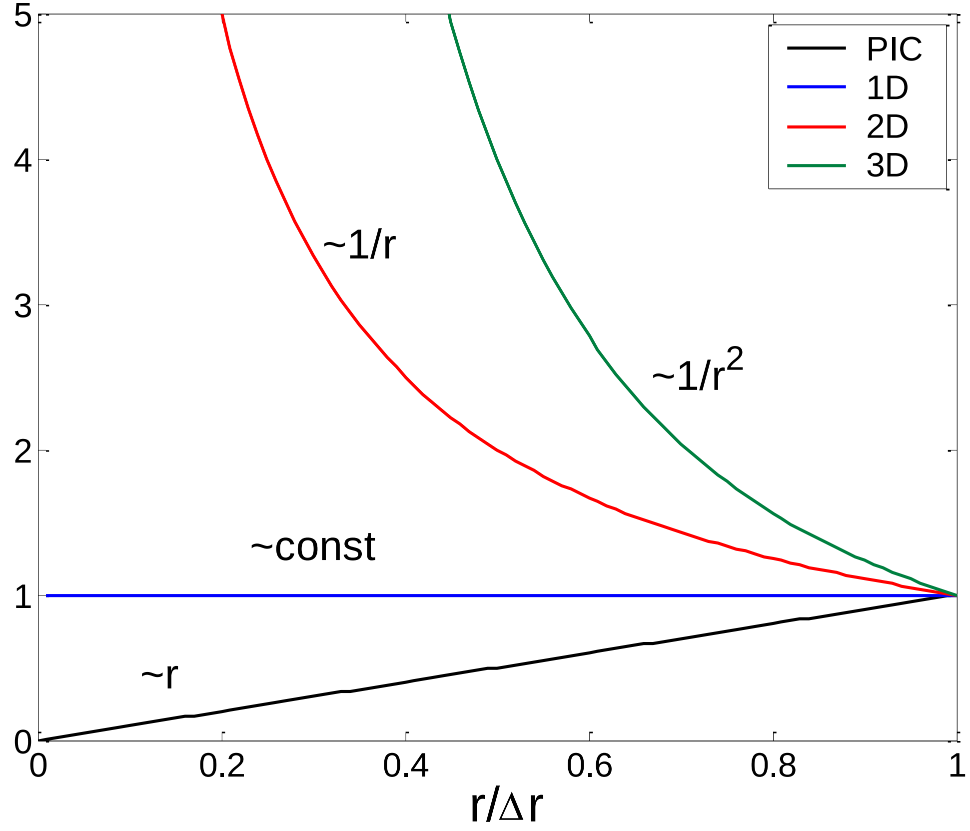
$$\left(\frac{\partial}{\partial t}+\vec{V}\frac{\partial}{\partial \vec{r}}+\frac{\vec{F}}{m}\frac{\partial}{\partial \vec{V}}\right) f\left(\vec{r},\vec{V},t\right) \approx 0$$

We need

$$\left(\frac{\partial}{\partial t}+\vec{V}\frac{\partial}{\partial \vec{r}}+\frac{\vec{F}}{m}\frac{\partial}{\partial \vec{V}}\right) f\left(\vec{r},\vec{V},t\right) = St$$

Reminder

$$\nu_{Coulumb} \sim \frac{n}{T^{3/2}}$$



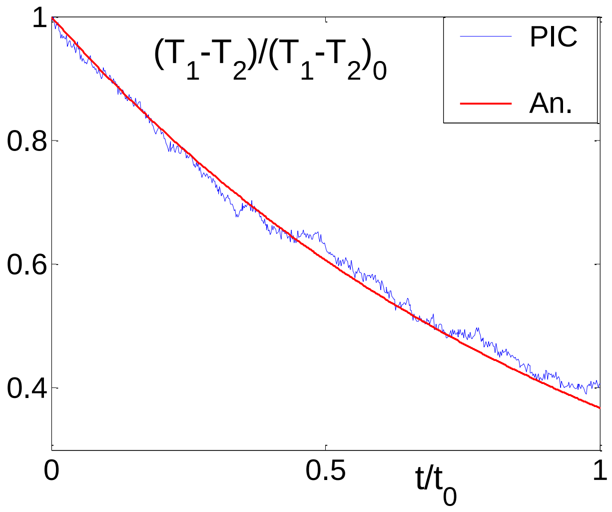
Interaction force between two particles inside the grid cell

Coulomb collision models

Linear model [2]

Maxwell-distribution ↓
Chandrasekhar coefficients
Force acting on particle ↓

$$\Delta\vec{V} = \vec{F}\Delta t + \sqrt{\Delta V_{\perp}^{2}\Delta t}\,\vec{R}_{1}\vec{e}_{\perp} + \sqrt{\Delta V_{\parallel}^{2}\Delta t}\,R_{2}\vec{e}_{\parallel}$$



Thermal equilibration of two-temperature plasma (BIT1 code)

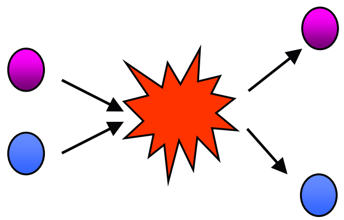
Nonlinear model

Calculation of Rothembluth potentials [3]
Force acting on particle

Requires extremely large number of particles

Binary collision model [4]

1. Choosing colliding pares
2. Colliding the particles

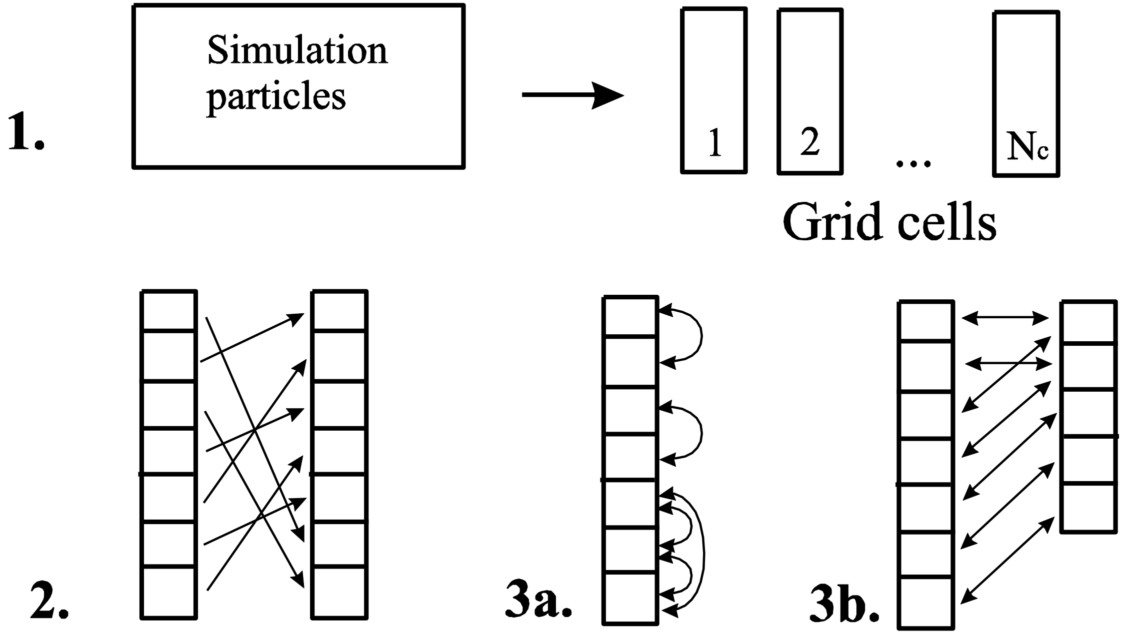


Binary collisions conserving momentum and energy

[2] A. Bergmann, Contrib. Plasma Phys., 38, 1998
[3] O.V. Batishchev, Phys. Plasmas, 3, 1996
[4] T. Takizuka and H. Abe, J. Comput. Phys., 25, 1977

Binary collision model

Choosing of colliding pares



Particle sorting

$$\Delta r_{PIC} \sim \lambda_{Debye}$$

All particles are collided

too expensive

Cumulative binary collision operator [5] – applicable for relatively uniform plasmas

Collision of two particles

$$\mathbf{V}' = \hat{\mathbf{O}}(\chi)\mathbf{V}$$

Scattering angle

$$P(\chi) = \frac{\chi}{\langle \chi^2 \rangle_{\Delta t}} \exp\left(-\frac{\chi^2}{2\langle \chi^2 \rangle_{\Delta t}} \right),$$

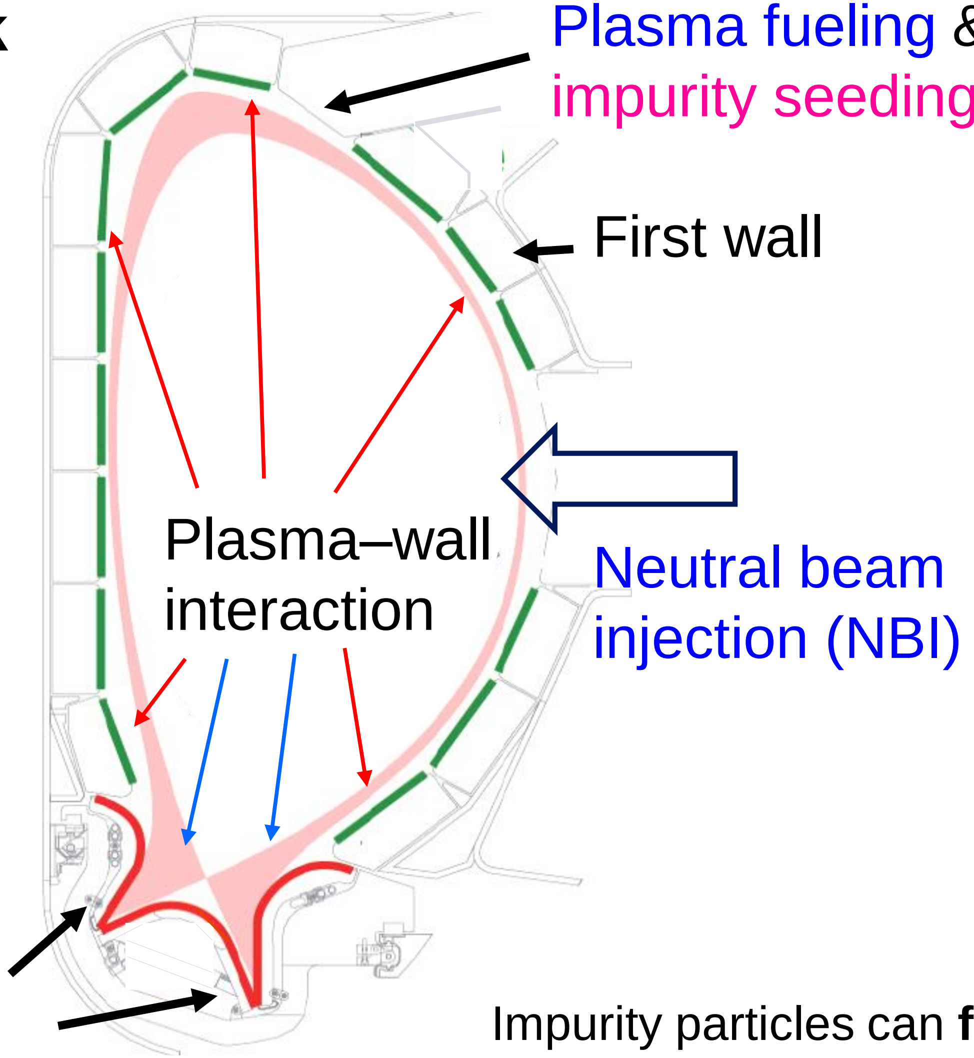
$$\langle \chi^2 \rangle_{\Delta t} \sim e^4 n \Delta t / V^3$$

[5] K. Nanbu, Phys. Rev., E 55, 1997

Questions?

Atoms and molecules in fusion devices

Tokamak cross section



- **Atomic and molecular fuel** (D, T, D_2, T_2): plasma fueling, NBI, plasma recycling
- Seeded **impurity particles** (*N*, *Ne*, *Ar*, *Xe*)
- Intristic **impurity particles**, sputtered due to plasma-wall interactions (*C*, *W*, *Be*, *Li*, *Fe*, *Sn*, …)
- Parasitic **impurity particles** penetrating into the plasma due to different processes (O, O_2,…)
- Fusion product impurity (*He*)
- Impurity particles used in different diagnostics (*Li*, …)

Impurity particles can **form molecules**: C_xH_y, N_xH_y, BeA, WA (A=H, N, O)

General principle of MC model

Deterministic model of particle motion

$$\frac{d}{dt}\vec{r}_i = \vec{V}_i, \quad \frac{d}{dt}\vec{V}_i = \frac{1}{m}\vec{F}_i,$$

$$\vec{F} = \vec{F}_{av.\,field} + \vec{F}_{collisions}$$

Deterministic + stochastic model of particle motion

$$\frac{d}{dt}\vec{r}_i = \vec{V}_i, \quad \frac{d}{dt}\vec{V}_i{}' = \frac{1}{m}\vec{F}^{\,i}_{av.\,field},$$

$$\vec{V}_i{}' \xrightarrow{\text{Stochastic, collision}} \vec{V}_i$$

$$P(t)$$

$$P(t) = 1 - \exp(-\upsilon t)$$

$$\upsilon = nu\sigma(u)$$

Collision event

$$\begin{pmatrix} \vec{V}_1 \\ \vec{V}_2 \end{pmatrix} \Rightarrow \begin{pmatrix} \vec{V}_1{}' \\ \vec{V}_2{}' \end{pmatrix}$$

Equations conserving momentum and energy

Different ways of choosing the collision partners*

1. Counter based models

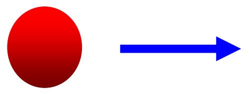
2. Non-counter based models: direct simulation MC (DSMC)

Counter based models

$$P(t) = 1 - \exp(-\upsilon t)$$
$$\upsilon = nu\sigma(u)$$

$$t_{col} = -\frac{\ln R}{\upsilon}, \quad R \in [0,1]$$

1. Calculation of average time between collisions
2. Colliding particle after t_{col} time.



$\mathbf{r}$, $\mathbf{V}$, t_{col}

For each particle one has to **calculate** and **curry** an **additional parameter** t_{col}

Too expensive!

Null collision method [6]

1. Calculation of shortest possible collision time $t_{col}^{\min} = -\frac{\ln R}{\upsilon_{\max}}$
2. Analyzing for collision after $t_{col}^{\min}$
3. Colliding these particles if $R' \le \frac{P}{P_{\max}} = \frac{1-\exp(-\nu t)}{1-\exp(-\nu_{\max} t)} \approx \frac{\nu}{\nu_{\max}}$

$t_{col}^{\min}$ is same for any particle of the given type – **less expensive!**

What if different collision types can take place?

[6] H.R. Skullerud, J. Phys. D., 1, 1968

Different collision types

Collision types[7]

$N_{collided} \rightarrow M_{products}$

- 2 → 2 - elastic, excitation, charge-exchange, …
- 2 → 1 - recombination (radiative)
- 2 → 3 - dissociation, ionization
- 2 → 4 - double ionization, dissociative ionization
- 3 → 2 - recombination (three-body)

$$t_{col}^{\min} = -\frac{\ln R}{\upsilon_{\max}}, \quad \upsilon = \sum \upsilon_i$$

If $R' \leq \frac{v_1}{v_{\max}}$, then collision 1 takes place

If $R' \leq \frac{v_1 + v_2}{v_{\max}}$, then collision 2 takes place

….

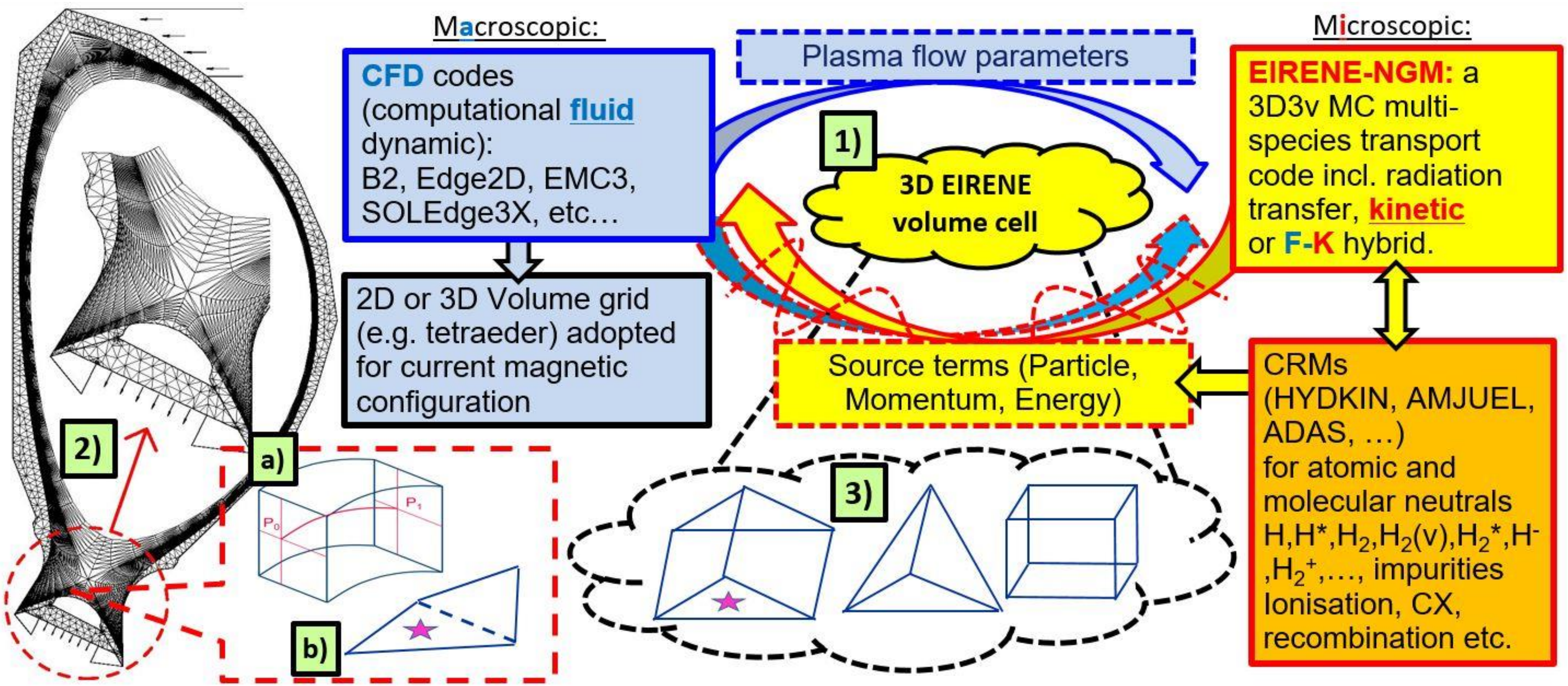
Frequently used in SOL simulating Linear MC codes (e.g. **EIRENE**)

Linear MC codes: target particles are not followed, but represent a background with given density, temperature and EDF

[7] D. Tskhakaya, Contr. Plasma Phys., (2008); (2016)

EIRENE basics

EIRENE-NGM iterative scheme with the CFD codes [8]: NGM – Neutral Gas Module; CFD - computational fluid dynamics; CRM - collisional-radiative model



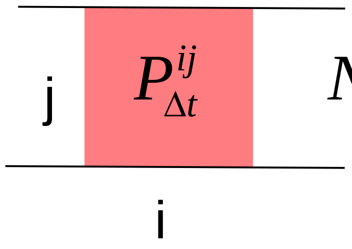
[8] https://www.eirene.de/Basics/basics.html

Questions?

Non-counter based models (DSMC)

Particles are sorted into the grid cells

i. Decision on collision



$$N_{\Delta t} = P_{\Delta t}^{ij}(\sigma) N_{ij}$$

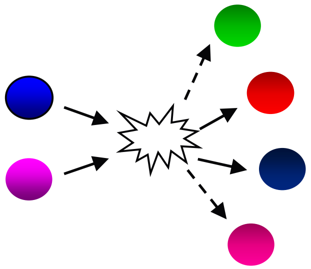
if yes

- Parameters in different cells are statistically independent
- Scales as $\sim N_{cell}$
- Null collisional method can be applied

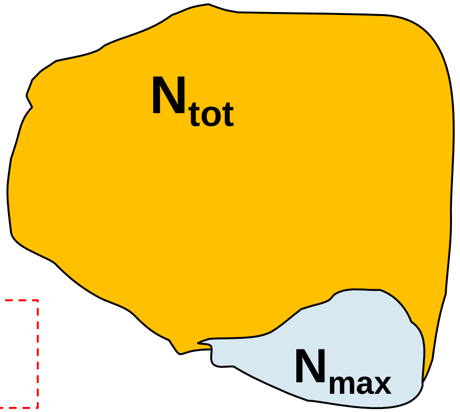
1. Calculation of maximum possible number of collided particles in each sell - N_{max}
2. Analyzing only N_{max} particles.

ii. Calculation of after-collision velocities

Binary collision model



particle number, energy and momentum are **conserved**



$$N_{max} = N_{tot} P_{max}(t) << N_{tot}$$

[9] G. A. Bird, Molecular Gas Dynamics and the Direct Simulation of Gas Flows, (1994).

Collision operators

Charge exchange: $D + D^{+} \rightarrow D^{+} + D$ $\begin{pmatrix} \vec{V}_1 \\ \vec{V}_2 \end{pmatrix} \Rightarrow \begin{pmatrix} \vec{V}_2 \\ \vec{V}_1 \end{pmatrix}$ $\sigma(E)$

Elastic: $e + D \rightarrow e + D$ $\vec{U} = \vec{V}_1 - \vec{V}_2$ $\vec{U}' = \hat{\mathbf{O}}(\theta)\vec{U}$ $\vec{U}'F\begin{pmatrix} \vec{V}_1 \\ \vec{V}_2 \end{pmatrix} \Rightarrow \begin{pmatrix} \vec{V}_1' \\ \vec{V}_2' \end{pmatrix}$ $\sigma(E,\theta)$

Excitation: $e + D \rightarrow e + D^{(n)}$ $\vec{U} = \vec{V}_1 - \vec{V}_2$ $\vec{U}' = \hat{\mathbf{O}}(\theta)\vec{U}$ $\vec{V}_1 \rightarrow \vec{V}_1' = \vec{V}_1 = \sqrt{1 - \frac{E_{th}}{E_0}}$

Ionization: $e + D \rightarrow 2e + D^{+}$ $\sigma(E,\theta,E_1,\theta_1)$ $\vec{U}'F\begin{pmatrix} \vec{V}_1' \\ \vec{V}_2 \end{pmatrix} \Rightarrow \begin{pmatrix} \vec{V}_1'' \\ \vec{V}_2' \end{pmatrix}$ $\sigma(E,\theta,n)$

Double ionization: $e + Ne \rightarrow 3e + Ne_n^{++}$ $\sigma(E,\theta,E_1,\theta_1,E_2,\theta_2,n)$