% !TEX root=/home/tavant/these/manuscript/src/manuscript.tex

\section{Elements of the 2D PIC-MCC simulations}

\subsection{Principe of the PIC simulations}

```
The \ac{PIC} simulation models the movement of particles on a fixed grid.

The grid is used to compute the electric field, in the electrostatic approximation

\begin{equation}
  \label{eq-poisson}
  \Delta \phi = - \frac{\rho}{\epsilon_0}
\end{equation}

where $\phi$ is the electric potential, $\rho$ is the charge density, and $\epsilon

The charge density $\rho$ is computed by depositing the particle over the cells, us

The particles moves following the Lorenz forces
\begin{equation}
  \label{eq-Lor}
  m \vec{a} = q E + q \vec{v} \times \vec{B}
\end{equation}
with $m$ and $q$ the particle mass and electric charge respectively.
The numerical particles followed in the simulations correspond to $q_f$ physical pa
\begin{equation}
  q_f = \frac{n V}{\Npc}
\end{equation}
with $n$ the particle density, $V$ the volume of a cell, and $\Npc$ the number of n
A large enough number of particle is needed in order to obtain physical results.
Indeed, insufficient number of particles leads to numerical heating \cite{ueda1994}
Usually, a minimum of 100 particles per cell are used, but recent results seem to e
```

\subsection{Monte Carlo collisions}

```
In \ac{PIC} simulations, collisions between charged and neutral particles can be mo
Instead, a Monte-Carlo algorithm can be used \cite{vahedi1995}.
This approach is very efficient, and allow scattering, momentum transfer and ioniza

The propellant used in \ac{HET} usually is \ac{Xe}, even if the recent constellatio
The cross sections used for modeling \ac{Xe} or other gases collisions are taken fr

Except is other with stated, the elastic, inelastic scattering and ionization react
The cross section values are summarised in \cref{fig-xexsection}.

\begin{table}[hbtp]
  \centering
```

```
    \caption{Reactions used in the PIC simulations}
    \label{tab-reactXe}
    \begin{tabular}{ccc}
      Reaction & Threshold & Reference\\
      {\it Elastic scattering} & &\\
      e + Xe = e + Xe   & --   & \cite{Lxcat_Xe,Lxcat_Xe2} \\
      {\it Excitation} & &\\
      e + Xe = e + Xe$^*$   & 8.315eV   & \cite{Lxcat_Xe,Lxcat_Xe2} \\
      e + Xe = e + Xe$^*$   & 9.447eV   & \cite{Lxcat_Xe,Lxcat_Xe2} \\
      e + Xe = e + Xe$^*$   & 9.917eV   & \cite{Lxcat_Xe,Lxcat_Xe2} \\
      e + Xe = e + Xe$^*$   & 11.7eV    & \cite{Lxcat_Xe,Lxcat_Xe2} \\
      {\it Ionization} & &\\
      e + Xe = e + Xe$^+$   & 8.315eV   & \cite{Lxcat_Xe,Lxcat_Xe2} \\

    \end{tabular}

  \end{table}


  \begin{figure}[hbtp]
    \centering
    \includegraphics[width=\defaultwidth]{figure/xenon_cross_section.pdf}
    \caption{Cross section values used in the Monte Carlo procedure \cite{Lxcat_Xe,Lx
    \label{fig-xexsection}
  \end{figure}
```

\section{Numerical implementation of the Particle in cell simulation}

%

% \LPPic is an explicit electrostatic \ac{PIC} code.

%

% Every time-steps, the simulation loop presented in \cref{fig-picloop} is computed.

%

% \begin{figure}[hbtp]

% \centering

% \includegraphics{picloop.png}

% \caption{\ac{PIC}-\ac{MCC} loop executed every time steps.}

% \label{fig-picloop}

% \end{figure}

%

% \subsection{Data used}

% In the \ac{PIC} simulation, there is two kind of data used:

% \begin{itemize}

% \item Particles

% \item Mesh

% \end{itemize}

%

```
% \paragraph{Particles}
% For each particles, are known its position $\vec{x}$ and its velocity $\vec{v}$.
% We can decouple the number of dimensions used for the velocity and the position.
% In most \ac{PIC}-\ac{MCC} simulations, the 3 directions of the velocity vector are followed in order to in order to take into account scattering.
% It is abbreviated as \acs{3V}.
%
% The dimension of the position depends of the dimension of the simulation domain, hence the mesh dimension.
% It is usual to find \acs{2D}\ac{3V} \ac{PIC} simulations, for particles with 3 directions on the velocity but 2 dimension in space.
%
% \subsection{Particle pusher}
% Integrating the movement equation \cref{eq-Lor} is deferent for magnetized and non-magnetized particles.
%
% For non-magnetized particles, we use \cite{birdsall1991} the leapfrog scheme
% \begin{align}\label{eq-leapfrog}
% v^t &= v^{t-1} + \frac{q}{m} E \dt, \
% x^t &= x^{t-1} + v^t \dt,
% \end{align}
% with the superscript $t$ designing the time step, $q$ and $m$ the particle electric charge and mass, $E$ the electric field at the particle position, and \dt the time step duration.
%
% It is important to note that the leapfrog induces a shift of $\frac{\dt}{2}$ between the position and the velocity, as illustrated in \cref{fig-leapfrog}.
% \begin{figure}[hbtp]
% \centering
% \includegraphics[width=\defaultwidth]{leapfrog.png}
% \caption{Illustration of the shift between the particle velocity and position.}
% \label{fig-leapfrog}
% \end{figure}
% This shift can leads to erroneous diagnostics when computing moments of the particles distribution.
% For instance, the mean velocity of an ensemble of $N$ particle at the instant $t$ is computed as:
% \begin{equation} \label{eq-meanv}
% \mean{v^t} = \frac{1}{N} \sum_i^N \lp v_i^t + \frac{q}{m} E_i \frac{\dt}{2} \rp.
% \end{equation}
% Other moments like the mean energy or heat flux follow the same correction.
% We can see that the error between $\mean{v}$ defined above and
% $$ \tilde{v} = \frac{1}{N} \sum_i^N v_i^t $$
% is
% $$\frac{q \dt}{2 m} \frac{1}{N} \sum_i^N E_i .$$
% Hence, the error in the diagnostic is large only in the region of large electric field.
%
% \paragraph{Magnetized particles}
% For magnetized particles, we use a modification of the leapfrog algorithm proposed by Boris \cite{boris1970}.
% It correspond to an operator splitting between the electrostatic acceleration and the magnetic rotation.
% This splitting is describe below:
% \begin{itemize}
% \item accelerate the particle during $\frac{\dt}{2}$ : $v^{t-\frac{\dt}{2}} = v^{t-1} + \frac{q}{m} E \frac{\dt}{2}$
% \item Rotate the particle velocity with the magnetic field
% \item accelerate the particle during $\frac{\dt}{2}$ : $v^t = v^{t-\frac{\dt}{2}} + \frac{q}{m} E \frac{\dt}{2}$
%
% \end{itemize}
%
%
% \subsection{Poisson equation solver}
% \label{subsec-poissonintro}
%
% The Poisson equation \cref{eq-poisson} is an elliptic equation.
% We can directly discretize the differential operator by finite volume on the cell mesh.
% The formal discretization is develop in \cref{sec-diel}, but a short summary is given here.
%
% In \ac{1D}, the obtained linear system is tridiagnonal.
% It can be solve directly using {\sc Thomas} algorithm, which simply stores the Gauss elimination's coefficient.
%
% In \ac{2D}, the linear system is pentadiagonal.
% A direct solver, like the $LU$ decomposition, would require a large amount a memory to store the factorisation matrices.
% On the other hand, as the time step is usually small in \ac{PIC} simulation, we expect the plasma potential $\phi$ not to change rapidly.
% Hence, an iterative solver using the previous solution as initial guess seems more reasonable on the memory storage and the computational time.
%
% In practice, we uses {\sc Hypre}'s multigrid solver to solve Poisson equation in \ac{2D}.
```