An Example of an Electromagnetic Particle Code

• As an example of a kinetic simulations we will use a one dimensional electromagnetic simulation code called KEMPO developed by Yoshiharu Omura and Hiroshi Matsumoto.

• More detailed information including instructions on how to run the code is available from http://www.terrapub.co.jp/e-library/cspp/index.html.

• We have included a version of the code on the class web pages.

• KEMPO is an example of class of codes known are particle in cell codes.

• In these codes the equation of motion of the particles in a plasma is solved self-consistently.
  – The particle motions for both ions and electrons are calculated in electric and magnetic fields.
  – The resulting changes in the electric and magnetic fields are calculated and then built back into the particle calculations.

• The KEMPO code is sufficiently flexible that it can be used for both test particle calculations (i.e. no self-consistent fields) or as an electrostatic code (changes in the electric field only).
The Basic Problem

- The electromagnetic field's are given by Maxwell's Equations where $\vec{J}$, $\rho$, $c$, $\varepsilon_0$, and $\mu_0$ are the current density, charge density, light speed, electric permittivity, and magnetic permeability respectively.

$$\nabla \times \vec{B} = \mu_0 \vec{J} + \frac{1}{c^2} \frac{\partial \vec{E}}{\partial t}$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \cdot \vec{E} = \frac{\rho}{\varepsilon_0}$$

$$\nabla \cdot \vec{B} = 0$$
The Basic Problem 2

• For this example the grid is assumed to be one-dimensional.
• The electric field \( E_x \) must satisfy Poisson's equation initially. Note this only has to be done at the beginning of the simulation since Ampere's Law will assure it is solved automatically.

\[
\frac{\partial E_x}{\partial x} = \frac{\rho}{\varepsilon_0}
\]

• The magnetic field component \( B_x \) should satisfy \( \frac{\partial B_x}{\partial x} = 0 \)

In a one-dimensional system this makes \( B_x \) constant.

• The code solves Maxwell's equations for the electric field \((E_x, E_y, E_z)\) and the magnetic field \((B_y, B_z)\).

• The current density \((J_x, J_y, J_z)\) and the charge density \( \rho \) are computed from the motion of a large number of particles.

• For particles of charge \( q \) and mass \( m \) the equation of motion is

\[
\frac{d\vec{v}}{dt} = \frac{q}{m} (\vec{E} + \vec{v} \times \vec{B})
\]

\[
\frac{dx}{dt} = v_x
\]

• In simulations \( \varepsilon_0 \) and \( m_0 \) can be defined arbitrarily provided \( \varepsilon_0 \mu_0 = \frac{1}{c^2} \)
The Grid Strategy

- The electric field, current density and magnetic field are defined at spatial grid points while the particles can take arbitrary positions. Interpolation is used to give the fields for calculating the trajectories.
- Full integer grids are at $i\Delta x$ ($i=1,2,3, \ldots N_x$) and half-integer grids at $(i + \frac{1}{2})\Delta x$.
- The quantities in the simulations are defined as shown on the right.
- The electric field and the current density must be assigned to the same grids since the current density contributes directly to the time dependent electric field.
- The time and spatial derivatives in Ampere's Law and Faraday's Law are centered differences.
How the Scheme Works: Time Sequencing

- There are two time sequences—full integer time \((n\Delta t)\) and half-integer time \((n+1/2)\Delta t\).
- Basically the electric field is integrated at full integer time and the magnetic field at half integer time.
- The integration is done by using the leap-frog method.
- The magnetic field is advanced twice by a half step to obtain intermediate values for the particle pushing field at the full-integer time.
- Particle positions \(x\) at the full integer time and velocities \(v\) at the half integer time are advanced by the leap-frog method.
- The positions are advanced twice so the current density can be calculated at the time integer time.
Digression on the Leap-Frog Method

- A Leap-Frog method is second order accurate in time as well as space.
- Consider again the advection equation we used as an example when discussing the solution of the MHD equations.

\[
\frac{\partial u}{\partial t} = -\nu \frac{\partial u}{\partial x}
\]

- The solution takes on the following form in a Leap-Frog system.

\[
u_{j}^{n+1} - u_{j}^{n-1} = -\frac{\nu \Delta t}{\Delta x} \left( u_{j+1}^{n} - u_{j-1}^{n} \right)
\]

- The time levels (the n's) in the time derivative term "leapfrog" over the time levels in the space derivative term. Note the \(u^{n-1}\) and \(u^{n}\) must be stored in order to calculate \(u^{n+1}\).
- The von Neumann stability analysis gives so the Courant condition is required.

\[
\xi^2 - 1 = -2i \xi \frac{\nu \Delta t}{\Delta x} \sin k \Delta x
\]

- There is no amplitude dissipation.
The Courant Condition

- Assume a quantity has a structure with a wavenumber $k$ a frequency $\omega$.

$$A(x, t) = A_0 e^{(ikx - i\omega t)}$$

- The derivative becomes

$$\frac{\Delta A}{\Delta x} = \frac{A(x_0 + \Delta x/2, t) - A(x_0 - \Delta x/2, t)}{\Delta x}$$

$$= \frac{e^{(ik\Delta x/2)} - e^{(-ik\Delta x/2)}}{\Delta x} A(x_0, t)$$

$$= i \frac{\sin(k\Delta x/2)}{\Delta x/2} A(x_0, t)$$

- Remember that $\Delta A/\Delta x$ represents $\partial A/\partial x$ so that in the difference equation the wavenumber $k$ is replaced by $K$.

$$K = \frac{\sin(k \Delta x/2)}{\Delta x/2}$$
The Courant Condition 2

- Similarly the frequency $\omega$ is replaced by $\Omega$ where
  \[ \Omega = \frac{\sin(\omega \Delta t/2)}{\Delta t/2} \]

- The dispersion relation for electromagnetic waves in a vacuum is $\omega^2 = c^2 k^2$

- The numerical dispersion relation becomes $\Omega^2 = c^2 K^2$

- For the maximum wavenumber occurring for $k_{\text{max}} = \pi/\Delta x$
  \[ \sin^2(\omega \Delta t/2) = \left( \frac{c \Delta t}{\Delta x} \right)^2 \]

- If $c \Delta t/\Delta x > 1$  $\omega$ becomes complex and we have a numerical instability.

- If $c \Delta t/\Delta x = 1$ the system is marginally stable. This is the Courant condition.
The Debye Length

• To avoid instability caused by the grid spacing $\Delta x$ should be close to the Debye length $\lambda_e$ given by

$$\lambda_e = \frac{v_{th,e}}{\omega_{pe}}$$

where $v_{th,e}$ and $\omega_{pe}$ are the thermal velocity and the plasma frequency of electrons.

• In the actual KEMPO code the grid spacing is set to

$$\Delta x \leq 3\lambda_e$$
How the Code Works: Initialization

• Define the charge density. At the grid point $x = X_i$ it is calculated by

$$\rho_i = \frac{1}{\Delta x} \sum_{j=1}^{N_p} q_j W(x_j - X_i)$$

where the particle shape function is given by

$$W(x) = 1 - \frac{|x|}{\Delta x}, \quad |x| \leq \Delta x$$

$$= 0, \quad |x| > \Delta x$$

• The initial electric field is calculated from Poisson's equation by

$$\frac{E_{x,i+1/2} - E_{x,i-1/2}}{\Delta x} = \frac{\rho_i}{\varepsilon_0}$$
How the Code Works: Solving Maxwell's Equations

- The current density $J_x$ by using charge conservation

$$J_{x,i+1/2}^{t+\Delta t/2} - J_{x,i-1/2}^{t+\Delta t/2} = -\frac{\Delta x}{\Delta t} \left( \rho_{i+1}^{t+\Delta t} - \rho_i^t \right)$$

- $J_y$ and $J_z$ are calculated by

$$J_{i+1/2}^{t+\Delta/2} = \frac{1}{\Delta x} \sum_{j}^{N_p} q_j v W(x_j - X_{i+1/2})$$

- This gives $J_y$ at half-integer grids but we need it at whole integer grids so the average is used

$$J_{y,i} = \frac{J_{y,i-1/2} + J_{y,i+1/2}}{2}$$

- Once we know current density we can calculate E and B by using Maxwell's equations.
How the Code Works: Solving Maxwell's Equations 2

- Advancing the electric field
  \[
  E_{y,i}^{t+\Delta t} = E_y^t + \Delta t \left[ -c^2 \frac{B_{z,i+1/2}^{t+\Delta t/2} - B_{z,i-1/2}^{t+\Delta t/2}}{\Delta x} - J_{y,i}^{t+\Delta t/2} \right]
  \]
  \[
  E_{z,i+1/2}^{t+\Delta t} = E_{z,i+1/2}^t + \Delta t \left[ c^2 \frac{B_{y,i+1}^{t+\Delta t/2} - B_{y,i}^{t+\Delta t/2}}{\Delta x} - J_{z,i+1/2}^{t+\Delta t/2} \right]
  \]

- Advancing the magnetic field
  \[
  B_{y,i}^{t+\Delta t/2} = B_{y,i}^{t-\Delta t/2} + \Delta t \left[ \frac{E_{z,i+1/2}^t - E_{z,i-1/2}^t}{\Delta x} \right]
  \]
  \[
  B_{z,i+1/2}^{t+\Delta t/2} = B_{z,i+1/2}^{t-\Delta t/2} + \Delta t \left[ \frac{E_{y,i+1}^t - E_{y,i}^t}{\Delta x} \right]
  \]
How the Code Works: Solving the Equation of Motion

• Next we must solve the equation of motion

\[
\frac{d\vec{v}}{dt} = \frac{q}{m} (\vec{E} + \vec{v} \times \vec{B}) \quad \frac{dx}{dt} = v_x
\]

• The difference equation is

\[
\frac{\vec{v}^{t+\Delta t/2} - \vec{v}^{t-\Delta t/2}}{\Delta t} = \frac{q_s}{m_s} \left( \vec{E}^t + \frac{\vec{v}^{t+\Delta t/2} + \vec{v}^{t-\Delta t/2}}{2} \times \vec{B}^t \right)
\]

• Define

\[
\vec{v}^- = \vec{v}^{t-\Delta t/2} + \frac{q_s}{m_s} \frac{\vec{E}^t \Delta t}{2}
\]

\[
\vec{v}^+ = \vec{v}^{t+\Delta t/2} - \frac{q_s}{m_s} \frac{\vec{E}^t \Delta t}{2}
\]
How the Code Works: Solving the Equation of Motion 2

- The actual code uses the Buneman-Boris method – this four step method assures strict conservation of kinetic energy in the cyclotron motion.

\[ \begin{align*}
1 & \quad \vec{v}^- = \vec{v}^{t+\Delta t/2} + \left( \frac{q}{m} \right)_s \vec{E}^t \frac{\Delta t}{2} \\
2 & \quad \vec{v}^0 = \vec{v}^- + \vec{v}^- \times \left( \frac{q}{m} \right)_s \vec{B}^t \frac{\Delta t}{2} \\
3 & \quad \vec{v}^+ = \vec{v}^- + \frac{2}{1 + \left( \left( \frac{q}{m} \right)_s \vec{B}^t \Delta t / 2 \right)^2} \vec{v}_0 \times \vec{B}^t \frac{\Delta t}{2} \\
4 & \quad \vec{v}^{t+\Delta t/2} = \vec{v}^2 + \left( \frac{q}{m} \right)_s \vec{E}^t \frac{\Delta t}{2}
\end{align*} \]
How the Code Works: Solving the Equation of Motion 3

- In advancing the velocity $v$ from $t-\Delta t/2$ to $t+\Delta t/2$ we need the electric and magnetic fields at the time $t$ at the particle position $x(t)$. The fields are linearly interpolated from adjacent grid points.

- A particle should not be influenced by the field due to its own charge. The electrostatic field $E_x$ is defined on half integer grids but has to be relocated to full-integer grids before the interpolation to cancel the electrostatic self-force.

- Similarly the magnetic field $B_y$ has to be relocated before interpolation from full-integer grids to half integer grids to cancel the magnetostatic force due to the current density $J_z$,

$$\frac{B_{y,i+1} - B_{y,i}}{\Delta x} = \mu_0 J_{z,i+1/2}$$

- The effect of this goes away if

$$B_{y,i+1/2} = \frac{B_{y,i} + B_{y,i+1}}{2}$$
How the Code Works: Solving the Equation of Motion 4

- In one time step, $\Delta t$, the particle positions $x$ advance twice each by a half time step.

\[
x^{t+\Delta t/2} = x^t + v^t_{x} \frac{\Delta t}{2}
\]

\[
x^{t+\Delta t/2} = x^{t+\Delta t/2} + v^t_{x} \frac{\Delta t}{2}
\]