iPic3D units and variables

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Chapter 1

iPIC3D units and normalized variables

1.1 Legend

Given a variable in code units ϕ (i.e. particle number density, a component of the electric field ...):

- The physical value to which ϕ corresponds is: $\bar{\phi}$.
- The value to which ϕ is normalized in the code is: $\tilde{\phi}$

The following relation holds:

$$\frac{\bar{\phi}}{\tilde{\phi}} = \phi.$$

1.2 iPIC3D dimensional equations (CGS)

Given a particle of species s, the particle equations for iPIC3D are:

$$\frac{d\bar{\mathbf{x}}}{d\bar{t}} = \bar{\mathbf{v}}$$

$$\frac{d\bar{\mathbf{v}}}{d\bar{t}} = \left(\frac{\bar{q}}{m}\right)_s \left(\bar{\mathbf{E}} + \frac{\bar{\mathbf{v}} \times \bar{\mathbf{B}}}{c}\right)$$

where $\bar{\mathbf{x}}$ is particle position, $\bar{\mathbf{v}}$ is particle velocity, $\bar{t}$ is time, $\bar{q}_s$ is particle charge, $\bar{m}_s$ is particle mass, $\bar{\mathbf{E}}$ is the electric field, $\bar{\mathbf{B}}$ is the magnetic field, c is the speed of light. The fields equations are:

$$\bar{\nabla}^2 \bar{\mathbf{E}} - \frac{1}{c^2}\frac{\partial^2 \bar{\mathbf{E}}}{\partial \bar{t}^2} = \frac{4\pi}{c^2}\frac{\partial \bar{\mathbf{J}}}{\partial \bar{t}} + 4\pi \bar{\nabla}\bar{\rho}$$

$$\frac{\partial \bar{\mathbf{B}}}{\partial \bar{t}} = -c\bar{\nabla} \times \bar{\mathbf{E}}$$

$$\bar{\rho} = \sum_s \bar{q}_s \int \bar{f}_s d\bar{\mathbf{v}}, \quad \bar{\mathbf{J}} = \sum_s \bar{q}_s \int \bar{\mathbf{v}} \bar{f}_s d\bar{\mathbf{v}}$$

where $\bar{f}_s$ is the particle distribution function.

1.3 iPIC3D non dimensional equations

The previous equations are solved by iPIC3D in the following non dimensional form:

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}$$

$$\frac{d\mathbf{v}}{dt} = \left(\frac{q}{m}\right)_s \left(\mathbf{E} + \frac{\mathbf{v}\times\mathbf{B}}{c_{ipic}}\right)$$

$$\nabla^2\mathbf{E} - \frac{1}{c_{ipic}^2}\frac{\partial^2\mathbf{E}}{\partial t^2} = \frac{4\pi}{c_{ipic}^2}\frac{\partial\mathbf{J}}{\partial t} + 4\pi\nabla\rho$$

$$\frac{\partial\mathbf{B}}{\partial t} = -c_{ipic}\nabla\times\mathbf{E}$$

$$\rho = \sum_s q_s \int f_s d\mathbf{v}, \quad \mathbf{J} = \sum_s q_s \int \mathbf{v} f_s d\mathbf{v}$$

where c_{ipic} is the value of the speed of light in ipic units (generally equal to 1). Comparing dimensional and non dimensional equations we get the following normalizations:

$$\tilde{x} = \tilde{d}_p; \quad \tilde{t} = \tilde{d}_p/c; \quad \tilde{v} = c$$

$$\tilde{E} = \left(\frac{\tilde{q}}{m}\right)^{-1} c^2/\tilde{d}_p; \quad \tilde{\rho} = \left(\frac{\tilde{q}}{m}\right)^{-1} c^2/\tilde{d}_p^2 \quad \tilde{B} = \left(\frac{\tilde{q}}{m}\right)^{-1} c^2/\tilde{d}_p;$$

$$\tilde{J} = \left(\frac{\tilde{q}}{m}\right)^{-1} c^3/\tilde{d}_p^2; \quad \tilde{f} = \tilde{\rho}/(c^3\tilde{q})$$

where $\tilde{d}_p$ is the normalizing proton inertial length, c is the speed of light and $\tilde{q}/\tilde{m}$ is the normalizing charge over mass ratio (this generally takes protons values, but that is not the only possible choice).

It is worth noticing that in order to have the time normalized to the inverse of the proton plasma frequency, the numerical value of the particle density in the code has to be chosen properly. We have that:

$$\bar{\omega}_{pp} = \left(\frac{4\pi\bar{n}_p e^2}{m_p}\right)^{1/2}$$

The last one can be written in the following form:

$$\tilde{t}^{-1}\omega_{pp} = \left(\frac{4\pi\tilde{n}_p n_p e^2}{m_p}\right)^{1/2}$$

Now considering that:

$$\bar{n}_p = \frac{\bar{\rho}}{e} = \frac{\tilde{\rho}\rho}{e}$$

and using what found before for $\tilde{t}$ and $\tilde{\rho}$, we get the following:

$$\omega_{pp} = (4\pi\rho)^{1/2}.$$

which means that in order to normalize time to the inverse of the proton plasma frequency, which means $\omega_{pp} = 1$, one must have:

$$\rho = \frac{1}{4\pi}$$

In the code this is done in the following way: in the input file ρ is set equal to 1, then it is immediately divided (inside the code) by 4π, this means that the actual numerical value of the charge density in the code at the beginning is $1/4\pi$ (even if in the input file it is set equal to 1).

Chapter 2

How do I compute energies in iPIC3D units?

The total energy in a PIC code is given by the summation of magnetic, electric and particle kinetic energy.

2.1 Magnetic energy

The magnetic energy in CGS is given by:

$$\int \frac{B^2}{8\pi} dV$$

The same expression is valid for iPIC3D. So, if you want to compute the magnetic energy in iPIC3D you shall compute:

$$E_M^{iP} = \frac{1}{8\pi} \sum_{i,j,k} B_{i,j,k}^2 \; \Delta x \Delta y \Delta z$$

2.2 Electric energy

The electric energy in CGS is given by:

$$\int \frac{E^2}{8\pi} dV$$

The same expression is valid for iPIC3D. So, if you want to compute the magnetic energy in iPIC3D you shall compute:

$$E_E^{iP} = \frac{1}{8\pi} \sum_{i,j,k} E_{i,j,k}^2 \; \Delta x \Delta y \Delta z$$

2.3 Kinetic energy

The kinetic energy is more tricky to compute. The general form is:

$$E_K = \sum_a \sum_p \frac{1}{2} m_\alpha v_{a,p}^2$$

where α is the particle species, m_α its mass, and $v_{\alpha,p}$ is the speed of the the $p-th$ particle (of species α). It is generally useful to separate the contributions to the kinetic energy into the bulk energy and the thermal energy. Let's consider now a single species and drop the index α, the average (bulk) speed is defined as:

$$\mathbf{V} = \frac{1}{N_p}\sum_p \mathbf{v_p}.$$

Using last expression we can write the velocity in this form:

$$\mathbf{v_p} = \mathbf{V} + \delta\mathbf{v_p}$$

Now we compute the modulus square of the last expression, we sum over the particles, we multiply by a factor $\frac{m}{2}$, and we get:

$$\frac{1}{2}m\sum_{p=1}^{N_p}|\mathbf{v_p}|^2 = \frac{1}{2}m\sum_{p=1}^{N_p}|\delta\mathbf{v_p}|^2 + \frac{1}{2}mN_p|\mathbf{V}|^2. \tag{2.1}$$

The three terms in last equations are the total E_K, thermal E_{th}, and bulk E_{bulk} kinetic energy:

$$\begin{aligned}
E_K &= \frac{1}{2}m\sum_{p=1}^{N_p}(v_{p,x}^2 + v_{p,y}^2 + v_{p,z}^2) \\
E_{th} &= \frac{1}{2}m\sum_{p=1}^{N_p}(v_{pth,x}^2 + v_{pth,y}^2 + v_{pth,z}^2) \\
E_{bulk} &= \frac{1}{2}mN_pV^2 = \frac{1}{2}mN_p(V_x^2 + V_y^2 + V_z^2)
\end{aligned}$$

where $\mathbf{v_p} = (v_{p.x}, v_{p.y}, v_{p.z})$, $\delta\mathbf{v_p} = (v_{pth.x}, v_{pth.y}, v_{pth.z})$, and $\mathbf{V} = (V_x, V_y, V_z)$. Diving equation 2.1 by N_p one gets:

$$\langle E_K\rangle = \langle E_{th}\rangle + \langle E_{bulk}\rangle.$$

The last expression is true for each components of the velocity:

$$\begin{aligned}
\langle E_{K,x}\rangle &= \langle E_{th,x}\rangle + \frac{1}{2}mV_x^2 \\
\langle E_{K,y}\rangle &= \langle E_{th,y}\rangle + \frac{1}{2}mV_y^2 \\
\langle E_{K,z}\rangle &= \langle E_{th,z}\rangle + \frac{1}{2}mV_z^2
\end{aligned}$$

2.3.1 Bulk kinetic energy

Let's consider particles of species α. The total bulk energy is given by:

$$E_{bulk} = \int \frac{1}{2}\rho_\alpha^m V_\alpha^2 dxdydz,$$

where ρ_α^m is the local mass density. We know that the current density $\mathbf{J}$ is (by definition):

$$\mathbf{J} = \rho_\alpha^c \mathbf{V},$$

where ρ_α^c is the charge density. If we know consider that $\rho_\alpha^m = \frac{q_\alpha}{m_\alpha}\rho_\alpha^m$, where q_α is the particle charge, we can write the bulk energy as a function of the current:

$$E_{bulk} = \int \frac{1}{2}\frac{J_\alpha^2}{\frac{q_\alpha}{m_\alpha}\rho_\alpha^c}\; dxdydz$$

Last expression can be computed in iPIC3D in the following way:

$$E_{bulk,\alpha}^{iP} = \sum_{i,j,k}\frac{1}{2}\frac{J_{\alpha,(i,j,k)}^2}{(qom)_\alpha \rho_{\alpha,(i,j,k)}}\;\Delta x\Delta y\Delta z$$

2.3.2 Thermal Energy

The thermal energy is given by:

$$E_{th,\alpha} = \int \frac{1}{2}\left(P_{xx} + P_{yy} + P_{zz}\right)\; dxdydz,$$

where Pij is the pressure tensor (see section on how to compute pressure tensor from iPIC3D data, Chapter 3). It is worth noticing that this relation must hold:

$$P_{xx} + P_{yy} + P_{zz} = P_{\perp 1} + P_{\perp 2} + P_{\|},$$

where $P_{\perp 1}$, $P_{\perp 2}$, and $P_{\|}$ are the diagonal components of the pressure tensor in the reference frame of the magnetic field, related to the perpendicular and parallel directions with respect to it. The thermal energy from iPIC3D data is:

$$E_{th,\alpha}^{iP} = \sum_{i,j,k}\frac{1}{2}\left(P_{xx,(i,j,k)} + P_{yy,(i,j,k)} + P_{zz,(i,j,k)}\right)\;\Delta x\Delta y\Delta z.$$

The pressure tensor used here is not the one given as an output by iPIC3D (see Chapter 3).

2.4 Total Energy

We arrived to the expression for the total energy in iPIC3D units:

$$E = \sum_{i,j,k}\left[\frac{B_{i,j,k}^2}{8\pi} + \frac{E_{i,j,k}^2}{8\pi} + \sum_\alpha \frac{1}{2}\frac{J_{\alpha,(i,j,k)}^2}{(qom)_\alpha \rho_{\alpha,(i,j,k)}} + \right.$$
$$\left. + \frac{1}{2}\left(P_{xx,(i,j,k)} + P_{yy,(i,j,k)} + P_{zz,(i,j,k)}\right)\right]\Delta x\Delta y\Delta z$$

2.5 Temperature and thermal velocity

The following formula holds for an ideal gas of species α:

$$U_a = \frac{3}{2}n_\alpha \kappa_B T_\alpha,$$

where U is the internal energy, κ_B the Boltzman constant, n_α the number density, and T_α the temperature. The factor three in the formula is due to the three possible directions of the thermal velocity, namely x, y, z.

In iPIC3D the internal (or thermal) energy is related to the pressure tensor P_{ij} by the formula:

$$E_{th,\alpha} = \sum_{i,j,k} \frac{1}{2}(P_{\alpha,xx} + P_{\alpha,yy} + P_{\alpha,zz})\Delta x \Delta y \Delta z. \tag{2.2}$$

Therefore, the following expression holds for the temperature:

$$n_\alpha T_{\alpha,ii} = P_{\alpha,ii}, \text{ for } i = x, y, z. \tag{2.3}$$

κ_B is equal to 1 in iPIC3D units. On the other hand the thermal energy has to be equal to:

$$E_{th,\alpha} = \sum_{i,j,k} \frac{1}{2}\rho^m_\alpha (v^2_{\alpha_{th,x}} + v^2_{\alpha_{th,y}} + v^2_{\alpha_{th,z}})\Delta x \Delta y \Delta z \tag{2.4}$$

Combining Equations 2.2, 2.3 and 2.4 we arrive to the following relation between temperature and thermal velocity:

$$T_{\alpha,ii} = m_\alpha v^2_{\alpha_{th,i}}$$

where $i = x, y, z$. Notice that the mass is normalized in code units. If the unit mass is the proton mass $m_p = 1$, the electron mass in code units will be $m_e = 1/|(qom)_e|$.

Chapter 3

How to compute true pressure tensor from iPIC3D output?

The definition of the pressure tensor in fluid theory is given by:

$$P_{ij} = \int m_\alpha v_i v_j f_\alpha(\mathbf{r}, \mathbf{v}, t) d^3v - m_\alpha n_\alpha V_i V_j$$

where m_α is the particle mass, f_α is the particle distribution function, n_α is the particle number density, and $\mathbf{V}$ is the mean velocity. The following equation holds for f_α:

$$\int f_\alpha(\mathbf{r}, \mathbf{v}, t) d^3r d^3v = N(t),$$

where $N(t)$ is the total number of particles at time t. In iPIC3D the following quantity is printed as output in each node: $P_{ij}^{iPIC} = 1/Vol_{cell} \sum_p q_\alpha * weight * u_i u_j$, where q_α is the particle charge *weight* is the particle weight with respect to the node, and Vol_{cell} is the cell volume. From this relation we get that:

$$\int m_\alpha v_i v_j f_\alpha(\mathbf{r}, \mathbf{v}, t) d^3v = \frac{P_{ij}^{iPIC}}{qom_\alpha}$$

where qom_α is the charge to mass ratio in code units. It is also easy to show that:

$$m_\alpha n_\alpha V_i V_j = \frac{J_{\alpha,i} J_{\alpha,j}}{qom_\alpha \rho_\alpha},$$

where ρ_α is the charge density. We arrive to the following expression for the true pressure tensor in iPIC3D units:

$$P_{ij,\alpha} = \frac{1}{qom_\alpha}\left(P_{ij,\alpha}^{iPIC} - \frac{J_{\alpha,i} J_{\alpha,j}}{\rho_\alpha}\right)$$

3.1 Magnetic field reference frame

Work in progress...

Chapter 4

How to compute beta in iPIC3D

The plasma β is defined as the ratio between the kinetic and magnetic pressure:

$$\beta = \frac{P}{\frac{B^2}{8\pi}},$$

where $P = \sum_\alpha P_\alpha$ is the sum of the pressures of each species. It is possible to define the β of a single species as

$$\beta_\alpha = \frac{P_\alpha}{\frac{B^2}{8\pi}}.$$

Now, considering that $P_\alpha = n_\alpha \kappa_B T_\alpha$, and that $\sqrt{\frac{\kappa_B T_\alpha}{m_\alpha}} = v_{th,\alpha}$, β_α can be written as follows

$$\beta_\alpha = 2\frac{v_{th,\alpha}^2}{c_{A,\alpha}^2},$$

where $c_{A,\alpha} = \sqrt{\frac{B^2}{4\pi m_\alpha n_\alpha}}$. Note that, if the ions are protons, $m_\alpha = 1.0$ and $n_\alpha = 1/4\pi$ at the initial time. Therefore, the Alfvén speed can be computed as $c_{A,i} = B$, and the electron Alfvén speed as $c_{A,e} = c_{A,i}\sqrt{\frac{m_i}{m_e}}$.

Chapter 5

How to get heat flux from iPic3D energy flux output

One of iPic3D outputs is the energy flux that is defined in the code as

$$\mathbf{EF}_\alpha = \frac{m_\alpha}{2} \int f_\alpha v^2 \mathbf{v} d^3 v$$

It is possible to extract from the latter the heat flux using the information on the first and the second order moments of the distribution function. The heat flux of a certain species α is defined as

$$\mathbf{h}_\alpha = \frac{1}{2} m_\alpha \int f_\alpha w^2 \mathbf{w} d^3 v,$$

where $\mathbf{w} = \mathbf{v} - \mathbf{V}$, $\mathbf{V}$ being the mean velocity defined as $\mathbf{V} = \frac{\int f_\alpha \mathbf{v} d^3 v}{\int f_\alpha d^3 v}$. Using the definition of the pressure tensor

$$P_{ij,\alpha} = m_\alpha \int f_\alpha w_i w_j d^3 v,$$

one arrives to the following expression for the $i-th$ component of the heat flux

$$h_{i,\alpha} = EF_{i,\alpha} - \frac{m_\alpha n_\alpha}{2} V_\alpha^2 V_{i,\alpha} - \frac{1}{2} P_{jj,\alpha} V_{i,\alpha} - V_{j,\alpha} P_{ji,\alpha}.$$

The last expression can be written as a function of iPic3D outputs as follows

$$h_{i,\alpha} = EF_{i,\alpha} - \frac{1}{2qom_\alpha} \frac{J_\alpha^2}{\rho_\alpha} J_{i,\alpha} - \frac{1}{2} P_{jj,\alpha} \frac{J_{i,\alpha}}{\rho_\alpha} - \frac{J_{j,\alpha}}{\rho_\alpha} P_{ji,\alpha},$$

where qom_α is the charge to mass ratio of species α in code units, and $P_{ij,\alpha}$ is the true pressure tensor of species α (not iPic3D "pressure" output).

Chapter 6

Relevant physical quantities in code units

We consider the case of a plasma made of ions and electrons. For protons $Z = 1$. The following holds provided that ion and electron charge density are $1/(4\pi)$. c_{ipic} is generally set equal to 1 in the code.

Ion cyclotron frequency

$$\bar{\Omega}_{ci} = \frac{Z\bar{e}\bar{B}_0}{\bar{m}_i\bar{c}}; \qquad \Omega_{ci} = \frac{B_0}{c_{ipic}}$$

Electron cyclotron frequency

$$\bar{\Omega}_{ce} = \frac{\bar{e}\bar{B}_0}{\bar{m}_e\bar{c}}; \qquad \Omega_{ce} = \Omega_{ci}\frac{m_i}{m_e} = \frac{B_0}{c_{ipic}}\frac{m_i}{m_e}$$

Ion plasma frequency

$$\bar{\omega}_{pi} = \left(\frac{4\pi\bar{n}_i Z_i^2\bar{e}^2}{\bar{m}_i}\right)^2; \qquad \omega_{pi} = 1.0$$

Electron plasma frequency

$$\bar{\omega}_{pe} = \left(\frac{4\pi\bar{n}_e\bar{e}^2}{\bar{m}_e}\right)^2; \qquad \omega_{pe} = \omega_{pi}\sqrt{\frac{m_i}{m_e}} = \sqrt{\frac{m_i}{m_e}}$$

Alfvén speed

$$\bar{c}_A = \frac{\bar{B}_0}{\sqrt{4\pi\bar{n}_i\bar{m}_i}}; \qquad c_A = B_0$$

Alfvén to light speed ratio

$$\bar{c}_A/\bar{c} = \frac{\bar{B}_0}{\sqrt{4\pi\bar{n}_i\bar{m}_i}\bar{c}}; \qquad c_A/c = B_0/c_{ipic}$$

Electron plasma to cyclotron frequency ratio

$$\frac{\bar{\omega}_{pe}}{\bar{\Omega}_{ce}} = \frac{\bar{\omega}_{pi}\sqrt{\frac{m_i}{m_e}}}{\bar{\Omega}_{ci}\frac{m_i}{m_e}}; \qquad \frac{\omega_{pe}}{\Omega_{ce}} = \frac{1}{\Omega_{ci}}\sqrt{\frac{m_e}{m_i}}$$