1 Introduction

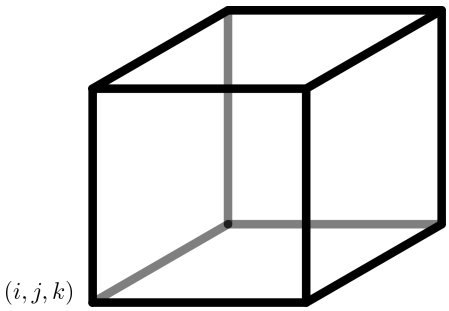
This document describes how field and hydro quantities are aranged on the underlying regular grid in VPIC (and most other particle in cell codes as well). If all of this introduces too many complications, we can always go back to the simplifying approximation that we have one value for each three components of the electric field (E_x, E_y, E_z) of the electric field vector $\mathbf{E} = (E_x, E_y, E_z)$ that is constant inside that cell. The same then applies to the magnetic field $\mathbf{B}$ with components B_x, B_y, B_z.

To explain why that is not the best possible approximation I will need a lot of pictures.

Contents

2 A simulation cell

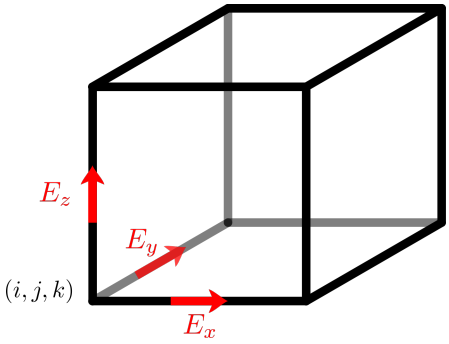
Let's take a representative grid cell:



The grid cell is labeled as (i, j, k) and by that we mean the the center of the cell is at position

$$\mathbf{r} = (i \cdot \Delta x, j \cdot \Delta y, k \cdot \Delta z) \quad . \tag{1}$$

However the components of the electric field are not all located at the center of the cell, but are actually arranged as follows:



In other words E_x is actually located at

$$\mathbf{r}_{e,x} = (i \cdot \Delta x, (j - 1/2) \cdot \Delta y, (k - 1/2) \cdot \Delta z) \tag{2}$$

and E_y and E_z are located at

$$\mathbf{r}_{e,y} = ((i - 1/2) \cdot \Delta x, j \cdot \Delta y, (k - 1/2) \cdot \Delta z) \tag{3}$$

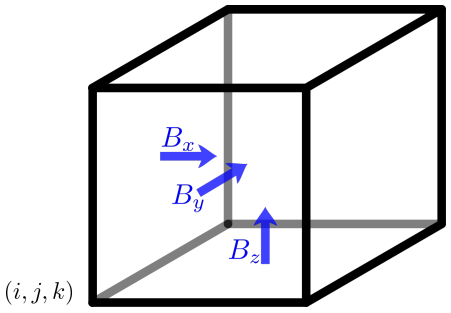
and

$$\mathbf{r}_{e,z} = ((i - 1/2) \cdot \Delta x, (j - 1/2) \cdot \Delta y, k \cdot \Delta z) \tag{4}$$

respectively.

The electric field components that are "owned" by one cell are not co-located, but are rather located at the lower, front and left edges of the cell[1]. This implies $\mathbf{r}_{e,x} \neq \mathbf{r}_{e,y} \neq \mathbf{r}_{e,z}$.

For the components of the magnetic field we find:



The x component of the magnetic field "points" in the x direction and is thus located where the face normal of the $y - z$ plane is located. The other two components are located at the other two face centers[2], at positions

$$\mathbf{r}_{b,x} = ((i - 1/2) \cdot \Delta x, j \cdot \Delta y, k \cdot \Delta z) \quad , \tag{5}$$

$$\mathbf{r}_{b,y} = (i \cdot \Delta x, (j - 1/2) \cdot \Delta y, k \cdot \Delta z) \quad , \tag{6}$$

$$\mathbf{r}_{b,z} = (i \cdot \Delta x, j \cdot \Delta y, (k - 1/2) \cdot \Delta z) \quad . \tag{7}$$

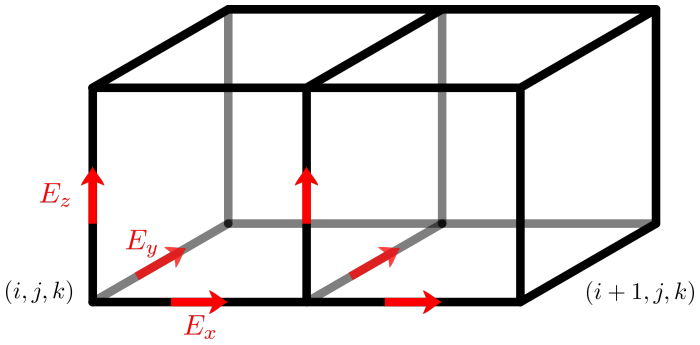
Note that none of the magnetic field components are co-located with any other magnetic field component nor any component of the electric field. We will get to the reason for that in section 6.

3 Neighbouring Cells

A simulation cells if of course never along, but surrounded by other simulation cells. For example there is another simulation cells onbe Δx further along the x axis with index $(i + 1, j, k()$:

[1] This makes sense when thinking about electrodynamics as an discrete exterior algebra. The electric field should then be composed of one-forms that are naturaly located at edges of the underlying (simplex) grid.

[2] Again that makes sense in a discrete exterior algbra, where the magnetic field should be two-form associated with faces. In 3d space, two-form can be represented by pseudo-vectors (3d - 2form = pseudo 1form) that indicate the vector normal to the face.



The electric field components of that cell are located at

$$\mathbf{r'}_{e,x} = ((i + 1) \cdot \Delta x, (j - 1/2) \cdot \Delta y, (k - 1/2) \cdot \Delta z) \quad , \tag{8}$$

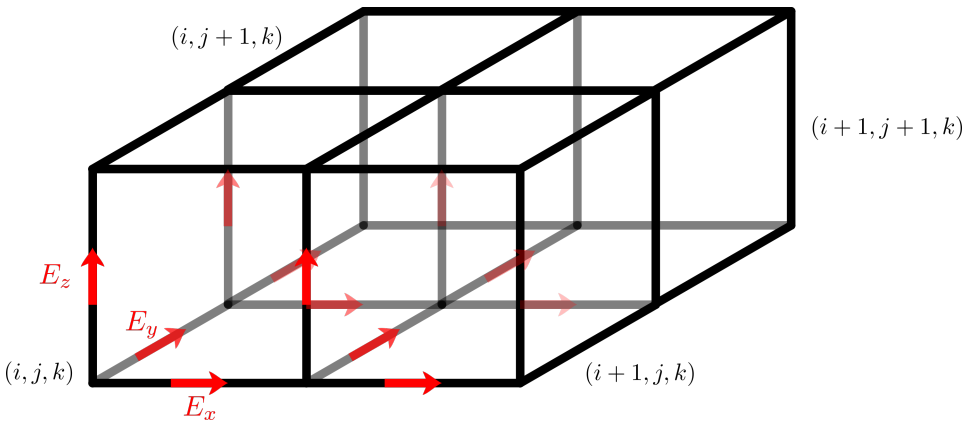
$$\mathbf{r'}_{e,y} = ((i + 1/2) \cdot \Delta x, j \cdot \Delta y, (k - 1/2) \cdot \Delta z) \tag{9}$$

and

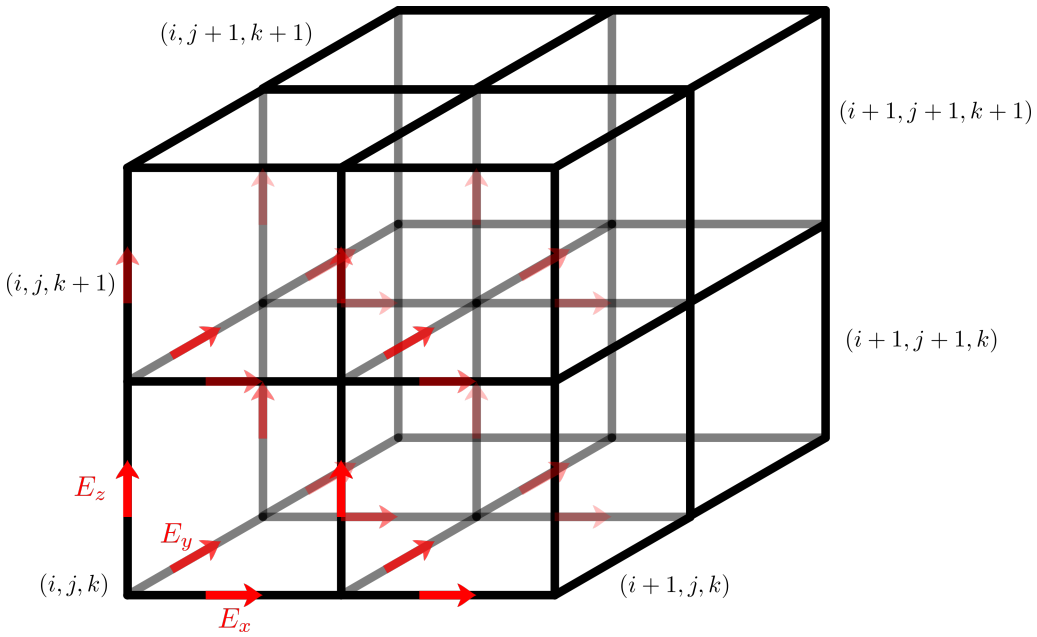
$$\mathbf{r'}_{e,z} = ((i + 1/2) \cdot \Delta x, (j - 1/2) \cdot \Delta y, k \cdot \Delta z) \quad , \tag{10}$$

respectively. The cell will also hold it's own values of the three components of the magnetic field, but for brevity I will not draw that as well nor write out their location explicitly.

There is also additional cells in the y direction, displaced by one Δy:

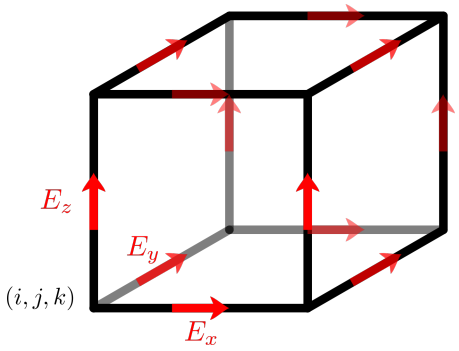


And even the z direction:



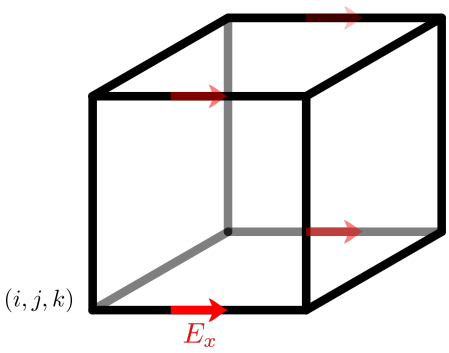
4 Interpolating Electric Field

To reduce the horrible clutter, let's get rid of all the other grid cells and only keep field components of the electric field that touch on of the twelve edges of our grid cell:



If we now want to figure out the value of E_x at some location inside the cell, we can not only use the value of that component at the left, front, bottom edges

but can also use the values of the cells behind $(i, j+1, k)$), on top($(i, j, k+1)$ and behind+ontop $(i, j+1, k+1)$.



None of those are any closer to for further from the cell center. So it is reasonable to interpolate linearly in both y and z, to whatever position inside the cell we are interested in.

Thus we get

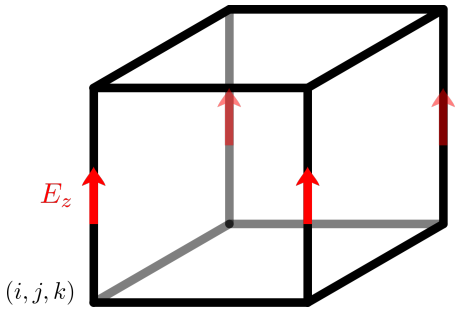
$$\begin{aligned} E_x((i+\varepsilon_1)\Delta x,&(j+\varepsilon_2)\Delta y,(k+\varepsilon_3)\Delta z) = \\ &(1/2-\varepsilon_3)\cdot(1/2-\varepsilon_2)\cdot E_x(i\Delta x, j\Delta y, k\Delta z) \\ &+(1/2-\varepsilon_3)\cdot(1/2+\varepsilon_2)\cdot E_x(i\Delta x, (j+1)\Delta y, k\Delta z) \\ &+(1/2+\varepsilon_3)\cdot(1/2-\varepsilon_2)\cdot E_x(i\Delta x, j\Delta y, (k+1)\Delta z) \\ &+(1/2+\varepsilon_3)\cdot(1/2+\varepsilon_2)\cdot E_x(i\Delta x, (j+1)\Delta y, (k+1)\Delta z) \end{aligned} \tag{11}$$

for $\varepsilon_i \in [-1/2, 1/2]$.

In principle we can also use additional cells to the left (right) of our cells and interpolate in that direction as well if the point we are interested in is left (right) of the cell center. But that is even more complicated and we will ignore it here[3].

If we want to determine the local value of E_z we basically do the same, but use the cells (i, j, k), $(i+1, j, k)$, $(i, j+1, k)$ and $(i+1, j+1, k)$

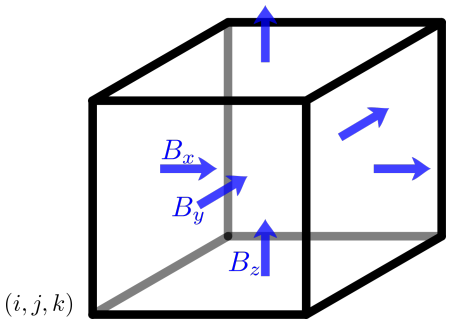
[3] A lot of other Particle-in-cell codes do just that when interpolation to the particle location, as well as using higher-order interpolation instead of simple bi-linear interpolation. The cost per particle during the simulation is greatly increased, but the number of required particles drops significantly, resulting in a complicated trade-off



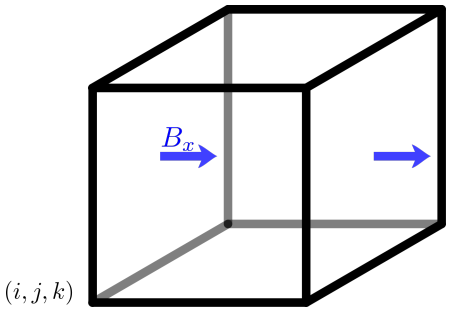
and interpolate their values for E_z in x and y.

5 Interpolating Magnetic Field

For the magnetic field, we have the values at the six faces of our grid cell:



If we want to interpolate the value of B_x, we can use the value at the left of cell (i, j, k) and the value at the right face (that properly belongs to cell $(i + 1, j, k)$.)



and calculate

$$\begin{aligned} B_x((i+\varepsilon_1)\Delta x,(j+\varepsilon_2)\Delta y,(k+\varepsilon_3)\Delta z) = \\ (1/2-\varepsilon_1)\cdot B_x(i\Delta x, j\Delta y, k\Delta z) \\ +(1/2+\varepsilon_1)\cdot B_x((i+1)\Delta x, j\Delta y, k\Delta z) \end{aligned} \tag{12}$$

The values for B_y or B_z would similarily be interpolated linearily in y or z respectively.

Again it is possible to also use cells above/below as well as in front of/ behind the "local" cell and interpolate in those directions as well or use higher order interpolation, but that is beyond the scope here that aims to match the interpolation order in VPIC.

6 Finite difference approximations of Curl

After the technical explanation of *how* top interpolate the staggered field components, let's briefly answer the question *why* one might want the stagger the field components in this way.

In the end this goes back to Maxwell's equations that describe the behaviour of the electric and magnetic field. Ignoring scaling factor such as the speed of light and the impedance of vaccuum, and looking only at the basic structure of the equation, we can write Maxwell's equations as

$$\nabla \times \mathbf{E} = -\frac{\partial}{\partial t}\mathbf{B} \tag{13}$$

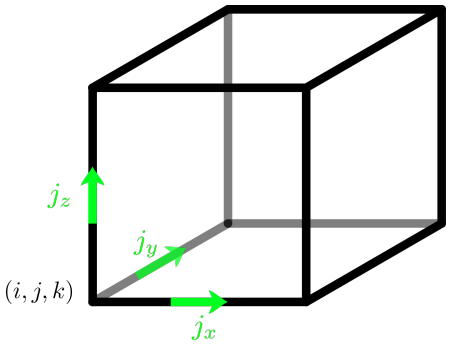
$$\nabla \times \mathbf{B} = \frac{\partial}{\partial t}\mathbf{E} + \mathbf{J} \tag{14}$$

$$\nabla \cdot \mathbf{E} = \rho \tag{15}$$

$$\nabla \cdot \mathbf{B} = 0 \quad . \tag{16}$$

In these equation ∇ is an operator, that in a standard cartesian basis is just a vector of the partial derivatives with respect to the coordinate directions. For a vector field $\mathbf{F}$ the expression $\nabla \times \mathbf{F}$ denotes the curl of the vector field and $\nabla \cdot \mathbf{F}$ denotes the divergence of the vector field.

The quantities ρ and $\mathbf{J}$ are the charge density and the current (density). In the particle-in-cell code these are calculated based on the particles and deposited onto in the grid. The method to do so is outside the scope of this document. For the purpose of manipulating Maxwell's equations we can just assume that they are known fixed quantities. The current density is a vector quantity with components j_x, j_y and j_z that are colocated with the electric field components:



If we take Faraday's Law in Eq. (13), we can approximate the (temporal) derivative of the magnetic field by a finite difference between the magnetic field $\mathbf{B}^n$ at time $t = n \cdot \Delta t$ and at a slightly later time $t = (n+1) \cdot \Delta t$ when it has value $\mathbf{B}^{n+1}$:

$$\nabla \times \mathbf{E} = -\frac{\mathbf{B}^{n+1} - \mathbf{B}^n}{\Delta t} \quad . \tag{17}$$

A simulation code such as VPIC typically wants to calculate the magnetic field at a later time, based on known quantities to follow the time evolution, so it

$$\mathbf{B}^{n+1} = \mathbf{B}^n - \nabla \times \mathbf{E} \cdot \Delta t \quad . \tag{18}$$

For the purposes here we will not talk about the temporal ordering too much, we will just assume that $\mathbf{E}$ is known at the time $(n + 1/2) \cdot \Delta t$ which is perfect to update $\mathbf{B}$ from $n \cdot \Delta t$ to $(n + 1) \cdot \Delta t$ and will concentrate on the spatial derivatives.

The curl of the electric field $\nabla \times \mathbf{E}$ is given by

$$\nabla \times \mathbf{E} = \left(\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z}, \frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x}, \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right) \quad . \tag{19}$$

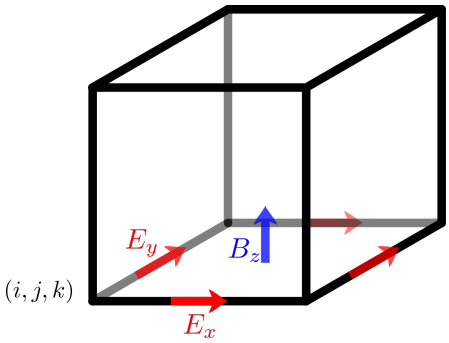
To eliminate repetition let's concentrate on the z component of $\nabla \times \mathbf{E}$ that is necessary to update B_z, the other two components work analogously. For this representative component we need finite difference approximations of partial derivatives such as $\partial E_x / \partial y$. In the easiest case we can just use

$$\frac{\partial E_x}{\partial y} \approx \frac{E_x \left(i \cdot \Delta x, (j + 1/2) \cdot \Delta y, (k - 1/2) \cdot \Delta z\right) - E_x \left(i \cdot \Delta x, (j - 1/2) \cdot \Delta y, (k - 1/2) \cdot \Delta z\right)}{\Delta y} \tag{20}$$

and

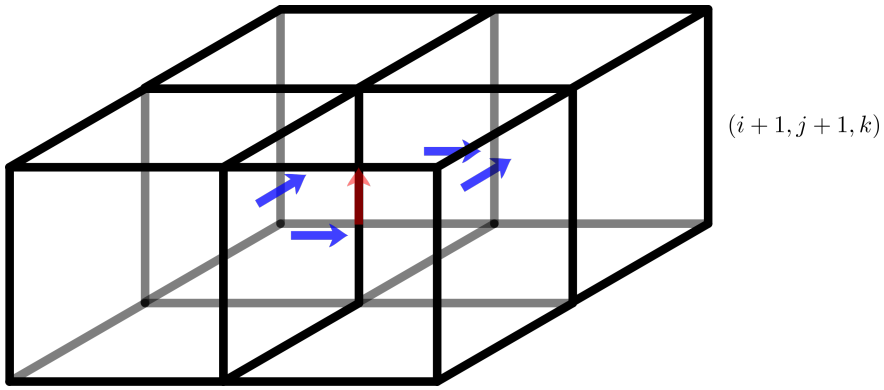
$$\frac{\partial E_y}{\partial x} \approx \frac{E_y \left((i + 1/2) \cdot \Delta x, j \cdot \Delta y, (k - 1/2) \cdot \Delta z\right) - E_y \left((i - 1/2) \cdot \Delta x, j \cdot \Delta y, (k - 1/2) \cdot \Delta z\right)}{\Delta x} \quad . \tag{21}$$

While the chosen locations look compliated at first they are just the value of E_x in cells (i, j, k) and $(i+1, j, k)$ as well as the value of E_y in cells (i, j, k) and $(i, j+1, k)$ which are readily available. And the finite difference approximation might look crude, but gives a good estimate for $(\nabla \times \mathbf{E})_z$ at $(i \cdot \Delta x, j \cdot \Delta y, (k - 1/2) \cdot \Delta z)$, which is exactly the location of B_z, as illustrated below:



Graphically we compute the curl by walking in a little closed loop around the field component for which the curl in needed in the field update.

And the great thing about the interleaved dual meshes with offset field components is, that this also works for $\nabla \times \mathbf{B}$, that is needed to update $\mathbf{E}$.



We can rewrite Ampere's equation from the form in Eq. (14) to

$$\mathbf{E}^{n+1/2} = \mathbf{E}^{n-1/2} + [\nabla \times \mathbf{B} - \mathbf{J}^n] \cdot \Delta t \quad . \tag{22}$$

The current density $\mathbf{J}$ is located where the electric field $\mathbf{E}$ is located as well and we can again approximate $\nabla \times \mathbf{B}$ by performing the walk along a little closed loop.

7 Diagnostics

After this (not so) short introduction to the finite-difference time-domain method and the wonders of the dual, staggered grids for electric and magnetic fields, let's consider how this influences the diagnostics we have been talking about so far. I will attempt to show how to implement the simplest version of each diagnostic (that ignores all the complications introduced by the staggered grids), as well as the next higher order that respects the staggering. Higher order implementations that try to queeze even more details out of the output by using even higher order stencils are beyond the scope of this write up.

7.1 Total Current

In this diagnositic the goal is to add the current from the electrons $\mathbf{J_e}$ with components $(J_{e,x}, J_{e,y}, J_{e,z})$ to the current of the ions $\mathbf{J_i}$ with components $(J_{i,x}, J_{i,y}, J_{i,z})$ to obtain the total current J_t. The x component of all currents is of course located at the same grid location, so the staggered mesh does not affect this diagnostic and we can simply calculate

$$\begin{aligned} J_{t,x} &= J_{e,x} + J_{i,x} \quad , \\ J_{t,y} &= J_{e,y} + J_{i,y} \quad , \\ J_{t,z} &= J_{e,z} + J_{i,z} \end{aligned}$$

element by element. Even opening two different hydro files for input and writing to a third file should be very straight forward.

7.2 Absolute Value of Current

In the naive version of this diagnostic we would compute

$$|J| = \sqrt{J_{t,x}^2 + J_{t,y}^2 + J_{t,z}^2} \tag{23}$$

element by element. This should still be straight forward.

If we are more careful we not that the three components of the current are not co-located by displaces by to the middle of the edges, just like the components of the electric field. Before adding them together we should interpolate them to a common location. The typical and sensible location is the bottom, left, front corner of the cell[4].

[4] This would also be a good location for charge density, because it would be easy to calculate the divergence of the current at that location.

So we should calculate

$$\begin{aligned}
\hat{j}_x = J_{t,x}((i-1/2)\cdot\Delta x,&(j-1/2)\cdot\Delta y,(k-1/2)\cdot\Delta z) = \\
&\frac{1}{2}\big[J_{t,x}((i-1)\cdot\Delta x,(j-1/2)\cdot\Delta y,(k-1/2)\cdot\Delta z + \\
&\quad J_{t,x}(i\cdot\Delta x,(j-1/2)\cdot\Delta y,(k-1/2)\cdot\Delta z\big] \\
\hat{j}_y = J_{t,y}((i-1/2)\cdot\Delta x,&(j-1/2)\cdot\Delta y,(k-1/2)\cdot\Delta z) = \\
&\frac{1}{2}\big[J_{t,y}((i-1/2)\cdot\Delta x,(j-1)\cdot\Delta y,(k-1/2)\cdot\Delta z + \\
&\quad J_{t,y}((i-1/2)\cdot\Delta x,j\cdot\Delta y,(k-1/2)\cdot\Delta z\big] \\
\hat{j}_z = J_{t,z}((i-1/2)\cdot\Delta x,&(j-1/2)\cdot\Delta y,(k-1/2)\cdot\Delta z) = \\
&\frac{1}{2}\big[J_{t,z}((i-1/2)\cdot\Delta x,(j-1/2)\cdot\Delta y,(k-1)\cdot\Delta z + \\
&\quad J_{t,z}((i-1/2)\cdot\Delta x,(j-1/2)\cdot\Delta y,k\cdot\Delta z\big]
\end{aligned}$$

and then get the absolute value of the current using

$$|J| = \sqrt{\hat{j}_x^2 + \hat{j}_y^2 + \hat{j}_z^2} \quad . \tag{24}$$

Two implementation details: It is possible to never explicitly calculate the average and instead get $|J|$ as half the square root of the squares of the current components at the relevant six locations. For the cells at the front, left and bottom boundary, where we can not access the neighbouring cell that we need to reinterpolate, it is ok to go back to the naive calculate shown in Eq. (23).

7.3 RMS Fluctuations of the Absolute Value of the Current

This diagnostic is tricky, regardless of the grid location issues discussed in this document as it needs a total reduction over the entire domain.

The quantity we are interested in can be defined as

$$j_{rms} = \frac{1}{\sum_{i,j,k} 1}\sqrt{\sum_{i,j,k} J_{t,x}^2 + J_{t,y}^2 + J_{t,z}^2} \tag{25}$$

and is noting but the root-mean-square of $|J|$. The factor in front of the square root just calculates the number of grid cells N.

The more careful version of this diagnostic would use the properly co-located components $\hat{j}_x$, $\hat{j}_y$ and $\hat{j}_z$ instead of the raw components of each cell.

7.4 Work done by Particles

The work done by particles and thus energy that is transferred from the particles to the electromagnetic field is given by the scalar product of the (total) current density $\mathbf{J}_t$ and the electric field $\mathbf{E}$

$$\begin{aligned} D &= \mathbf{j} \cdot \mathbf{E} \\ &= J_{t,x}E_x + J_{t,y}E_y + J_{t,z}E_z \quad . \end{aligned} \tag{26}$$

In some cases it might also make sense to calulate D separately for electrons and ions, i.e. use the current from their respective hydro outputs, instead of forming the total current $\mathbf{J}_t$ first. Either way we do not have any extra complications introduced by the grid here as $\mathbf{J}$ and $\mathbf{E}$ are co-located.

7.5 Parallel Electric Field

Parallel in this context means parallel to the local magnetic field. So in other words we are looking for the component of the electric field along the magnetic field. If we ignore the complications due to the grid, this is given by

$$E_\parallel = \frac{E_x B_x + E_y B_y + E_Z B_Z}{\sqrt{B_x^2 + B_y^2 + B_z^2}} \quad . \tag{27}$$

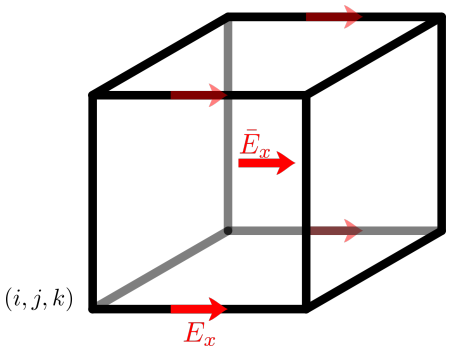
This requires to read all six components of the field output and write a new scalar quantity to the output and can be done on a point-by-point basis.

The problem is that in the actual grid none of the six components are co-located and it is not even clear to which location in the grid one would want to reinterpolate. One could interpolate the electric field to the corner of the cell, in the same way as it is done for the current in diagnostic 7.2 and average over four locations of each component of the magnetic field to also bring it to the corner of the cell. Below I instead decided to interpolate everything to the center of the cell, which is equivalent to the choise of $\epsilon_i = 0$ in sections 4 and 5.

For the electric field at the cell center we get

$$\begin{aligned} \bar{E}_x = E_x(i \cdot \Delta x, j \cdot \Delta y, k) \cdot \Delta z) = \\ \frac{1}{4}\big[E_x(i \cdot \Delta x, (j-1/2) \cdot \Delta y, (k-1/2) \cdot \Delta z) + \\ E_x(i \cdot \Delta x, (j+1/2) \cdot \Delta y, (k-1/2) \cdot \Delta z) + \\ E_x(i \cdot \Delta x, (j-1/2) \cdot \Delta y, (k+1/2) \cdot \Delta z) + \\ E_x(i \cdot \Delta x, (j+1/2) \cdot \Delta y, (k+1/2) \cdot \Delta z)\big] \end{aligned} \tag{28}$$

which can be illustraded by



Analogously we get

$$\begin{aligned}\bar{E}_y = E_y(i\cdot\Delta x, j\cdot\Delta y, k)\cdot\Delta z) = \\ \frac{1}{4}\big[E_y((i-1/2)\cdot\Delta x, j\cdot\Delta y, (k-1/2)\cdot\Delta z)+ \\ E_y((i+1/2)\cdot\Delta x, j\cdot\Delta y, (k-1/2)\cdot\Delta z)+ \\ E_y((i-1/2)\cdot\Delta x, j\cdot\Delta y, (k+1/2)\cdot\Delta z)+ \\ E_y((i+1/2)\cdot\Delta x, j\cdot\Delta y, (k+1/2)\cdot\Delta z)\big]\end{aligned} \tag{29}$$

and

$$\begin{aligned}\bar{E}_z = E_z(i\cdot\Delta x, j\cdot\Delta y, k)\cdot\Delta z) = \\ \frac{1}{4}\big[E_z((i-1/2)\cdot\Delta x, (j-1/2)\cdot\Delta y, k\cdot\Delta z)+ \\ E_z((i+1/2)\cdot\Delta x, (j-1/2)\cdot\Delta y, k\cdot\Delta z)+ \\ E_z((i-1/2)\cdot\Delta x, (j+1/2)\cdot\Delta y, k\cdot\Delta z)+ \\ E_z((i+1/2)\cdot\Delta x, (j+1/2)\cdot\Delta y, k\cdot\Delta z)\big]\end{aligned} \tag{30}$$

for the other two components.

For the magnetic field interpolations is somewhat simpler as we only need to average over the two components at the lower and upper interface of the cell in each direction to get that component of the magnetic field at the center. In terms of algebra that is

$$\begin{aligned}\bar{B}_x = B_x(i\cdot\Delta x, j\cdot\Delta y, k)\cdot\Delta z) = \\ \frac{1}{2}\big[B_x(i-1/2)\cdot\Delta x, j\cdot\Delta y, k\cdot\Delta z)+ \\ B_x(i+1/2)\cdot\Delta x, j\cdot\Delta y, k\cdot\Delta z)\big]\end{aligned} \tag{31}$$

$$\begin{aligned}\bar{B}_y = B_y(i\cdot\Delta x, j\cdot\Delta y, k)\cdot\Delta z) = \\ \frac{1}{2}\big[B_y(i\cdot\Delta x, (j-1/2)\cdot\Delta y, k\cdot\Delta z)+ \\ B_y(i\cdot\Delta x, (j+1/2)\cdot\Delta y, k\cdot\Delta z)\big]\end{aligned} \tag{32}$$

$$\begin{aligned}\bar{B}_z = B_z(i\cdot\Delta x, j\cdot\Delta y, k)\cdot\Delta z) = \\ \frac{1}{2}\big[B_z(i\cdot\Delta x, j\cdot\Delta y, (k-1/2)\cdot\Delta z)+ \\ B_z(i\cdot\Delta x, j\cdot\Delta y, (k+1/2)\cdot\Delta z)\big]\end{aligned} \tag{33}$$

In term of the field components at the center of the cell, the parallel electric field there is

$$\bar{E}_{\parallel} = \frac{\bar{E}_x\bar{B}_x + \bar{E}_y\bar{B}_y + \bar{E}_z\bar{B}_z}{\sqrt{\bar{B}_x^2 + \bar{B}_y^2 + \bar{B}_z^2}} \quad . \tag{34}$$

7.6 Local Fields for a particle

For each particle we know the cell (i, j, k) that contains the particles, as well as the fractional position d_x, d_y, and d_z in that cell, where $d_i \in [-1; 1]$[5].

The electric field $E_{p,x}$ is the given by

$$\begin{aligned}\bar{E}_{p,x} =& \frac{1-d_y}{2}\frac{1-d_z}{2}E_x(i\cdot\Delta x, (j-1/2)\cdot\Delta y, (k-1/2)\cdot\Delta z) + \\ & \frac{1+d_y}{2}\frac{1-d_z}{2}E_x(i\cdot\Delta x, (j+1/2)\cdot\Delta y, (k-1/2)\cdot\Delta z) + \\ & \frac{1-d_y}{2}\frac{1+d_z}{2}E_x(i\cdot\Delta x, (j-1/2)\cdot\Delta y, (k+1/2)\cdot\Delta z) + \\ & \frac{1+d_y}{2}\frac{1+d_z}{2}E_x(i\cdot\Delta x, (j+1/2)\cdot\Delta y, (k+1/2)\cdot\Delta z) \quad .\end{aligned} \tag{35}$$

At this point we should not that the interpolation in diagnostic 7.5 is just the special case with $d_x = d_y = d_z = 0$, which denotes the center of the cell. We should also note that VPIC interpolates to the location of the particle differently, by computing $\bar{E}_x$ and $\partial\, E_x/\partial y$, $\partial\, E_x/\partial z$ and $\partial^2\, E_x/\partial y\partial z$ at the cell center first and then interpolates using

$$\bar{E}_{p,x} = \bar{E}_x + d_y\cdot\frac{\partial\, E_x}{\partial y} + d_z\cdot\left(\frac{\partial\, E_x}{\partial z} + d_y\cdot\frac{\partial^2\, E_x}{\partial y\partial z}\right) \quad . \tag{36}$$

As far as I can tell this is purely done for performance and should give identical results and stability to the method in Eq. (35).

[5] Contrary to what most other codes used and what was used in section 4 and 5 the fractional part is not limited to $[-1/2; 1/2]$ but uses the range $[-1; 1]$, which introduces a bunch of factors $1/2$ in the following equations.

The other two components of the electric field can interpolated similarily:

$$\begin{aligned}\bar{E}_{p,y} =& \frac{1-d_x}{2}\frac{1-d_z}{2}E_y((i-1/2)\cdot\Delta x, j\cdot\Delta y, (k-1/2)\cdot\Delta z) + \\ & \frac{1+d_x}{2}\frac{1-d_z}{2}E_y((i+1/2)\cdot\Delta x, j\cdot\Delta y, (k-1/2)\cdot\Delta z) + \\ & \frac{1-d_x}{2}\frac{1+d_z}{2}E_y((i-1/2)\cdot\Delta x, j\cdot\Delta y, (k+1/2)\cdot\Delta z) + \\ & \frac{1+d_x}{2}\frac{1+d_z}{2}E_y((i+1/2)\cdot\Delta x, j\cdot\Delta y, (k+1/2)\cdot\Delta z) \quad . \end{aligned} \tag{37}$$

$$\begin{aligned}\bar{E}_{p,z} =& \frac{1-d_x}{2}\frac{1-d_y}{2}E_x((i-1/2)\cdot\Delta x, (j-1/2)\cdot\Delta y, k\cdot\Delta z) + \\ & \frac{1+d_x}{2}\frac{1-d_y}{2}E_x((i+1/2)\cdot\Delta x, (j+1/2)\cdot\Delta y, k\cdot\Delta z) + \\ & \frac{1-d_x}{2}\frac{1+d_y}{2}E_x((i-1/2)\cdot\Delta x, (j-1/2)\cdot\Delta y, k\cdot\Delta z) + \\ & \frac{1+d_x}{2}\frac{1+d_y}{2}E_x((i+1/2)\cdot\Delta x, (j+1/2)\cdot\Delta y, k\cdot\Delta z) \quad . \end{aligned} \tag{38}$$

For the magnetic field again only two components have to be interpolated

$$\begin{aligned}\bar{B}_{p,x} =& \frac{1-d_x}{2}B_x((i-1/2)\cdot\Delta x, j\cdot\Delta y, k\cdot\Delta z) + \\ & \frac{1+d_x}{2}B_x((i+1/2)\cdot\Delta x, j\cdot\Delta y, k\cdot\Delta z) \quad , \end{aligned} \tag{39}$$

$$\begin{aligned}\bar{B}_{p,y} =& \frac{1-d_y}{2}B_y(i\cdot\Delta x, (j-1/2)\cdot\Delta y, k\cdot\Delta z) + \\ & \frac{1+d_y}{2}B_y(i\cdot\Delta x, (j+1/2)\cdot\Delta y, k\cdot\Delta z) \quad , \end{aligned} \tag{40}$$

and

$$\begin{aligned}\bar{B}_{p,z} =& \frac{1-d_z}{2}B_z(i\cdot\Delta x, j\cdot\Delta y, (k-1/2)\cdot\Delta z) + \\ & \frac{1+d_z}{2}B_z(i\cdot\Delta x, j\cdot\Delta y, (k+1/2)\cdot\Delta z) \quad . \end{aligned} \tag{41}$$

VPIC itself again does the interpolation to the particle location by computing $\bar{B}_i$ and $\partial B_i/\partial i$ at the cell center and then uses

$$\bar{B}_{p,i} = \bar{B}_i + d_i \cdot \frac{\partial B_i}{\partial i} \quad , \tag{42}$$

but not numerical necessity for that is visible.

7.7 Parallel Electric Field at Particle Positions

Once the field components are interpolated to the location of the particle, as per diagnostic 7.6, it is straight forwards to calculate the local electric field there:

$$\bar{E}_{p,\parallel} = \frac{\bar{E}_{p,x}\bar{B}_{p,x} + \bar{E}_{p,y}\bar{B}_{p,y} + \bar{E}_{p,z}\bar{B}_{p,z}}{\sqrt{\bar{B}_{p,x}^2 + \bar{B}_{p,y}^2 + \bar{B}_{p,z}^2}} \quad . \tag{43}$$

7.8 Magnetic Fieldlines

Magnetic field lines follow the magnetic field. This can either be seen as tautological or as the definition of a field line. To make a more useful statement we can restate the condition in the following way:

A fieldline that goes through point $\mathbf{x}_1 = (x_1, y_1, y_2)$ where the magnetic field is $\mathbf{b} = (b_x, b_y, b_z)$ will also go through point $\mathbf{x}_2 = (x_2, y_2, z_2) = (x_1 + d_x, y_1 + d_y, z_1 + d_z)$. The infinitesimal steps d_x, d_y and d_z are related to the magnetic field by the condition

$$\frac{d_x}{b_x} = \frac{d_y}{b_y} = \frac{d_z}{b_z} \quad . \tag{44}$$

So if we want to trace a field line from a starting point, we can interpolate the magnetic field to that point and calculate

$$d_x = \frac{b_x}{\sqrt{b_x^2 + b_y^2 + b_z^2}} \cdot \Delta \tag{45}$$

$$d_y = \frac{b_y}{\sqrt{b_x^2 + b_y^2 + b_z^2}} \cdot \Delta \tag{46}$$

$$d_z = \frac{b_s}{\sqrt{b_x^2 + b_y^2 + b_z^2}} \cdot \Delta \tag{47}$$

and then move from the starting point by a distance d_x, d_y, d_z to the next point. There, we interpolate the magnetic field again, determine new d_x, d_y, d_z and continute the process. The parameter Δ sets the step length and will typically be a small fraction (10^{-3} to 10^{-1}) of a cell size.

If ArrayUDF is a good fit for this type of analysis, we might want to perform this for thousands of field lines (this is where the parallelism in ArrayUDF might come in) and using a Runge-Kutta type integration instead of the simple Euler type integration given in Eqs. (45)-(47).