Implicit centered symmetric scheme for thermal conduction in MHD

In MHD calculations, writing an implicit scheme for anisotropic heat conduction is not an easy task. As we'll show later, the heat conduction cannot be expressed as a global function in the anisotropic nonlinear conduction case. The implicit centered symmetric scheme satisfies the self adjointness at cell corners and has the desirable property that the perpendicular numerical diffusion is independent of the conductivity ratio. Moreover, it allows large time steps.

1. General Equation

The general heat conduction equation can be written as:

$$\frac{\partial T}{\partial t} = -\nabla \bullet q \quad (1)$$

where $q = -\vec{b}n(\kappa_{\|} - \kappa_{\perp})\vec{b}\bullet\nabla T - n\kappa_{\perp}\nabla T$ (2)

b are the unit vector pointing on the field direction, κ are the thermal conductivities along and perpendicular to the field direction, n is the number density of particles. In our calculation, $\kappa_{\|}$ and $\kappa_{\perp}$ should be considered as analytic functions of T.

2. The simplest case and Crank Nicholson scheme

The simplest case is the isotropic diffusion. In this case, we can write $\kappa_{\|} = \kappa_{\perp} = \kappa$, the equation then becomes:

$$\frac{\partial T}{\partial t} = \nabla \bullet(\kappa\nabla T)$$

here n is grouped into κ . In this case, T at each grid points can be solved directly using implicit scheme. Consider z as a function of T that satisfies:

$$z = \int \kappa \, dT$$

We can then write the equation as:

$$\frac{\partial T}{\partial t} = \nabla^2 z$$

Now take the difference at point (i,j), we get:

$$\frac{T_{i,j}^{m+1} - T_{i,j}^{m}}{dt} = \frac{z_{i+1,j}^{m+1/2} - 2z_{i,j}^{m+1/2} + z_{i-1,j}^{m+1/2}}{dx^2} + \frac{z_{i,j+1}^{m+1/2} - 2z_{i,j}^{m+1/2} + z_{i,j-1}^{m+1/2}}{dy^2} \quad (3)$$

here the superscripts and subscripts indicates time step and grids, respectively. The time step m+1/2 are present because we are using an implicit Crank Nicholson scheme:

$$z_{i,j}^{m+1/2} = \frac{z_{i,j}^{m} + z_{i,j}^{m+1}}{2}$$

A more general scheme can be derived by considering putting in a relaxation factor w:

$$z_{i,j}^{m+1/2} = wz_{i,j}^{m} + (1-w)z_{i,j}^{m+1}$$

or other ways of averaging over the two time steps. The above equation involves T at time steps m and m+1, where time step m values are known but time step m+1 values are to be solved. Since z are just functions of T, we therefore have an equation set that only involves T at time steps m+1 as unknowns. Unfortunately, since z in most cases are nonlinear functions of T, this equation set is nonlinear and not easy to solve. To linearize the equations, we can do a Taylor expansion on z:

$$z_{i,j}^{m+1/2} = wz_{i,j}^{m} + (1-w)z_{i,j}^{m+1} = wz_{i,j}^{m} + (1-w)[z_{i,j}^{m} + (\frac{\partial z}{\partial T})_{i,j}^{m}(T_{i,j}^{m+1} - T_{i,j}^{m})]$$

but remember that we have:

$$z = \int \kappa \, dT$$

Thus we get:

$$z_{i,j}^{m+1/2} = wz_{i,j}^{m} + (1-w)[z_{i,j}^{m} + \kappa_{i,j}^{m}(T_{i,j}^{m+1} - T_{i,j}^{m})]$$

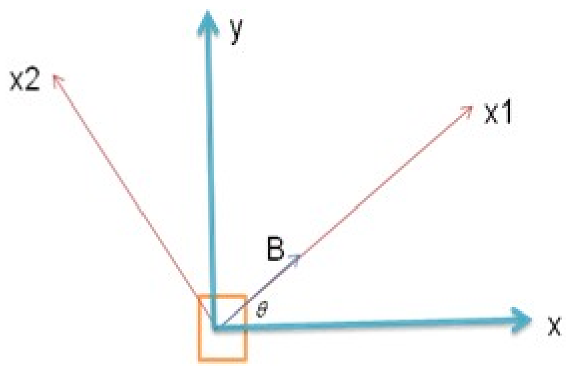
This is a linear function of T. Substituting this expression into (3), we then get an linear equation that involves T at grids (i,j), (i+1,j), (i,j+1), (i-1,j), (i,j-1). By putting the corresponding coefficients into the linear solver, we can solve this equation system to get the solution at t=m+1.

3. Difficulty in an anisotropic case

Things becomes more difficult in the anisotropic case. Consider the general equation (2), this equation can be equivalently written as:

$$\vec{q} = \vec{q}_{\parallel} + \vec{q}_{\perp} = -\kappa_{\parallel}(\nabla T)_{\parallel} - \kappa_{\perp}(\nabla T)_{\perp}$$

Now let's look at what happens when doing the differentials. Let's first define a local coordinate aligned with the B field as shown in graph (1).



graph (1)

Then we have:

$$\vec{q} = -\kappa_{\parallel}\frac{\partial T}{\partial x_1}\hat{x}_1 - \kappa_{\perp}\frac{\partial T}{\partial x_2}\hat{x}_2$$

This is just:

$$\vec{q} = -\kappa_{\parallel}(\frac{\partial T}{\partial x}\frac{\partial x}{\partial x_1} + \frac{\partial T}{\partial y}\frac{\partial y}{\partial x_1})\hat{x}_1 - \kappa_{\perp}(\frac{\partial T}{\partial x}\frac{\partial x}{\partial x_2} + \frac{\partial T}{\partial y}\frac{\partial y}{\partial x_2})\hat{x}_2$$

Using the coordinate transform we have the rotation:

$$\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

from the new coordinate to (x,y). Thus:

$$\vec{q} = -\kappa_{\parallel}(\frac{\partial T}{\partial x}\cos\theta + \frac{\partial T}{\partial y}\sin\theta)(\cos\theta\hat{x} + \sin\theta\hat{y}) - \kappa_{\perp}(\frac{\partial T}{\partial x}(-\sin\theta) + \frac{\partial T}{\partial y}\cos\theta)(-\sin\theta\hat{x} + \cos\theta\hat{y})$$

$$= (-\kappa_{\parallel}\frac{\partial T}{\partial x}\cos^2\theta - \kappa_{\parallel}\frac{\partial T}{\partial y}\sin\theta\cos\theta - \kappa_{\perp}\frac{\partial T}{\partial x}\sin^2\theta + \kappa_{\perp}\frac{\partial T}{\partial y}\cos\theta\sin\theta)\hat{x}$$

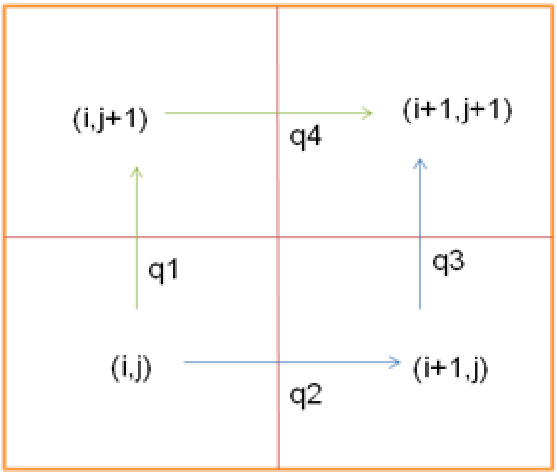
$$+(-\kappa_{\parallel}\frac{\partial T}{\partial x}\cos\theta\sin\theta - \kappa_{\parallel}\frac{\partial T}{\partial y}\sin^2\theta + \kappa_{\perp}\frac{\partial T}{\partial x}\sin\theta\cos\theta - \kappa_{\perp}\frac{\partial T}{\partial y}\cos^2\theta)\hat{y}$$

Substituting into equation (1), we then get:

$$\frac{\partial T}{\partial t} = -\frac{\partial}{\partial x}(\kappa_{\parallel}\frac{\partial T}{\partial x}\cos^2\theta) - \frac{\partial}{\partial y}(\kappa_{\parallel}\frac{\partial T}{\partial y}\sin^2\theta) - \frac{\partial}{\partial x}(\kappa_{\perp}\frac{\partial T}{\partial x}\sin^2\theta) - \frac{\partial}{\partial y}(\kappa_{\perp}\frac{\partial T}{\partial y}\cos^2\theta)$$

$$+[-\frac{\partial}{\partial y}(\kappa_{\parallel}\frac{\partial T}{\partial x}\cos\theta\sin\theta) - \frac{\partial}{\partial x}(\kappa_{\parallel}\frac{\partial T}{\partial y}\sin\theta\cos\theta) + \frac{\partial}{\partial y}(\kappa_{\perp}\frac{\partial T}{\partial x}\sin\theta\cos\theta) + \frac{\partial}{\partial x}(\kappa_{\perp}\frac{\partial T}{\partial y}\cos\theta\sin\theta)]$$

Notice the term in the bracket, this term is nonzero when the conductivity is anisotropic. When the conductivities on the two directions are two universal constants, the cross terms can still exist. These cross terms are caused by the transverse flux which is illustrated by graph (2). In this graph we can see that the total heat flowing into grid (i+1, j+1) is different depending on the path chosen.



graph(2)

Since the heat transfer is anisotropic, q1, q2, q3, q4 do not equal each other. Thus the result at i+1, j+1 depends on the actual path by which the energy is transferred. If the problem is isotropic, we have q1=q2, q3=q4, then these two paths are equivalent, the transport does not depend on the path, we end up getting a Laplacian for the source term. If the conductivity is not locally dependent, we have q1=q3, q2=q4, again the transport is path independent.

In summary, in the nonlinear anisotropic case, it is impossible to write the source term into a Laplacian, we are therefore forced to calculate the fluxes at each interfaces.

4. implicit centered symmetric scheme

Let's look at the heat flux on x direction. Using equation (3), the x direction flux should be:

$$q_x = -b_x n(\kappa_{\|} - \kappa_{\perp})(b_x \frac{\partial T}{\partial x} + b_y \frac{\partial T}{\partial y}) - n\kappa_{\perp}\frac{\partial T}{\partial x} \quad (4)$$

This flux exist at (i+1/2, j), (i+1/2, j+1) and so on.

To calculate this flux at (i+1/2, j), we first calculate the corner value, i.e. the flux at (i+1/2, j+1/2). (From now on (i+1/2, j) will be written as (1/2, 0) for convenience.)

Here we should first expand the expression into a form for which linear Taylor expansion is possible. As before, we define:

$z_1 = \int \kappa_{\|} dT$, $z_2 = \int \kappa_{\perp} dT$

Expanding equation (4), we get:

$$q_x = -b_x n(b_x \frac{\partial z_{\|}}{\partial x} + b_y \frac{\partial z_{\|}}{\partial y}) - b_y n(b_y \frac{\partial z_{\perp}}{\partial x} - b_x \frac{\partial z_{\perp}}{\partial x})$$

here bx, by, n should be evaluated using interpolation:

$$b_{x,1/2,1/2} = (b_{x,1/2,0} + b_{x,1/2,1})/2$$

$$b_{y,1/2,1/2} = (b_{y,0,1/2} + b_{y,1,1/2})/2$$

$$\frac{4}{n_{1/2,1/2}} = \frac{1}{n_{0,0}} + \frac{1}{n_{1,0}} + \frac{1}{n_{0,1}} + \frac{1}{n_{1,1}}$$

The fluxes

$$(\frac{\partial z}{\partial x})_{1/2,1/2} = \frac{z_{1,0} - z_{0,0} + z_{1,1} - z_{0,1}}{2dx}$$

$$(\frac{\partial z}{\partial y})_{1/2,1/2} = \frac{z_{0,1} - z_{0,0} + z_{1,1} - z_{1,0}}{2dy}$$

Substituting everything into (4), we get:

$$q_{x,1/2,1/2} = -b_{x,1/2,1/2} n_{1/2,1/2} (b_{x,1/2,1/2} \frac{z_{\|1,0} - z_{\|0,0} + z_{\|1,1} - z_{\|0,1}}{2dx} + b_{y,1/2,1/2} \frac{z_{\|0,1} - z_{\|0,0} + z_{\|1,1} - z_{\|1,0}}{2dy})$$
$$- b_{y,1/2,1/2} n_{1/2,1/2} (b_{y,1/2,1/2} \frac{z_{\perp 1,0} - z_{\perp 0,0} + z_{\perp 1,1} - z_{\perp 0,1}}{2dx} - b_{x,1/2,1/2} \frac{z_{\perp 0,1} - z_{\perp 0,0} + z_{\perp 1,1} - z_{\perp 1,0}}{2dy}) \quad (5)$$

Keep in mind that z are unknown which can be written as

$$z_{i,j} = wz^m_{i,j} + (1-w)z^{m+1}_{i,j} = wz^m_{i,j} + (1-w)[z^m_{i,j} + \kappa^m_{i,j}(T^{m+1}_{i,j} - T^m_{i,j})] \quad (6)$$

Equation (5) with (6) is the final form of linearized difference scheme. Similarly, we can calculate heat flux on y direction.

With the heat fluxes at corners (1/2,1/2),(1/2,-1/2),(-1/2,1/2) and (-1/2,-1/2) calculated, we can get the fluxes at the surfaces:

$$q_{x,1/2,0} = (q_{x,1/2,1/2} + q_{x,1/2,-1/2})/2$$

$$q_{x,-1/2,0} = (q_{x,-1/2,1/2} + q_{x,-1/2,-1/2})/2$$

$$q_{y,0,1/2} = (q_{y,1/2,1/2} + q_{y,-1/2,1/2})/2$$

$$q_{y,0,-1/2} = (q_{y,1/2,-1/2} + q_{y,-1/2,-1/2})/2$$

They are:

$$q_{x,1/2,0} = -\frac{b_{x,1/2,1/2} n_{1/2,1/2}}{2}(b_{x,1/2,1/2}\frac{z_{\parallel 1,0}-z_{\parallel 0,0}+z_{\parallel 1,1}-z_{\parallel 0,1}}{2dx} + b_{y,1/2,1/2}\frac{z_{\parallel 0,1}-z_{\parallel 0,0}+z_{\parallel 1,1}-z_{\parallel 1,0}}{2dy})$$
$$-\frac{b_{y,1/2,1/2} n_{1/2,1/2}}{2}(b_{y,1/2,1/2}\frac{z_{\perp 1,0}-z_{\perp 0,0}+z_{\perp 1,1}-z_{\perp 0,1}}{2dx} - b_{x,1/2,1/2}\frac{z_{\perp 0,1}-z_{\perp 0,0}+z_{\perp 1,1}-z_{\perp 1,0}}{2dy})$$
$$-\frac{b_{x,1/2,-1/2} n_{1/2,-1/2}}{2}(b_{x,1/2,-1/2}\frac{z_{\parallel 1,-1}-z_{\parallel 0,-1}+z_{\parallel 1,0}-z_{\parallel 0,0}}{2dx} + b_{y,1/2,-1/2}\frac{z_{\parallel 0,0}-z_{\parallel 0,-1}+z_{\parallel 1,0}-z_{\parallel 1,-1}}{2dy})$$
$$-\frac{b_{y,1/2,-1/2} n_{1/2,-1/2}}{2}(b_{y,1/2,-1/2}\frac{z_{\perp 1,-1}-z_{\perp 0,-1}+z_{\perp 1,0}-z_{\perp 0,0}}{2dx} - b_{x,1/2,-1/2}\frac{z_{\perp 0,0}-z_{\perp 0,-1}+z_{\perp 1,0}-z_{\perp 1,-1}}{2dy})$$

$$q_{x,-1/2,0} = -\frac{b_{x,-1/2,1/2} n_{-1/2,1/2}}{2}(b_{x,-1/2,1/2}\frac{z_{\parallel 0,0}-z_{\parallel -1,0}+z_{\parallel 0,1}-z_{\parallel -1,1}}{2dx} + b_{y,-1/2,1/2}\frac{z_{\parallel -1,1}-z_{\parallel -1,0}+z_{\parallel 0,1}-z_{\parallel 0,0}}{2dy})$$
$$-\frac{b_{y,-1/2,1/2} n_{-1/2,1/2}}{2}(b_{y,-1/2,1/2}\frac{z_{\perp 0,0}-z_{\perp -1,0}+z_{\perp 0,1}-z_{\perp -1,1}}{2dx} - b_{x,-1/2,1/2}\frac{z_{\perp -1,1}-z_{\perp -1,0}+z_{\perp 0,1}-z_{\perp 0,0}}{2dy})$$
$$-\frac{b_{x,-1/2,-1/2} n_{-1/2,-1/2}}{2}(b_{x,-1/2,-1/2}\frac{z_{\parallel 0,-1}-z_{\parallel -1,-1}+z_{\parallel 0,0}-z_{\parallel -1,0}}{2dx} + b_{y,-1/2,-1/2}\frac{z_{\parallel -1,0}-z_{\parallel -1,-1}+z_{\parallel 0,0}-z_{\parallel 0,-1}}{2dy})$$
$$-\frac{b_{y,-1/2,-1/2} n_{-1/2,-1/2}}{2}(b_{y,-1/2,-1/2}\frac{z_{\perp 0,-1}-z_{\perp -1,-1}+z_{\perp 0,0}-z_{\perp -1,0}}{2dx} - b_{x,-1/2,-1/2}\frac{z_{\perp -1,0}-z_{\perp -1,-1}+z_{\perp 1,0}-z_{\perp 1,-1}}{2dy})$$

$$q_{y,0,1/2} = -\frac{b_{y,1/2,1/2} n_{1/2,1/2}}{2}(b_{x,1/2,1/2}\frac{z_{\parallel 1,0}-z_{\parallel 0,0}+z_{\parallel 1,1}-z_{\parallel 0,1}}{2dx} + b_{y,1/2,1/2}\frac{z_{\parallel 0,1}-z_{\parallel 0,0}+z_{\parallel 1,1}-z_{\parallel 1,0}}{2dy})$$
$$+\frac{b_{x,1/2,1/2} n_{1/2,1/2}}{2}(b_{y,1/2,1/2}\frac{z_{\perp 1,0}-z_{\perp 0,0}+z_{\perp 1,1}-z_{\perp 0,1}}{2dx} - b_{x,1/2,1/2}\frac{z_{\perp 0,1}-z_{\perp 0,0}+z_{\perp 1,1}-z_{\perp 1,0}}{2dy})$$
$$-\frac{b_{y,-1/2,1/2} n_{-1/2,1/2}}{2}(b_{x,-1/2,1/2}\frac{z_{\parallel 0,0}-z_{\parallel -1,0}+z_{\parallel 0,1}-z_{\parallel -1,1}}{2dx} + b_{y,-1/2,1/2}\frac{z_{\parallel -1,1}-z_{\parallel -1,0}+z_{\parallel 0,1}-z_{\parallel 0,0}}{2dy})$$
$$+\frac{b_{x,-1/2,1/2} n_{-1/2,1/2}}{2}(b_{y,-1/2,1/2}\frac{z_{\perp 0,0}-z_{\perp -1,0}+z_{\perp 0,1}-z_{\perp -1,1}}{2dx} - b_{x,-1/2,1/2}\frac{z_{\perp -1,1}-z_{\perp -1,0}+z_{\perp 0,1}-z_{\perp 0,0}}{2dy})$$

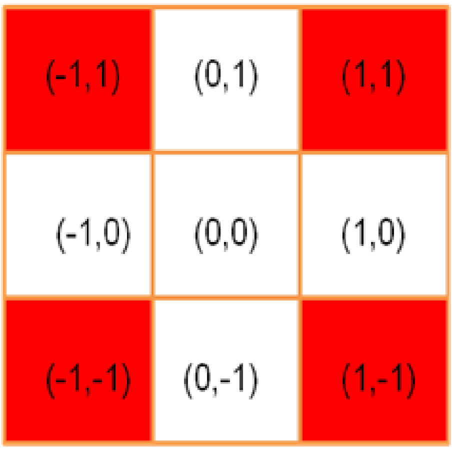
$$q_{y,0,-1/2} = -\frac{b_{y,1/2,-1/2} n_{1/2,-1/2}}{2} \left(b_{x,1/2,-1/2} \frac{z_{\|1,-1} - z_{\|0,-1} + z_{\|1,0} - z_{\|0,0}}{2dx} + b_{y,1/2,-1/2} \frac{z_{\|0,0} - z_{\|0,-1} + z_{\|1,0} - z_{\|1,-1}}{2dy}\right)$$

$$+ \frac{b_{x,1/2,-1/2} n_{1/2,-1/2}}{2} \left(b_{y,1/2,-1/2} \frac{z_{\perp 1,-1} - z_{\perp 0,-1} + z_{\perp 1,0} - z_{\perp 0,0}}{2dx} - b_{x,1/2,-1/2} \frac{z_{\perp 0,0} - z_{\perp 0,-1} + z_{\perp 1,0} - z_{\perp 1,-1}}{2dy}\right)$$

$$- \frac{b_{y,-1/2,-1/2} n_{-1/2,-1/2}}{2} \left(b_{x,-1/2,-1/2} \frac{z_{\|0,-1} - z_{\|-1,-1} + z_{\|0,0} - z_{\|-1,0}}{2dx} + b_{y,-1/2,-1/2} \frac{z_{\|-1,0} - z_{\|-1,-1} + z_{\|0,0} - z_{\|0,-1}}{2dy}\right)$$

$$+ \frac{b_{x,-1/2,-1/2} n_{-1/2,-1/2}}{2} \left(b_{y,-1/2,-1/2} \frac{z_{\perp 0,-1} - z_{\perp -1,-1} + z_{\perp 0,0} - z_{\perp -1,0}}{2dx} - b_{x,-1/2,-1/2} \frac{z_{\perp -1,0} - z_{\perp -1,-1} + z_{\perp 0,0} - z_{\perp 0,-1}}{2dy}\right)$$

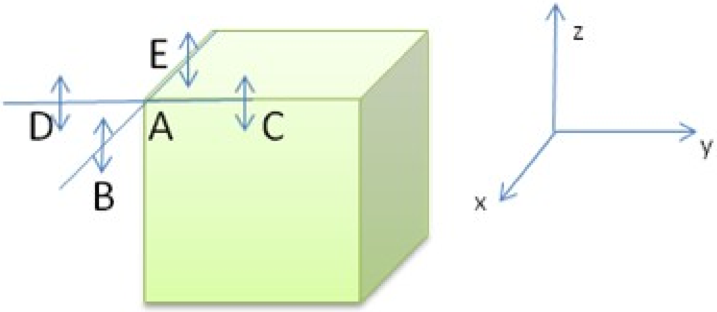
Now, by writing z as linear functions of T at time m+1, we can again get a set of linear equations. The stencil to be used in this case is shown in graph (3).



graph (3)

Here we see that in addition to the traditional cross shaped stencil, four corner cells (painted in red) are needed. This is exactly because in the anisotropic case, the transverse flux matters!

In a 3-D case, the symmetric problem works the same. Consider the cubic cell in graph (4). We first find out the flux at the eight corners: (1/2, 1/2, 1/2), (1/2, 1/2, -1/2) etc. For example, to get the z direction flux at point A, we should average over point B, C, D and E. After getting all of the corner fluxes, we can compute the fluxes at the centers of the edges, and finally average over the edges of a certain surface to get the flux into that surface.



graph (4)

5. AMR of the diffusion equation

To consider the AMR of the diffusion algorithm, we can start from the simplest case. Suppose that we have a discretized mesh shown in graph (5). In this mesh, (0,0) is on level 0, (3/4,-1/4) is on level 1, (9/8,-3/8) is on level 2. Let's look the discretized equation at (3/4,-1/4) in this case. The equation should be:

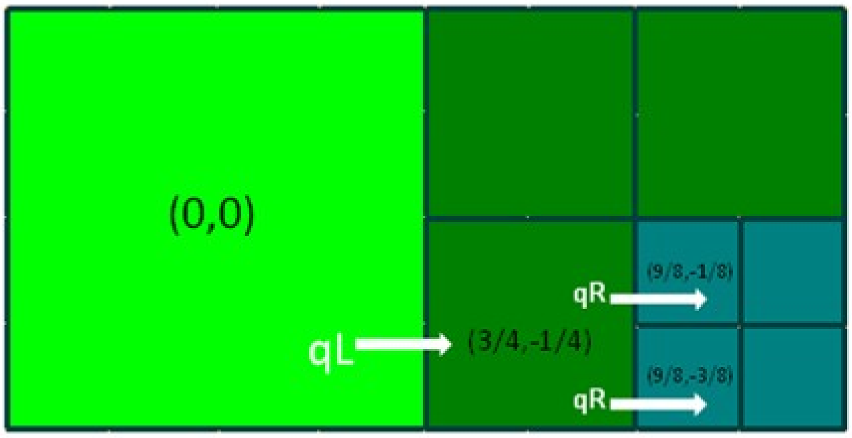
$$\frac{\partial T}{\partial t} = \nabla \bullet (\kappa \nabla T)$$

On the x direction, it's just:

$$\frac{T^1_{3/4,-1/4} - T^0_{3/4,-1/4}}{dt} = \frac{q_L - q_R}{9dx/16}$$

where q are the fluxes indicated in the graph. Positive means going right. qL is located 3/8 from

(3/4, -1/4), qR is located 3/16 from (3/4, -1/4).



graph (5)

So once we get the expression for q in this configuration, we can do the implicit calculation.

Again define z as:

$$z = \int \kappa \, dT$$

Then:

$$q = \nabla z$$

We can write down:

$$q_L = \frac{z_{0,0} - z_{3/4,-1/4}}{3dx/4}$$

$$q_R = \frac{z_{3/4,-1/4} - z_{9/8,-3/8}}{3dx/8} + \frac{z_{3/4,-1/4} - z_{9/8,-1/8}}{3dx/8}$$

here, z should be expanded into:

$$z_{i,j}^{m+1/2} = w z_{i,j}^{m} + (1-w) z_{i,j}^{m+1}$$

The m+1 time step z are nonlinear functions of the unknown T, thus we can linearize the equations by Taylor expansion to the first order.

In an anisotropic case, it is better to use a symmetric discretization. We first compute the corner fluxes, that would depend on the configuration of that corner. For example, point A in graph (5) is surrounded by cells of level 0,0,0 and 1. The flux in this case is different from the case when the corner is surrounded by cells of level 0, 0, 1, 1… and so on. Thus we need to determine different patterns that may surround a corner and find out the corner flux in each of the configuration. In 3D, there are 8 corners, each corner is surrounded by 8 cells, this makes the problem complicated (all of these cells has to be considered because the transverse fluxes, as we have shown before, cannot be ignored in an anisotropic case!).