PDE Poisson problem

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https://software.intel.com/en-us/forums/intel-math-kernel-library/topic/782777

To summarize, you want to solve the problem

$\Delta u = \nabla \cdot \vec{p}$ in $\Omega = [0,1]^3$
With boundary conditions
$u(\vec{x})$ periodic in x, y directions and 0-neumann in z direction

The specific p being used is the piecewise constant function
$\vec{p}(x,y,z) = [0,0,1]$ if $z > 1/2$
$\vec{p}(x,y,z) = [0,0,-1]$ if $z <= 1/2$

Note that the function $\vec{p}$ is technically not differentiable, but if we relax our requirements from functions to distributions , it has weak divergence equal to 2 * delta function along $z = 1/2$
($i.e. \quad div(\vec{p}) = 2\delta\left(z - \frac{1}{2}\right)$)

This could be done weakly using distributions and integration by parts, but may not work so well in the context of finite differences with explicit computation of divergence of p. You use a centered difference in the code based on component pz in direction z which essentially smears out the dirac delta function and perturbs the solution a little, but you may still obtain convergence to true solution with refinement of mesh...

The first thing we should do is to check that this system is well defined and consistent. A typical check is to integrate both sides of pde over domain and then use integration by parts (or multidimensional version of the same) to reduce to boundary integrals where we can use the bc data. We start with

$$\int_\Omega \Delta u \, d\,\vec{x} = \int_\Omega \nabla \cdot \vec{p} \, d\,\vec{x}\,.$$

Integrating both sides by parts against the implicit 1 function and simplifying, we obtain the requirement that

$$\int_{\partial\Omega} \nabla u \cdot \vec{n} \, d\,\vec{x} = \int_{\partial\Omega} \vec{p} \cdot \vec{n} \, d\,\vec{x}\,.$$

Notice that $\vec{n}$ is $\vec{p}$ on z boundaries so $\vec{p} \cdot \vec{n} = 1$ on z boundaries and $\vec{p} \cdot \vec{n} = 0$ on periodic boundaries. Simplifying, the rhs, this reduces to the weak requirement that

$$\int_{\partial\Omega} \nabla u \cdot \vec{n} \, d\,\vec{x} = 2.$$

The periodicity requirement says that u(0,y,z) is equal to u(1,y,z) so that (assuming that our solution is at least once differentiable,) we also have du/dx(0,y,z) = du/dx(1,y,z) and since $\vec{n} = [-1,0,0]$ for x=0 and $\vec{n} = [1,0,0]$ for x=1, $\nabla u(0,y,z) \cdot \vec{n}(0,y,z) = -\nabla u(1,y,z) \cdot \vec{n}(1,y,z)$. Thus the sum of integrals over x=0 and x=1 is 0. (We will see this issue again even in we assume only weak differentiability later)

Likewise u(x,0,z) = u(x,1,z) leads to the same conclusion for the y periodic boundaries.

Thus, our consistency requirement simplifies to

$$\int_{z=0} \nabla u \cdot \vec{n}\, d\,\vec{x} + \int_{z=1} \nabla u \cdot \vec{n}\, d\,\vec{x} \;= 2$$

But this cannot happen since we assumed $\nabla u \cdot \vec{n} = 0$ along z=0 and z=1. In otherwords, the system is not consistent as written and no possible solution exists. If we want both boundaries to have the same bc, the only recourse is to set the neumann boundary condition to be 1. There are many possiblilities if we don't assume they are constant and the same.

With neumann boundary condition = 1 on z boundaries, then this system is consistent and can admit a solution.

Let us now see if we can come up with a family of solutions to this system. We do not have a strong solution since divergence of p is not technically defined, but if we expand to weak solutions (assume p and u are distributions, not functions) to the pde, we can have a little wiggle room. (note 1: if you have used distributions, you may have seen something like this before in an applied analysis course. If not, then there is some fun reading and learning that you can do on your own :))

The Dirac delta function, the Heaviside or step function and the ramp function are weakly related by integration and differentiation. I will use without proof (see any text on distributions and weak derivatives from applied/functional analysis) that the Dirac delta function $\delta(x)$ is the weak derivative of the Heaviside or step function H(x) = 0 for x<0 = 1 for x>=0 which is the weak derivative of the ramp function max(0,x). Technically speaking this should all be done under integrals and multiplied by smooth test functions, but the idea is clear enough as is...

Your stated system can be written weakly as

$$\Delta u(x, y, z) = 2\,\delta(z - 1/2)$$

Which has weak gradient family of solutions with a scaled and shifted step function (or Heaviside function) in z component ie (= -1 for z<1/2 and 1 for z>1/2)

$$\nabla u \;=\; \left[\, a, b, 2H\left(z - \frac{1}{2}\right) - 1 \;+ c\right]$$

And a full family of weak solutions is the following:

$$u(x, y, z) = ax \;+ by \;+ \max\left(0, z - \frac{1}{2}\right) + \max\left(0, \frac{1}{2} - z\right) \;+ cz \;+ d$$

Now, the boundary conditions can be applied:

Periodic bc in x and y set $a = b = 0$
0-Neumann bc in z along z=0: $\nabla\, u(z = 0) = [0{,}0, -1 + c]$ and since $\vec{n} = [0{,}0, -1]$ we must have $c = 1$ to get $\nabla u \cdot \vec{n} = 0$
0-Neumann bc in z along z=1: $\nabla\, u(z = 1) = [0{,}0{,}1 + c]$ and since $\vec{n} = [0{,}0{,}1]$ we must have $c = -1$ to get $\nabla u \cdot \vec{n} = 0$

This is a contradiction, so this setup does not have a solution as described with neumann boundary condition = 0.

We could change it to be 1 - Neumann bc on both sides. In which case $c = 0$ and our family of solutions is

$$u(x, y, z) = \max\left(0, z - \frac{1}{2}\right) + \max\left(0, \frac{1}{2} - z\right) + \mathrm{d}$$

Notice that there is still a constant which makes this a family of solutions instead of a single one. Ie, the matrix system would be singular will a one dimensional null space.

Our Poisson solver will handle this singularity although it will give you a warning that the solution is singular. You should expect this and ignore it for what it is: a warning. The LU solver will provide one of the many solutions to the resulting singular system, then the Poisson solver will calculate the approximate integral of solution and subtract it off so that we return the approximately mean 0 solution. In the above weak solution, this would probably correspond to setting d = -1/4. Finally, it will test the computed solution against the provided exact solution. If you did not provide an exact solution or you are not close to the provided exact solution, then it will report error. If the system is not solvable (ie you have given inconsistent data) then it will fail with error as well.