

Deal.ii

1. ONE DIMENSIONAL EXAMPLE, FINITE VOLUME METHOD

1.1. Governing equations:

$$\frac{\partial}{\partial x} \left(\kappa \frac{\partial \phi}{\partial x} \right) = 0, \quad 0 \leq x \leq 1, \quad \kappa = \text{const.} \quad (1)$$

The reason why I use partial derivatives, and write the second order derivative like this, is because the notation is closer to the more complicated system I would like to solve later on.

1.2. Boundary conditions:

- $x = 0$ $\phi = 0$
- $x = 1$ constant flux I_{app} (i.e. $\kappa \frac{\partial \phi}{\partial x} = I_{app}$)

1.3. Solution.

The analytical solution is given by

$$\phi(x) = \frac{I_{app}}{\kappa} x \quad (2)$$

1.4. Integral Formulation.

We formulate equation (1) in integral formulation for a constant κ

$$\kappa \int_V \frac{\partial}{\partial x} \left(\frac{\partial \phi}{\partial x} \right) dV = 0, \quad (3)$$

Using Gauss' divergence theorem in 1D, we replace the volume integration with a surface integration

$$\kappa \int_S \left(\frac{\partial \phi}{\partial x} \right) dS = 0 \quad (4)$$

1.5. Discretization. We want to use n_x cell-centered finite volumes of constant width $h = \Delta x = \Delta y = \Delta z = \frac{1}{n_x}$, cell interfaces located at $f_i = ih$, $0 \leq i \leq n_x$ and cell centers located at $x_i = (i - 1/2)h = \left\{ \frac{h}{2}, \frac{3h}{2}, \dots, 1 - \frac{h}{2} \right\}$, $1 \leq i \leq n_x$. Figure 1 shows the setup of the finite volume method for $n_x = 7$ volumes. The discrete unknowns ϕ_i will be an approximation to the solution at $x = x_i$. Therefore, our system has n_x unknowns.

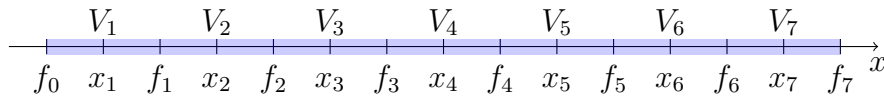


FIGURE 1. 1D Finite Volume setup

For each control volume, we then approximate equation (4) to obtain n_x equations for the n_x unknowns. For example for control volume V_5 in Figure 1, this would read:

$$\kappa \left[\int_{f_4} \frac{\partial \phi}{\partial x} dS + \int_{f_5} \frac{\partial \phi}{\partial x} dS \right] \quad (5)$$

$$= \kappa \left[- \left(\frac{\phi_5 - \phi_4}{h} \right) + \left(\frac{\phi_6 - \phi_5}{h} \right) \right] h^2 = 0, \quad (6)$$

where we have chosen an outward pointing normal vector (i.e. positive for f_5 and negative for f_4). The equations for all control volumes $2, \dots, n_x - 1$ will yield similar equations of the form.

$$\kappa \left[\left(\frac{\phi_{i-1} - \phi_i}{h} \right) + \left(\frac{\phi_{i+1} - \phi_i}{h} \right) \right] h^2 = 0, \quad 2 \leq i \leq n_x - 1 \quad (7)$$

For the two boundary conditions, the boundary fluxes lead to the following equations:

$$\kappa \left[\left(\frac{\phi_{\text{left}} - \phi_1}{h/2} \right) + \left(\frac{\phi_2 - \phi_1}{h} \right) \right] h^2 = 0 \quad i = 1 \quad (8)$$

$$\kappa \left(\frac{\phi_{n_x-1} - \phi_{n_x}}{h} \right) h^2 - I_{app} h^2 = 0 \quad i = n_x \quad (9)$$

RESIDUAL AND JACOBIAN FORMULATION

Because ultimately, we would like to solve a time-dependent, non-linear problem, we will denote the linear system to be solved $J\delta = -R$, where $R \in \mathbb{R}^{n_x \times 1}$ is the nonlinear residual, and $J \in \mathbb{R}^{n_x \times n_x}$ is the Jacobian matrix. The solution $\delta \in \mathbb{R}^{n_x \times 1}$ will be the incremental update in a Newton-Raphson scheme, but for this *linear* problem, the solution will be given by $\phi_i = \delta_i$.

2. ASSEMBLY FUNCTION

In our assembly function, we need to fill the matrix J and right-hand size $-R$ with the right entries. Similar to the `step-12/12b` tutorials, we can split the task into three distinct tasks for cells, boundaries and faces:

2.1. **Cell.** nothing to be done, later, add time-derivative term here

2.2. **Boundary.** Below is the assembly part for the boundary faces

Algorithm 1 boundary faces at $x = 0$

```

1: for each face  $f$  in BoundaryFaces  $x = 0$  do
2:    $x_i \leftarrow \text{CellCenters}[\text{right\_cell}(f)]$ 
3:   Residuals[ $i$ ]+ =  $\kappa \left( \frac{\phi_{\text{left}} - \phi_i}{h/2} \right) h^2$ 
4:   Jacobian[ $i, i$ ]+ =  $-\kappa \frac{2}{h/2} h^2$ 
5: end for
```

Algorithm 2 boundary faces at $x = 1$

```

1: for each face  $f$  in BoundaryFaces  $x = 1$  do
2:    $x_i \leftarrow \text{CellCenters}[\text{left\_cell}(f)]$ 
3:   Residuals[ $i$ ]+ =  $-I_{app} h^2$ 
4: end for
```

2.3. **Interior Faces.** Below is the assembly part for the interior faces

Algorithm 3 interior face (visit each face once)

```

1: for each face  $f$  in BoundaryFaces  $x = 1$  do
2:    $x_l \leftarrow \text{CellCenters}[\text{left\_cell}(f)]$ 
3:    $x_r \leftarrow \text{CellCenters}[\text{right\_cell}(f)]$ 
4:   flux =  $\kappa \left( \frac{\phi_r - \phi_l}{h} \right) h^2$ 
5:   Residuals[ $l$ ]+ = flux
6:   Residuals[ $r$ ]+ = -flux
7:   Jacobian[ $l, l$ ]+ =  $-\kappa \frac{1}{h} h^2$ 
8:   Jacobian[ $r, r$ ]+ =  $-\kappa \frac{1}{h} h^2$ 
9:   Jacobian[ $l, r$ ]+ =  $\kappa \frac{1}{h} h^2$ 
10:  Jacobian[ $r, l$ ]+ =  $\kappa \frac{1}{h} h^2$ 
11: end for
```

3. PLAN ON HOW TO IMPLEMENT IN DEAL.II

- use elements of type FE_DGQ
- for a start (maybe even forever), the degree of the element can be zero (i.e. piecewise constant), like in a piecewise constant finite volume scheme.
- build on `step-12` or `step-12b` tutorial and mainly change the three assembly functions as defined above as well as the boundary conditions.
- I hard-coded these functions in the appended `nik-step12.cc` file that produces the correct matrix and solution for the special case of $\kappa = h = 1$ and $I_{app} = -1$.

4. QUESTIONS

I think starting from the `step-12` or `step-12b` tutorials seems to be a suitable choice since they already use discontinuous elements.

My concrete questions for the forum are the following.

- How should I best write the three functions for the matrix assembly with as less hard-coding as possible?
- How can I best access the values of the current cell and neighbor cell (i.e. ϕ_{me} and $\phi_{neighbor}$) in (7)?

When I was trying to find resources for the derivation of a weak form using the discontinuous Galerkin method for (1), there were many different methods in chapter 1 of Rivière [1], some with penalty terms etc., which I think might be more complicated to implement. I really like the simplicity of the finite volume method but would like to use the provided DG tools in `deal.ii`

REFERENCES

1. Rivière, B. *Discontinuous Galerkin Methods for Solving Elliptic and Parabolic Equations* eprint: <https://epubs.siam.org/doi/pdf/10.1137/1.9780898717440>. <https://epubs.siam.org/doi/abs/10.1137/1.9780898717440> (Society for Industrial and Applied Mathematics, 2008).