Finite Volume Methods

A short Introduction to Principles and Concepts

Kenny Erleben
Department of Computer Science

University of Copenhagen

The Finite Volume Method (FVM)

- FVM is a method for discretizing PDEs into a system of equations. Just like the FDM or FEM methods treated elsewhere in these course slides.

- FVM is different in how it works. It has a more geometric flavor to it. One simply takes the "equations" and cuts the integral of these into geometric sub-pieces.

- Once the sub-integrals are obtained one reworks the integral version of the equations using various techniques. The most important is the application of the Gauss-Divergence theorem. This is similar to the weak-form reformulation that is critical in the FEM approach.

- Practical FVM often borrows from FDM or FEM methods when mathematically manipulating the equations into a discrete form. Hence, it can sometimes from a practical viewpoint be difficult to "categorize" a method as FVM.

The Finite Volume Method (FVM)

- FVM is different from FEM in that it takes a direct approach to getting the volume integrals and not a variational approach (using test functions) as done in FEM. Nor is it an approximation (using shape functions) of the central component of the FVM method.

- Compared to the FDM method the FVM method is more easily applied to unstructured meshes (like FEM) whereas FDM is more tricky for unstructured meshes.

- FDM is quite powerful for formal verification through analyzing the Taylor remainder terms. This is not so obviously done for the FVM method. In our opinion, FVM appears to be more an art form when deciding volume types and mesh layout, sub-techniques in discretization.

- In these slides we work our way through a portfolio of such techniques by going over examples and study group problems.

The General Recipe of FVM

One often works with FVM in the following way

Step 0 Get Governing Equation and Boundary Conditions

Step 1 Pick a volume type, design a mesh layout

Step 2 Apply FVM on the chosen mesh to get a system of equations

Step 3 Verify if the obtained system of equations are "well posed". If not go back to step 1 and try the process again with different choices.

To our knowledge, there is no formal structured way to make decisions; this is in our experience trial & error and knowledge/experience-based approach.

Verification Techniques

There are some typical methods one can apply to verify if the discretization worked out.

- Analyze Numerical Traits:
    - Fill-pattern,
    - Eigenvalues,
    - Spectral radius of any resulting matrices.

  These often reflect symmetries and properties of the original equations, also these reflect if the discrete equations can be numerically solved at all.

Verification Techniques

Ground Truth:

- Setup instances of your problem with known solutions.
  - For physical problems one can often try and simulate "equilibrium" states of the system. If a solver can not "stay" in equilibrium then something is wrong.
  - Testing reflections of the problem setup, like flipping the x-axis or so can be a good technique to test if FVM works (when symmetry is expected).
  - Often one solves for numerical solutions of balance/conservation equations. Hence, it is a good idea to verify if the discrete quantities are "conserved" too. This can be used to analyze numerical dissipation.

Verification Techniques

Convergence Studies:

- Analyze what happens when mesh-elements and time-step sizes are reduced. Solutions should not change too much when increasing spatial-temporal resolution.

FVM Overview of Ideas and Techniques

In the rest of these slides, we will now introduce the ideas, concepts, and ideas of using FVM.

- We start by defining a toy problem that we will use to illustrate the mathematical concepts and techniques of FVM.

- We walk through the techniques one by one, starting with discrete conservation, then the Gauss-Divergence theorem, and so on. These are all done on some "abstract" notion of a control volume V with surface S.

- When we have an idea of the mathematical techniques used in FVM then we will define specific concrete examples of control volumes.

- Armed with knowledge of mesh layout and FVM math steps we set out to work out a concrete example: the Navier-Stokes equations.

A Toy Example

A toy PDE example, given the known vector function $\mathbf{f}(\mathbf{u})$, and a scalar function $g(\mathbf{u})$, and the equation

$$\frac{\partial g(\mathbf{u})}{\partial t} + \nabla \cdot \mathbf{f}(\mathbf{u}) = \mathbf{0}$$

We wish to find an $\mathbf{u}$-solution, t can be viewed as time. One may think of $\mathbf{u}$ as some velocity field. It is not important what this equation models, for now, it is simply a mathematical problem to study.

This problem is only for educational purposes. Imagine the toy problem describes some balance or conservation law. We call this the "governing" equation as it describes the "dynamics" of our whole domain.
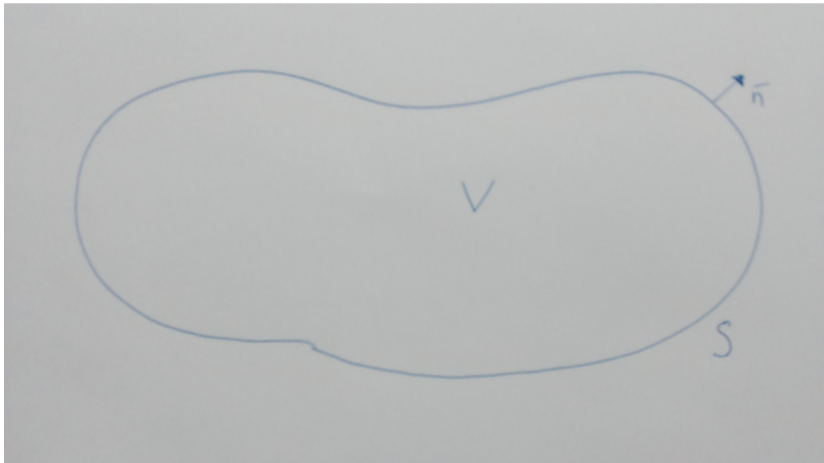
Start with putting PDE into Integral Form

Integrate PDEs over the arbitrary but fixed volume V with surface S

$$\frac{\partial g(\mathbf{u})}{\partial t} + \nabla \cdot \mathbf{f}(\mathbf{u}) = \mathbf{0}$$

$$\int_V \left(\frac{\partial g(\mathbf{u})}{\partial t} + \nabla \cdot \mathbf{f}(\mathbf{u}) \right) dV = \int_V \mathbf{0} dV = \mathbf{0}$$

$$\int_V \frac{\partial g(\mathbf{u})}{\partial t} dV = - \int_V \nabla \cdot \mathbf{f}(\mathbf{u}) dV$$
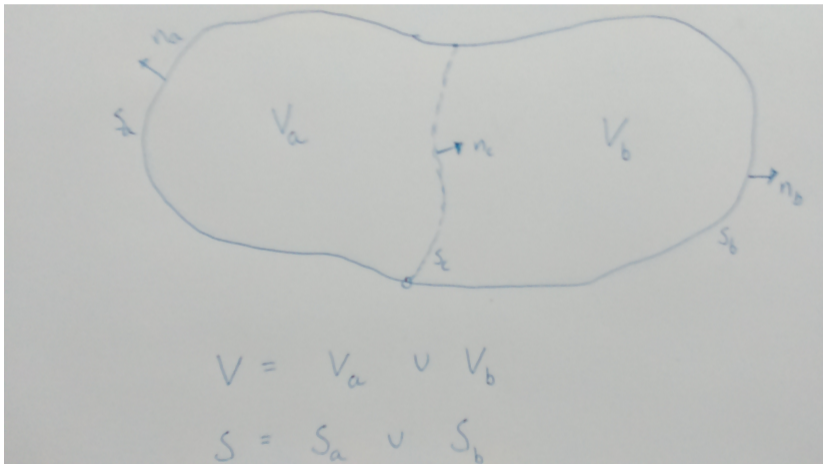
Using Gauss-Divergence theorem $\int_V \nabla \cdot \mathbf{f}(\mathbf{u}) dV = \int_S \mathbf{f}(\mathbf{u}) \cdot \mathbf{n} dS$,

$$\int_V \frac{\partial g(\mathbf{u})}{\partial t} dV = - \int_S \mathbf{f}(\mathbf{u}) \cdot \mathbf{n} dS.$$

The "global" volume

Split into "local" sub volumes

$$V = V_a \cup V_b$$

$$S = S_a \cup S_b$$

Local and Global Conservation Properties of FVM

If

- V_a and V_b shares common boundary S_c
- The boundary of V_a be $S_a \cup S_c$
- The boundary of V_b be $S_b \cup S_c$

Write integral forms over the sub-volumes and add them up

$$\int_{V_a} \frac{\partial g(\mathbf{u})}{\partial t} dV = - \left(\int_{S_a} \mathbf{f}(\mathbf{u}) \cdot \mathbf{n}_a dS + \int_{S_c} \mathbf{f}(\mathbf{u}) \cdot \mathbf{n}_c dS \right)$$

$$\int_{V_b} \frac{\partial g(\mathbf{u})}{\partial t} dV = - \left(\int_{S_b} \mathbf{f}(\mathbf{u}) \cdot \mathbf{n}_b dS + \int_{S_c} \mathbf{f}(\mathbf{u}) \cdot (-\mathbf{n}_c) dS \right)$$

Integrals of the common boundary cancel.

Conservation (Continued)

We have on the left-hand side

$$\int_{V_a \cup V_b} \frac{\partial g(\mathbf{u})}{\partial t} dV = \int_{V_a} \frac{\partial g(\mathbf{u})}{\partial t} dV + \int_{V_b} \frac{\partial g(\mathbf{u})}{\partial t} dV$$

and on the right-hand side after the substitution of the equation from previous slide

$$\int_{V_a \cup V_b} \frac{\partial g(\mathbf{u})}{\partial t} dV = -\int_{S_a} \mathbf{f}(\mathbf{u}) \cdot \mathbf{n}_a dS - \int_{S_b} \mathbf{f}(\mathbf{u}) \cdot \mathbf{n}_b dS$$

$$= -\int_{S_a \cup S_b} \mathbf{f}(\mathbf{u}) \cdot \mathbf{n} dS,$$

where $S_a \cup S_b$ is the boundary of $V_a \cup V_b$.

Insight on Conservation

The governing equation holds both for individual smaller volumes but also for the larger global volume

This means conservation is guaranteed by design on both the local scale (individual volumes) and global scale (the large volume).

Typical Traits of the Trade

We will now study typical discretization approaches used when working with FVM

- Use Gauss-Divergence theorem to change volume integrals into surface integrals
- Exploit piecewise continuous integrals
- Pull time-derivatives outside of integrals
- Apply numerical integration to solve integrals and finite-difference methods to deal with time-derivatives

This is an ordered list of steps to apply.

The Gauss Divergence Theorem

Used to rewrite volume integrals into surface integrals. It takes the generic form,

$$\int_V \nabla \cdot \mathbf{F} dV = \int_S \mathbf{F} \cdot \mathbf{n} dS,$$

where $\mathbf{F}$ is any vector field, V is a closed connected set, and S is the boundary of V having $\mathbf{n}$ as the outward unit-normal. There is a physical interpretation of this.

- Right-hand side gives the flux of $\mathbf{F}$ through the surface S. That is how much $\mathbf{F}$ transports into our V volume.
- The left-hand side tells how much of $\mathbf{F}$ is removed or added inside the volume V.
- Hence, left-side and right-aside express a balance law saying that the change of $\mathbf{F}$ inside the volume must equal the amount of $\mathbf{F}$ transported through the boundary surface S of V.

Exploit Piecewise Continuous Integral

After having applied the Gauss-Divergence theorem to our Toy problem, We have,

$$\int_V \frac{\partial g(\mathbf{u})}{\partial t} dV = - \int_S \mathbf{f}(\mathbf{u}) \cdot \mathbf{n} dS.$$

For the sake of example let us now assume,

- Boundary S is piece-wise continuous

The consequence is that we replace the right-hand-side with summation over the continuous pieces to obtain,

$$\int_V \frac{\partial}{\partial t} g(\mathbf{u}) dV = - \sum_e \int_{s_e} \mathbf{f}(\mathbf{u}) \cdot \mathbf{n} dS.$$

Using the Leibniz's Rule for Differentiation under the Integral Sign

After having exploited the piecewise continuous boundary surface to rewrite into a summation of surface integrals, We have,

$$\int_V \frac{\partial}{\partial t} g(\mathbf{u}) dV = - \sum_e \int_{s_e} \mathbf{f}(\mathbf{u}) \cdot \mathbf{n} dS.$$

Again for the sake of example, we will assume V is independent of time t,

- This allows us to exchange the integration and differentiation on the left-hand-side

This is often the case as one writes up the initial volume integrals using the reference coordinate space or material coordinate space of the problem. Then

$$\frac{\partial}{\partial t} \int_V g(\mathbf{u}) dV = - \sum_e \int_{s_e} \mathbf{f}(\mathbf{u}) \cdot \mathbf{n} dS.$$

The Midpoint Approximation Rule

We have

$$\frac{\partial}{\partial t} \int_V g(\mathbf{u}) dV = -\sum_e \int_{S_e} \mathbf{f}(\mathbf{u}) \cdot \mathbf{n} dS.$$

If

- The outward unit normal $\mathbf{n}$ is constant along each S_e part

Then when we use the midpoint approximation rule we obtain,

$$\frac{\partial}{\partial t} \left[g(\mathbf{u})\right]_c V = -\sum_e \left[\mathbf{f}(\mathbf{u})\right]_e \cdot \mathbf{n}_e l_e,$$

where l_e is the area of the S_e surface. The bracket and sub-script notation refer to the term being evaluated at the midpoint of the subscripted entity.

Some Remarks

- $\big[g(\mathbf{u})\big]_c$ interpreted as the "volume" mean value of $g(\mathbf{u})$ stored at the volume center denoted by the label, c, similar meaning applies to $\big[g(\mathbf{u})\big]_e$, the value at surface midpoint with label e.

- Usually

$$\big[g(\mathbf{u})\big]_c = g(\big[\mathbf{u}\big]_c)$$

Higher order approximations (computation time vs. accuracy tradeoffs)

- Midpoint rule replaced with any kind of Riemann Sum, Gaussian Quadrature, Simpsons Rule etc..

Applying Finite Differences

Apply finite difference on the left-hand side

$$\frac{V}{\Delta t}\left(\left[g(\mathbf{u}(t+\Delta t))\right]_c - \left[g(\mathbf{u}(t))\right]_c\right) = -\sum_e \left[\mathbf{f}(\mathbf{u}(t))\right]_e \cdot \mathbf{n}_e l_e.$$

The final discrete version of the original integral form

$$\int_V \frac{\partial g(\mathbf{u})}{\partial t}dV = -\int_S \mathbf{f}(\mathbf{u}) \cdot \mathbf{n}dS.$$

The discrete form can often be written compactly as

$$\mathbf{Au} = \mathbf{b}$$

In practice, matrices are rarely assembled but rather kept implicit.

Are there more steps?

So far we covered the "core" discretization approaches. There is more to be said on these matters. For instance how does one compute $[\mathbf{u}]_c$ or $[\mathbf{u}]_e$ and similar terms. There are two things to consider in dealing with this

- The mesh layout - at what location in the mesh (vertices, edges, or volumes) do we store/associate the discrete values of $\mathbf{u}$?
- What type of control volume is used for an unknown field? Note, that it is not uncommon to use more than one type of control volume - one for each unknown field being solved for.

Sometimes it is possible to make convenient design choices. Other times one is confronted with not having a needed value stored at a given location.

The Mesh Layout

There is no right and wrong here, it all depends on the "problem" being solved. Often one will see

- Scalar quantities (like pressure, mass density, viscosity, temperature etc.) are often stored at volume (also called cell) centers.
- Vector quantifies (like velocity, force) are often stored at vertices
- Flux terms (like normal components of vectors etc.) are often stored on edges.

A mesh layout like the above is referred to as a staggered mesh. If all quantities were stored at say vertices one would term it a collocated grid.

Different Control Volume Types

A few examples of control volumes for staggered grid types
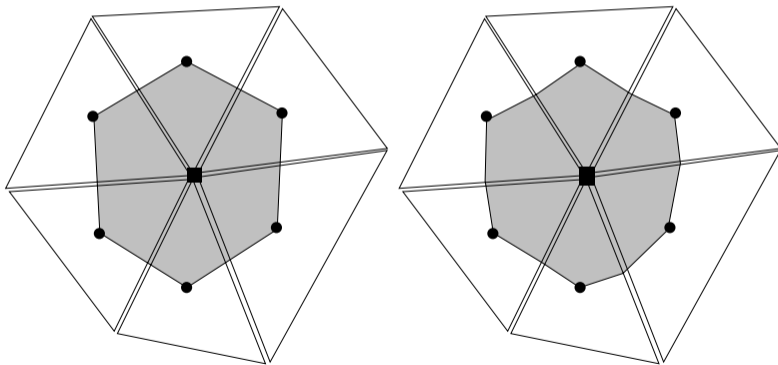
The centroid dual control volume and the median dual control volume.

Dealing with the further steps?

We will now use the incompressible Navier Stokes equations as a a concrete more complex example for showing

- How to apply upwind FDM schemes
- How to use shape functions (FEM techniques) for estimating derivatives at sample positions
- How to linearize non-linear terms (like advection).

Our Discretization Example

Our choices

- Incompressible Navier Stoke equations
- Unstructured mesh – Triangle mesh
- Staggered grid – Scalar values at triangle centers – Vector values at vertices
- Centroid dual control volume for Navier Stokes equation and Triangle control volume for incompressibility constraint equation.

Assumptions

- Regular mesh – close to equilateral triangles – all angles close to $60°$

The Integral Form of Navier Stokes Equations

Newtonian Incompressible Fluids for control volume V with boundary S

$$\int_S \rho \mathbf{u} \cdot \mathbf{n} \, dS = 0$$

$$\frac{\partial}{\partial t} \int_V \rho \mathbf{u} \, dV + \int_S \rho \mathbf{u} \left(\mathbf{u} \cdot \mathbf{n} \right) dS = \int_S \mathbf{T} \mathbf{n} \, dS - \int_S \left(p \mathbf{I} \right) \mathbf{n} \, dS + \int_V \rho \mathbf{b} \, dV$$

where $\mathbf{T}$ is the shear strain rate tensor and $\mathbf{I}$ is the identity tensor.

(Hint: You can read about Newtonian fluids in slide deck 7, note that we made the notation change in the current slide deck of of using the symbol $\mathbf{T}$ instead of $\mathbf{D}$.)

The Discrete Volume Conservation

We use triangle control volumes storing ρ at the triangle centers.

$$\underbrace{\int_{S_c} \rho \mathbf{u} \cdot \mathbf{n} dS}_{\approx \sum_{e \in S_c} M_e} = 0,$$

$$\sum_{e \in S_c} M_e = 0.$$

where M_e is the discrete mass flux.

The Discrete Navier Stokes equations

We use a vertex-centered centroid dual-control volume

$$\underbrace{\frac{\partial}{\partial t} \int_{V_c} \rho \mathbf{u} dV}_{\approx U_c} + \underbrace{\int_{\Gamma_c} \rho \mathbf{u} \left(\mathbf{u} \cdot \mathbf{n}\right) dS}_{\approx \sum_{e \in \Gamma_c} A_e} = \underbrace{\int_{\Gamma_c} \mathbf{T} \mathbf{n} dS}_{\approx \sum_{e \in \Gamma_c} D_e} - \underbrace{\int_{\Gamma_c} \left(p \mathbf{I}\right) \mathbf{n} dS}_{\approx \sum_{e \in \Gamma_c} P_e} + \underbrace{\int_{V_c} \rho \mathbf{b} dV}_{\approx B_c}$$

$$U_c + \sum_{e \in \Gamma_c} A_e = \sum_{e \in \Gamma_c} \left(D_e + P_e\right) + B_c$$

Notice the two equations in our problem use different kinds of control volumes.

The Mass Flux Term (1/2)

We have the triangle control volume c where e is the edge from vertex node i to node j.
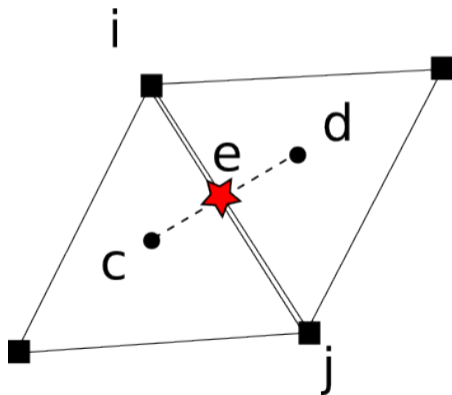
By our construction, we have defined a discrete flux term,

$$M_e \equiv \rho_e \mathbf{u}_e \cdot \mathbf{n}_e l_e$$

We will adopt averaging to numerically approximate the last terms,

$$\mathbf{u}_e == \equiv \frac{1}{2} \left(\mathbf{u}_i + \mathbf{u}_j \right)$$

$$\rho_e \equiv \frac{1}{2} \left(\rho_c + \rho_d \right)$$

The Mass Flux Term (2/2)

We have the triangle control volume *c* where *e* is the edge from vertex node *i* to node *j*.

Another option is to apply an upwind approximation instead of averaging,

$$\rho_e \equiv \begin{cases} \rho_c & ; \mathbf{u}_e \cdot \mathbf{n}_e \geq 0 \\ \rho_d & ; \mathbf{u}_e \cdot \mathbf{n}_e < 0 \end{cases}$$

where $\mathbf{n}_e$ is outward unit normal and l_e is edge length. This can be an advantage when dealing with transport type of problems as averaging tends to add too much numerical dissipation in such cases.
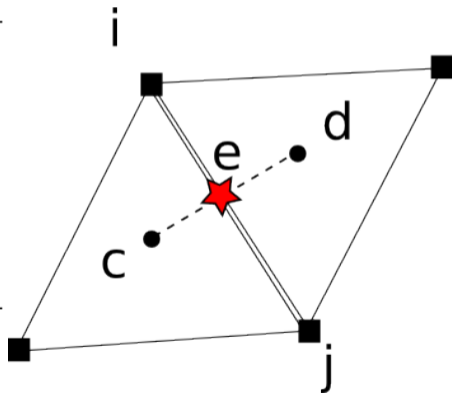
The Advection Term (1/2)

We will now use Picard linearization to deal with the nonlinear dependence in $\mathbf{u}$, notice the fixed point iteration index k
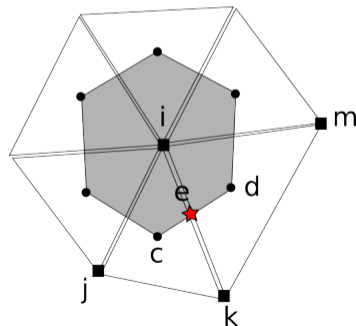
Hence, by construction, we now have the discrete advection term

$$A_e^{k+1} \equiv \mathbf{u}_e^{k+1}(\rho_e^k \mathbf{u}_e^k \cdot \mathbf{n}_e)l_e$$

We apply the final numerical approximations by using averaging, Hence,

$$\mathbf{u}_c \equiv \frac{1}{3}\left(\mathbf{u}_i + \mathbf{u}_j + \mathbf{u}_k\right), \mathbf{u}_d \equiv \frac{1}{3}\left(\mathbf{u}_i + \mathbf{u}_k + \mathbf{u}_m\right)$$

$$\mathbf{u}_e \equiv \frac{1}{2}\left(\mathbf{u}_c + \mathbf{u}_d\right), \rho_e \equiv \frac{1}{2}\left(\rho_c + \rho_d\right)$$
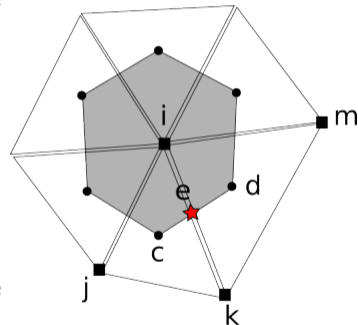
The Advection Term (2/2)

A simpler scheme may be adopted if we assume the edge going from i to k is orthogonal to the edge from c to d and intersects at the mid-points,

$$\mathbf{u}_e \equiv \frac{1}{2} \left(\mathbf{u}_i + \mathbf{u}_k \right)$$

$$\rho_e \equiv \frac{1}{2} \left(\rho_c + \rho_d \right)$$

The alternative upwind scheme would then apply the rule

$$\mathbf{u}_e^{k+1} \equiv \begin{cases} \mathbf{u}_i^{k+1} & ; \mathbf{u}_e^k \cdot \mathbf{n}_e \geq 0 \\ \mathbf{u}_j^{k+1} & ; \mathbf{u}_e^k \cdot \mathbf{n}_e < 0 \end{cases}$$

Remember our $60°$ mesh assumption!
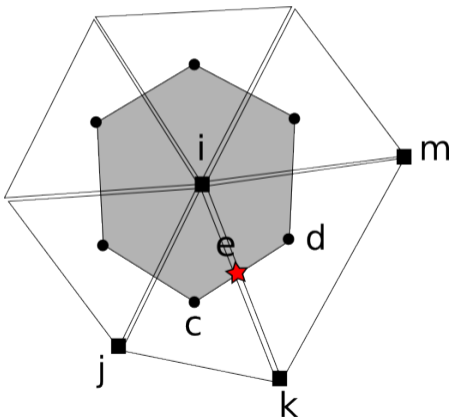
The Pressure Term

By construction, we defined the discrete pressure term to be

$$P_e = p_e \mathbf{n}_e l_e$$

Next, we apply averaging as the final numerical approximation,

$$p_e = \frac{1}{2} \left(p_c + p_d \right)$$

There are no velocity-term so it does not make sense to apply any upwind approximations here.
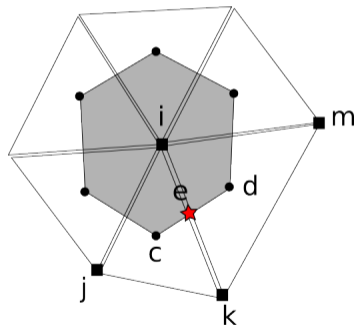
The Diffusion Term (1/2)

By construction, we have defined the discrete diffusion term to be

$$D_e = T_e \mathbf{n}_e l_e$$

where the stress tensor is defined as follows

$$T_{e,ij} = \mu \left(\frac{\partial \mathbf{u}_{e,i}}{\partial \mathbf{x}_j} + \frac{\partial \mathbf{u}_{e,j}}{\partial \mathbf{x}_i} \right)$$

We need a numerical approximation for the $\frac{\partial \mathbf{u}_e}{\partial \mathbf{x}}$ term,
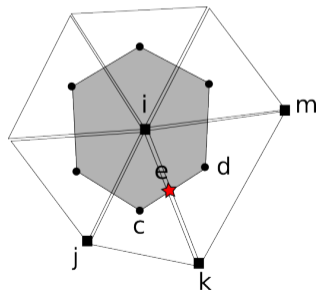
Observe that $\mathbf{u}_{e,i}$ means the ith component of $\mathbf{u}$ at location e. Similar $\mathbf{x}_i$ means the ith component of $\mathbf{x}$ and not the $\mathbf{x}$-value at vertex i.

The Diffusion Term (2/2)

To numerically approximate $\frac{\partial \mathbf{u}_e}{\partial \mathbf{x}_i}$ we will use the idea of having a linear FEM line segment going from c to d. Taking the derivative of the interpolation of $\mathbf{u}$ with linear shape function yields,

$$
\begin{aligned}
\frac{\partial \mathbf{u}_e}{\partial \mathbf{x}_i} &= \frac{\partial}{\partial \mathbf{x}_i} \left(t\mathbf{u}_d + (1-t)\mathbf{u}_c \right) \\
&= \left(\frac{\partial}{\partial t} \left(t\mathbf{u}_d + (1-t)\mathbf{u}_c \right) \frac{\partial t}{\partial \mathbf{x}_i} \right) \\
&= \frac{\mathbf{u}_d - \mathbf{u}_c}{\mathbf{x}_{d,i} - \mathbf{x}_{c,i}}
\end{aligned}
$$

Observe that $\mathbf{x}_{d,i}$ means the ith component of $\mathbf{x}$ at location d

The Magnetostatic Problem (1/4)

Let us introduce a new PDE problem that we can use as a case study for learning about the FVM method. We will start with writing up the Maxwell Equations in general differential form

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}$$

$$\nabla \cdot \mathbf{B} = 0$$

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

$$\nabla \times \mathbf{B} = \mu_0 \left(\mathbf{J} - \varepsilon 0 \frac{\partial \mathbf{E}}{\partial t} \right)$$

Next, we will simplify these using facts about magnetostatics.

The Magnetostatic Problem (2/4)

In the magnetostatic case, we have no currents and no charges, no motion, and hence all time derivatives are zero. Using these facts Maxwell's equations simplify to the following form,

$$\nabla \cdot \mathbf{B} = 0$$
$$\nabla \times \mathbf{H} = 0$$

Notice we have no **E** field either as there is no motion of the magnetic flux nor any charges.

The Magnetostatic Problem (3/4)

It is known that Magnetization is explicitly induced by the relation

$$\mathbf{B} = \mu_0 \left(\mathbf{M} + \mathbf{H} \right)$$

The equation $\nabla \times \mathbf{H} = \mathbf{0}$ has the general solution $\mathbf{H} = -\nabla\phi$ where ϕ is a scalar potential field. (Self Study: try and prove this). Now $\mathbf{B} = \mu_0 \left(\mathbf{M} + \mathbf{H} \right)$ becomes

$$\mathbf{B} = \mu_0 \left(\mathbf{M} - \nabla\phi \right)$$

The Magnetostatic Problem (4/4)

By substitution of $\mathbf{B} = \mu_0 \left(\mathbf{M} - \nabla \phi \right)$ into our simplified version of the Maxwell Equation we obtain,

$$\nabla \cdot \mathbf{B} = \mu_0 \left(\nabla \cdot \mathbf{M} - \nabla \cdot \nabla \phi \right) = 0$$

Rearranging the equation and cleaning up we get

$$\nabla \cdot \nabla \phi = \nabla \cdot \mathbf{M}$$

This is a Poisson equation to solve for ϕ. This is the governing equation of the Magnetostatic problem. We will work with this problem is the Assignments.

Facts about eigenvalues of ∇^2 (1/5)

It will be instructive to study the Poisson equation type from a little mathematical angle. In particular learning about its eigenvalues will give us insights about what to expect later on when we have to solve our discrete system of equations that we obtain with the FVM method.

Given the eigenvalue problem with eigenvalue λ and eigenvalue function v

$$-\nabla^2 v = \lambda\, v$$

We multiply by v and take the area integral,

$$\int_A \lambda v^2\, dA = \lambda \int_A v^2\, dA = -\int_A v\left(\nabla^2 v\right)\, dA$$

Facts about eigenvalues of ∇^2 (2/5)

Recall product rule $(f\,g)' = f'\,g + f\,g'$ giving integration by parts

$$\int f\,g'dx = \int (f\,g)'dx - \int f'\,gdx$$

Recall $\nabla^2 v = \sum_i \frac{\partial^2 v}{\partial x_i^2}$, Letting $f \equiv v$ and $g' \equiv \frac{\partial^2 v}{\partial x_i^2}$ then substitution into,

$$\int_A \lambda v^2 dA = \lambda \int_A v^2 dA = -\int_A v\left(\nabla^2 v\right)\ dA$$

Give us

$$\lambda \int_A v^2 dA = -\int_A v\left(\nabla^2 v\right)\ dA = \int_A \nabla v^T \nabla v\ dA - \int_A v\left(\nabla \cdot v\right)\ dA$$

Facts about eigenvalues of ∇^2 (3/5)

So

$$\lambda \int_A v^2 dA = \int_A \nabla v^T \nabla v \, dA - \int_A v \left(\nabla \cdot v \right) \, dA$$

Gauss divergence theorem gives

$$\lambda \int_A v^2 dA = \int_A \nabla v^T \nabla v \, dA - \underbrace{\int_S v \left(\nabla v \cdot \mathbf{n} \right) \, dS}_{\equiv 0}$$

The surface integral becomes zero due to our Neumann boundary conditions

$$\lambda \int_A v^2 dA = \int_A \nabla v^T \nabla v \, dA$$

Facts about eigenvalues of ∇^2 (4/5)

So we now have

$$\lambda \int_A v^2 dA = \int_A \nabla v^T \nabla v \, dA$$

We now observe

- If v is constant on A then $\nabla v = 0$ and we must have $\lambda = 0$
- If v is varying on A then $\nabla v \neq 0$ and $\lambda > 0$

From this, we conclude

- All $\lambda \geq 0$ for $-\nabla^2$ or $\lambda \leq 0$ for ∇^2 (Observe the sign flip in ∇^2).

Facts about eigenvalues of ∇^2 (5/5)

Assume u is a particular solution for $\nabla^2 u = b$. Let us use a simple affine transform $w \equiv a\,u + c$ where $a, b \in \mathbb{R}$. We want to know for what values a and b that w also will be a solution

$$\nabla^2 w = b$$
$$\nabla^2 (a\,u + c) = b$$
$$a\,\nabla^2 u + \nabla^2 c = b$$
$$a\,\nabla^2 u = b$$

We observe that we must have $a = 1$, but c can be any value. Hence, we have a one-dimensional family of general solution $w = u + c$. We expect at least one zero-eigenvalue.

Problem with Discontinuous Integrands (1/6)

Consider a term such as $\nabla \cdot \mathbf{M}(\mathbf{x})$ as seen in the magnetostatic case study. Its volume integral counterpart being

$$\int_A \underbrace{\nabla \cdot \mathbf{M}(\mathbf{x})}_{\equiv f(\mathbf{x})} \, dA$$

By the first fundamental theorem of calculus, we require the integrated $f(\mathbf{x})$ to be a continuous real-valued function. For the sake of serving as a learning example, we now define $\mathbf{M}$ in such a way that it is $\mathbf{0}$ outside a unit disk and constant inside,

$$\mathbf{M} \equiv \begin{cases} \mathbf{0} & \text{if } \| \mathbf{x} \| \le 1 \\ (0, -1)^T & \text{if } \| \mathbf{x} \| > 1 \end{cases}$$

Problem with Discontinuous Integrands (2/6)

Given this setup, we may now consider the following cases:

- If a control volume is completely outside the unit disk. Here $\mathbf{M} = \mathbf{0}$ and $f(\mathbf{x})$ is continuous and our integral makes sense in this case.
- If the control volume is completely inside then $\mathbf{M}$ is constant everywhere and our integrand is again a continuous function.
- Finally, if the control volume partially overlaps the unit disk. Then M jumps from one value inside the unit circle to another value outside the unit disk. Hence the integrated is discontinuous and the integral can not be solved.

Let us now study how to solve such a challenge.

Problem with Discontinuous Integrands (3/6)

One possible remedy is to split volume integral into a summation over integrals over piece-wise continuous domains. In our case study that means splitting A into two domains corresponding to the two regions of different constant M-values.

$$\int_A f(\mathbf{x})dA = \int_{A_{\text{inside}}} f(\mathbf{x})dA + \int_{A_{\text{outside}}} f(\mathbf{x})dA$$

The concept is illustrated below

A_{outside}

A_{inside}

$M = (0,0)^{\mathsf{T}}$

$M = (0,-1)^{\mathsf{T}}$
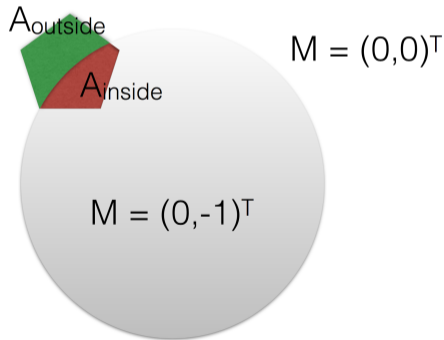
Problem with Discontinuous Integrands (4/6)

- After having split the control volume the FVM steps can be redone, hence Gauss-Divergence theorem leads to surface integrals
- Notice the shared surface along O_1 and I_1, here O_1 is treated as outside the unit disk and I_1 as inside the unit disk. Notice that the original control volume edge made from O_2 and I_2 has been cut into two pieces. All other edges are unaffected by the splitting.
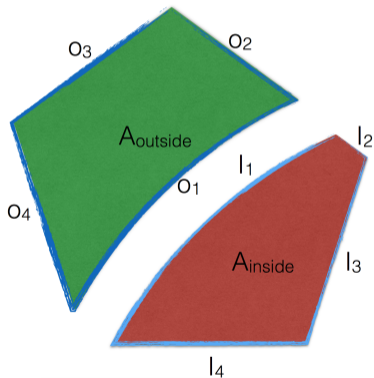
Problem with Discontinuous Integrands (5/6)

Further insights

- One does not actually have to create split geometries of control volumes that partially overlap discontinuous domains. The split can be done virtually on the fly when writing code that evaluates the integrals. The downside is that it adds a few if-statements to the code.

- The discontinuity in **M** comes from the physical magnet boundary which we have represented implicitly in our model by defining **M**. Alternatively, we could have represented the physical boundary explicitly in the mesh and made sure that the control volumes were designed such that their boundaries were conforming to the physical boundaries. The downside is that it can require a different mesh layout, a re-meshing, or both.

Problem with Discontinuous Integrands (6/6)

In summary

Remeshing to make boundaries conforming

Change
grid layout & control volume type
to make
boundaries conforming
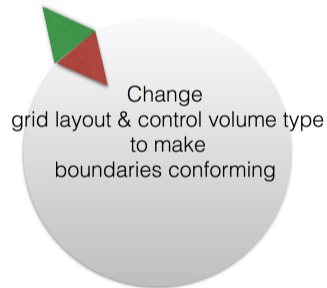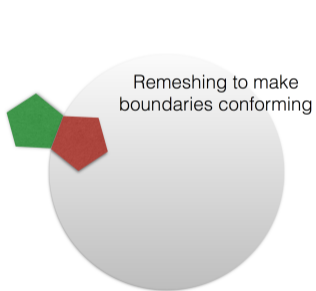
Assignment

The FVM integral form is explained on Page 10.

- How does the FVM conversion to integral form compare to what you did in the FEM method? Explain the difference in this rewriting as integral form step. (Hint: Test function?)

Assignment

Page 18 explains how to exploit a piecewise continuous boundary surface to rewrite our surface integral into a summation of surface integrals.

- Why is it clever to replace the closed surface integral with a summation over piecewise continuous integrals? (Hint: Consider using piecewise linear surfaces and solving integrals numerically)

Assignment

Page 19 explains how to deal with time-derivatives.

- Why is it clever to "pull" time-derivative outside the integral sign? (Hint: Think about using Finite Difference Methods (FDM) for discretizing the time-derivative)

Assignment

Page 22 explains how to apply numerical approximations in the FVM method.

- Discuss why we have postponed applying the numerical approximations as the last thing to do in the very last steps of the FVM method.

Assignment

- Use the simple **f**-function given by $\mathbf{f}(\mathbf{u}) \equiv \mathbf{u}$ and the simple scalar function $g(\mathbf{u}) \equiv (u_x + u_y)$ and derive the final discrete equation for the toy problem

$$\frac{V}{\Delta t} \left(\left[g(\mathbf{u}(t + \Delta t)) \right]_c - \left[g(\mathbf{u}(t)) \right]_c \right) = - \sum_e \left[\mathbf{f}(\mathbf{u}(t)) \right]_e \cdot \mathbf{n}_e l_e.$$

  Observe the 2D unknown vector field **u** depends on both time and position.

- Use a regular 2D grid as your computational mesh with equal cell spacing along the x and y axes. Store **u** at the center of the square cells. (Hint: Consider how to compute $\left[\mathbf{u} \right]_e$? That is the **u**-values at the edge midpoints). Draw the mesh layout.

Assignment

This is a continuation of Page 57

- You may use an alternative mesh layout where u_x is stored at the vertical edge centers and u_y is stored at the horizontal edge centers. No values are stored at the volume centers. (Hint: Consider how to compute $\begin{bmatrix} \mathbf{u} \end{bmatrix}_c$? That is the **u**-values at the volume centers). Draw the mesh layout.

- Show how your discrete toy problem from the previous slide is assembled into a linear system $\mathbf{Au} = \mathbf{b}$ (Hints: Notice the similarity to putting FDM update schemes into matrix form or doing the FEM assembly process).

Be careful when working with your discrete equation. You now have a single integral over each square control volume in your mesh. Label the control volumes by c.

Assignment

The integral form of the incompressible Navier-Stokes equations is shown on Page 28.

- Derive in full detail the integral form of the incompressible Navier Stokes equations from their corresponding differential form counterpart

$$\nabla \cdot \rho \mathbf{u} = 0$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \rho \left(\mathbf{u} \cdot \nabla \right) \mathbf{u} = \nabla \cdot \mathbf{T} - \nabla p + \rho \mathbf{b}$$

Assignment

On page 37 we used linear FEM to do numerical approximation in an FVM method.

- Work out the details of how to find the term $\frac{\partial t}{\partial \mathbf{x}_i}$. In 2D we have $x_0 = x$ and $x_1 = y$, so given a point on the line $p(t) = (x(t), y(t))^T$ we have

$$x(t) = t\, x_d + (1 - t)\, x_c$$
$$y(t) = t\, y_d + (1 - t)\, y_c$$

In the general notation

$$\mathbf{x}_i(t) = t\, \mathbf{x}_{d,i} + (1 - t)\, \mathbf{x}_{c,i}$$

(Hint: use the equation above to write t as a function of $\mathbf{x}_i$.

Assignment

Use the discrete Navier-Stokes equations from Page 30 as your starting point.

- Ignore the advection term and write out the formulas for all the coefficients of the **u**-terms in the discretisation
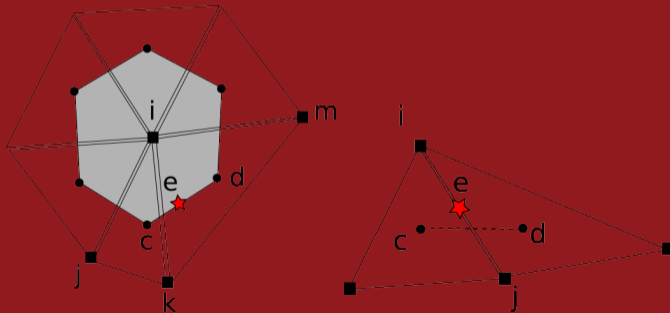
$$U_c = \sum_{e \in \Gamma_c} (D_e + P_e) + B_c$$

Explain how this can be assembled into a linear system like **Au** = **b**. Repeat the process for the discrete equation

$$\sum_{e \in S_c} M_e = 0.$$

Assignment

Recall all the discretization examples we have shown from Page 30 to 37. Consider what happens if you encounter meshes like the ones shown here.

Explain problems and possible solutions (Hint look for cross-diffusion in text books)

Assignment

We will work on the Magnetostatic problem as given on Page 41. Compute a solution $\phi(\mathbf{x}) : \mathbb{R}^2 \mapsto \mathbb{R}$ where $\mathbf{x} \in \mathbb{R}^2$. The problem is

$$\nabla^2 \phi(\mathbf{x}) = \nabla \cdot \mathbf{M}(\mathbf{x}) \quad \forall \mathbf{x} \in \mathcal{A}$$

where $\mathcal{A}$ is the the closed box $[-3..3] \times [-1..1]$ and $\mathbf{M}(\mathbf{x}) : \mathbb{R}^2 \mapsto \mathbb{R}^2$ is defined as zero outside the unit disk and $\mathbf{M} = (0, -1)^T$ everywhere else. At the vertex closest to the north pole of the unit disk boundary we have $\phi = 0$. At every other boundary point of the box we have $D(\phi, \mathbf{n}) = \nabla \phi^T \mathbf{n} = 0$ where $\mathbf{n}$ is the outward unit vector normal at the boundary. Remember that $\nabla^2 = \nabla \cdot \nabla$ and $\nabla = (\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2})^T$.

- Derive and implement a finite volume method scheme (Hint: use FDM to approximate directional derivative $\nabla \phi(\mathbf{x})^T \mathbf{n}$).

Assignment

Continued from Page 63.

- Assume the domain can be "nicely" triangulated
- Discuss grid layout and control volume types carefully! (Hint: handed out code store ϕ at vertices and use the vertex-centered centroid dual control volume)
- If you have time try and change the control volume to use a triangle control volume.

Hints: Think about how to deal properly with control volumes that are partial outside and inside the disk where **M** is defined. What is the problem with FVM for such control volumes?

Assignment

- Write out all the details and sub-steps in showing the integration by parts re-write on Page 43 that results in

$$-\int_A v\left(\nabla^2 v\right)\, dA = \int_A \nabla v^T \nabla v\, dA - \int_A v\left(\nabla \cdot v\right)\, dA$$

Assignment

Consider the theory covered on Pages 42-46. Assume some nonlinear transform $f(u(x))$ of the particular solution $u(x)$ to the general solution $w(x) = f(u(x))$.

- Prove $\nabla^2 w = b$ can be written as,

$$\frac{\partial^2 f}{\partial x^2} \left(\frac{\partial u}{\partial x}\right)^2 + \frac{\partial f}{\partial x}\frac{\partial^2 u}{\partial x^2} = b$$

- Prove that we must have $\frac{\partial u}{\partial x} \neq 0$, $\frac{\partial f}{\partial x} = 1$ and $\frac{\partial^2 f}{\partial x^2} = 0$ in order for u and w to be a solution for $\nabla^2(\cdot) = b$.

  This proves that only the affine transform exists which can produce another particular solution, hence we have exactly one zero-eigenvalue.

Assignment

- In the Magnetostatic cast study problem on Pages 63-64 we may choose to ignore the problem of **M** being discontinuous. What does this "solution" correspond to having done with the magnet boundary surface? That is what is the actual shape of the magnet that would give rise to the computed solution?

Assignment

- Handling Embedded Surfaces, read the paper "Tetrahedral Embedded Boundary Methods for Accurate and Flexible Adaptive Fluids Abstract" by Christopher Batty, Stefan Xenos, and Ben Houston, Eurographics 2010.

- Based on the paper describe ways to deal with embedded surfaces in an unstructured triangle mesh.

- Consider the magnetostatic case study again. Can any of the techniques from the Batty et al. 2010 paper be reapplied to improve this case study problem?