Specialized Numerical Methods for Transport Phenomena

The finite element method: Transient and transport problems

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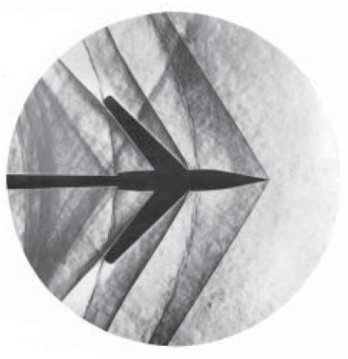

Outline

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Motivation

So far, we have only investigated steady-state Poisson problems such as the heat transfer equation. In many situations, we are interested in solving transient problems. For example, the transient heat equation:

$$\rho C_p \frac{\partial T}{\partial t} = k \nabla^2 T$$

with an initial condition describing $T(\boldsymbol{x})$ and boundary conditions.
We have an additional term that we need to consider, which is the time derivative.
There are two approaches we can consider:

- Interpolate in time using a Lagrange polynomial (space-time FEM)
- Use a finite difference approach. **This is generally the approach we take**.

Euler's method

You most likely have already seen at some place during your curriculum that one way to approximative time derivative is to use a finite difference scheme. For example:

$$\frac{\partial c}{\partial t} \approx \frac{c^{t+\Delta t} - c^{t}}{\Delta t}$$

is called Euler's method.

We generally distinguish between two families of Euler's method:

- Explicit: All terms at the right-hand-side are taken at time t
- Implicit: All terms at the right-hand side are taken at time $t + \Delta t$

An example

Let's consider the following system of ODEs:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \alpha x - \beta xy$$
$$\frac{\mathrm{d}y}{\mathrm{d}t} = \delta xy - \gamma y$$

Lets solve it using both implicit and explicit Euler

In the context of FEM

Solving transient problems in FEM is done in the same exact fashion. Let's take our PDE:

$$\rho C_p \frac{\partial T}{\partial t} = k \nabla^2 T$$

We discretize the equation in time:

$$\frac{T^{t+\Delta t} - T^{t}}{\Delta t} = \alpha \nabla^2 T$$

where $\alpha = k/\rho C_p$. Now let's see what happens when we solve it using explicit or implicit Euler.

Weak form: Explicit Euler

The weak form we obtain is:

$$\int_{\Omega} \left(\frac{1}{\Delta t} u T^{t+\Delta t} \right) \mathrm{d}\Omega = \int_{\Omega} \left(\frac{1}{\Delta t} u T^{t} - \alpha \nabla u \nabla T^{t} \right) \mathrm{d}\Omega$$

And fully discretized it is:

$$\sum_{j} T_j^{t+\Delta t} \int_{\Omega} \left(\frac{1}{\Delta t} \phi_i \phi_j \right) \mathrm{d}\Omega = \int_{\Omega} \left(\frac{1}{\Delta t} \phi_i T^{t} - \alpha \nabla \phi_i \nabla T^{t} \right) \mathrm{d}\Omega$$

Some conclusions:

- We still need to a solve a linear system, even if the scheme is explicit?
- There is a stability criterion.

Weak form: Implicit Euler

The weak form we obtain is:

$$\int_{\Omega} \left(\frac{1}{\Delta t} u T^{t+\Delta t} + \alpha \nabla u \nabla T^{t+\Delta t} \right) \mathrm{d}\Omega = \int_{\Omega} \left(\frac{1}{\Delta t} u T^{t} \right) \mathrm{d}\Omega$$

And fully discretized it is:

$$\sum_j T_j^{t+\Delta t} \int_{\Omega} \left(\frac{1}{\Delta t} \phi_i \phi_j + \alpha \nabla \phi_i \nabla \phi_j \right) \mathrm{d}\Omega = \int_{\Omega} \left(\frac{1}{\Delta t} \phi_i T^{t} \right) \mathrm{d}\Omega$$

We recognize two key blocks that have a specific name:

- $\phi_i \phi_j$: It is called the mass matrix. It models the inertia of a system.
- $\nabla \phi_i \nabla \phi_j$: It is called the stiffness matrix.

These names come from solid mechanics.

Alternatives

We have seen only one approach (Euler's method) to treat the transient terms. We can do the same thing with all sort of time-stepping schemes:

- Backward finite difference (BDF) from order 1 to order n
- Runge-Kutta methods (RK, IRK, DIRK, SDIRK, etc.)
- And so on and so forth...

This is an active research field. The same idea always applies, but the devil is in the details (as always).

Outline

Motivation

The advection-diffusion equation arises in several physical phenomena and it is defined for a scalar c follows:

$$\boldsymbol{v} \cdot \nabla c - D\nabla^2 c = 0$$

where $\boldsymbol{v}$ is a velocity vector. In 1D this equation can be written as follows:

$$v_x \frac{\mathrm{d}c}{\mathrm{d}x} - D\frac{\mathrm{d}^2 c}{\mathrm{d}x^2} = 0$$

Let us check the dimensions of this equation and find its dimensionless form.

Consequences

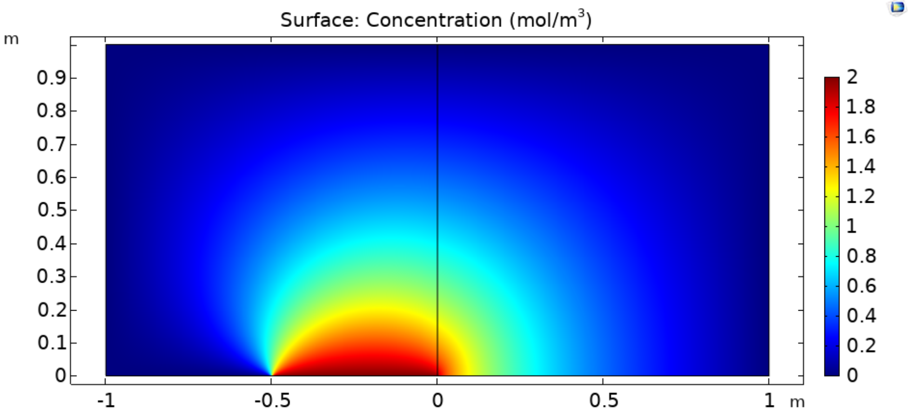
$$\underbrace{\bar{\boldsymbol{v}} \cdot \nabla c}_{\text{Advection}} - \frac{1}{\mathrm{Pe}} \underbrace{\nabla^2 c}_{\text{Diffusion}} = 0$$

The behavior of the solution depends on the ratio between the two mechanisms and it is represented by the Peclet number $\mathrm{Pe} = \frac{VL}{D}$.

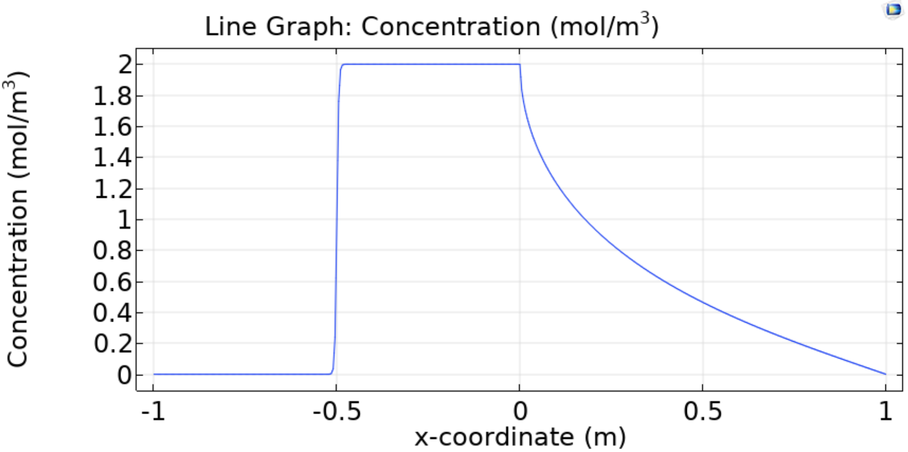
Two limits occur:

- Diffusion dominates when $\mathrm{Pe} \leq 1$
- Advection dominates when $\mathrm{Pe} \gg 1$

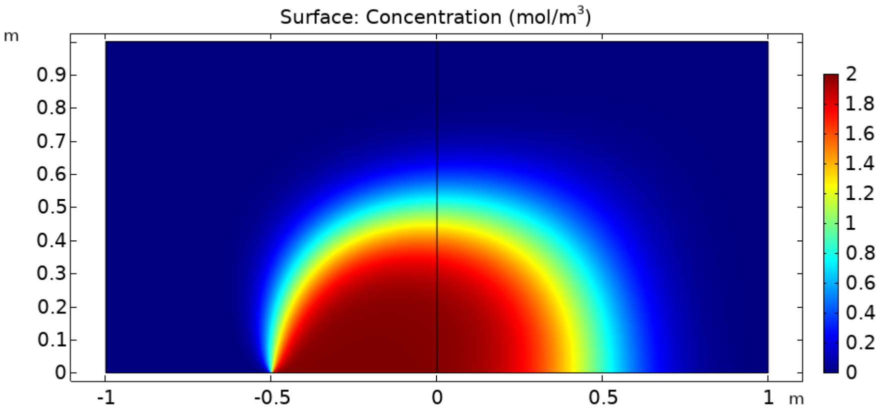
$\mathrm{Pe} = 1$ - **Strong diffusion**



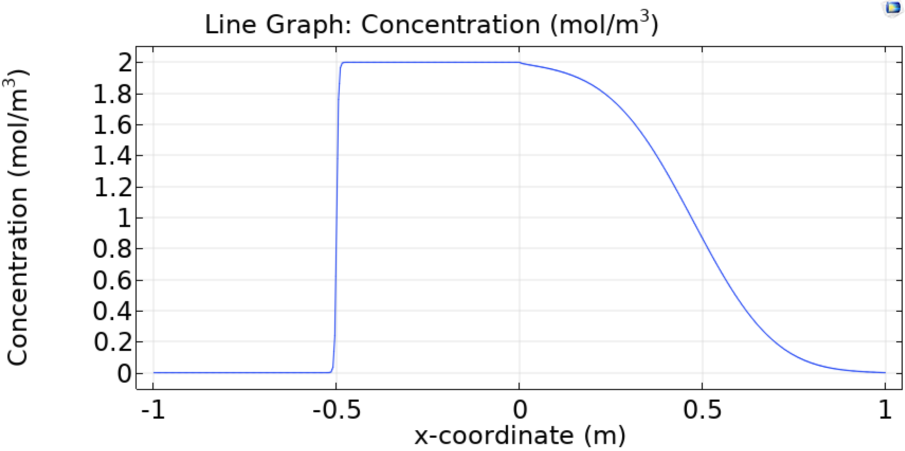
$\mathrm{Pe} = 1$ - **Strong diffusion**



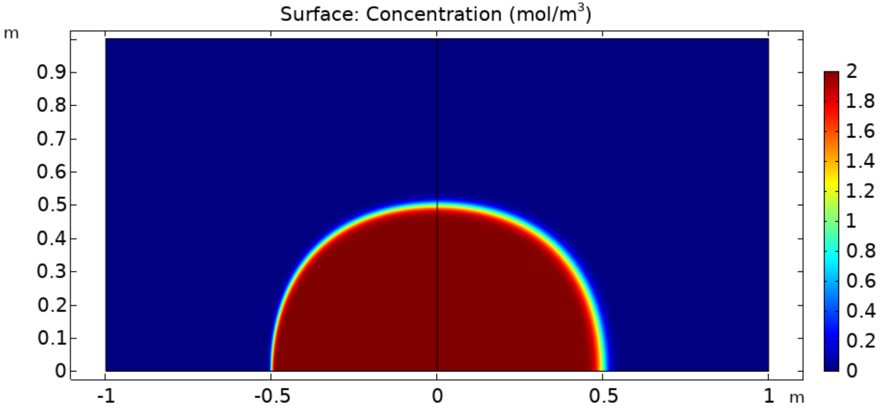
$\mathrm{Pe} = 100$ - **Balanced**



$\mathrm{Pe} = 100$ - **Balanced**



$\mathrm{Pe} = 10^4$ - **Advection dominates**



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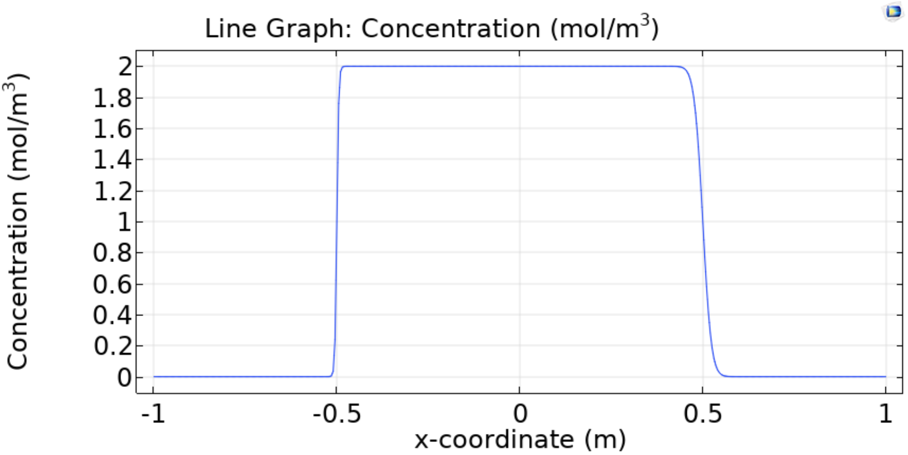


Toy problem 1 (TP1)

Solve the following equation:

$$v\frac{\partial c}{\partial x} - D\frac{\partial^2 c}{\partial x^2} = 0$$

on domain $\Omega = [0, L]$ with the following boundary conditions:

$$c(x = 0) = 0$$
$$c(x = L) = 1$$

and $v = 1$.

TP1: Dimensionless

We first write it in its dimensionless form in terms of the Pe number:

$$\frac{\partial c}{\partial \bar{x}} - \frac{1}{\mathrm{Pe}} \frac{\partial^2 c}{\partial \bar{x}^2} = 0$$

Then, we find the boundary conditions for the new variable $\bar{x}$:

$$c(\bar{x} = 0) = 0 \quad c(\bar{x} = 1) = 1$$

There is an analytical solution for this problem:

$$c = \frac{\exp(\mathrm{Pe}\,\bar{x}) - 1}{\exp(\mathrm{Pe}) - 1}$$

Toy problem 2 (TP2)

We want to solve the same equation but with a right hand side and different boundary conditions:

$$\frac{\mathrm{d}c}{\mathrm{d}\bar{x}} - \frac{1}{\mathrm{Pe}}\frac{\mathrm{d}^2c}{\mathrm{d}\bar{x}^2} = 1$$

on a domain $\Omega = [0, 1]$ with $v = 1$ and $c(0) = c(1) = 0$.

The analytical solution for this problem is given as follows:

$$c = x - \frac{\exp\left(-\mathrm{Pe}(1-x)\right) - \exp\left(-\mathrm{Pe}\right)}{1 - \exp\left(-\mathrm{Pe}\right)}$$

Finite element formulation

Let us establish the weak form of the problem with Dirichlet boundary conditions:

$$\boldsymbol{v} \cdot \nabla c - \frac{1}{\mathrm{Pe}} \nabla^2 c = 0$$

Note that we do it for the dimensionless form and with tensor notation so that it is valid for all dimensions.

Solution

Weak form:

$$\int_{\Omega} u\boldsymbol{v} \cdot \nabla c \,\mathrm{d}\Omega + \int_{\Omega} \frac{1}{\mathrm{Pe}} \nabla u \cdot \nabla c \,\mathrm{d}\Omega = 0$$

Which from now on we will note:

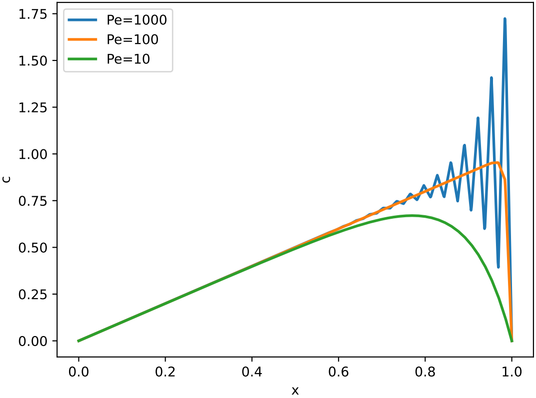
$$(\boldsymbol{v} \cdot \nabla c, u)_{\Omega} + (1/\mathrm{Pe} \nabla c, \nabla u)_{\Omega} = 0$$

with $c, u \in H^1(\Omega)$.

TP2: Solution as function of Pe

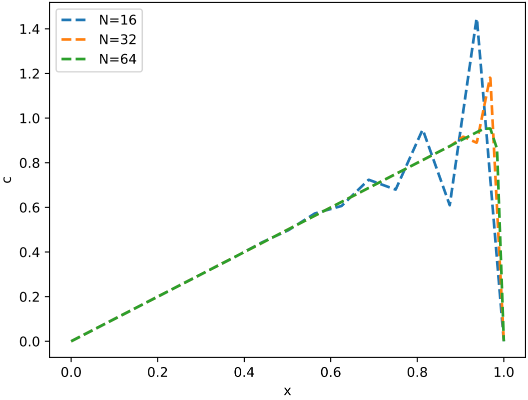
$$\frac{\mathrm{d}c}{\mathrm{d}x} - \frac{1}{\mathrm{Pe}}\frac{\mathrm{d}^2 c}{\mathrm{d}x^2} = 1$$

On domain $\Omega = [0, 1]$ with $c(0) = c(1) = 0$.

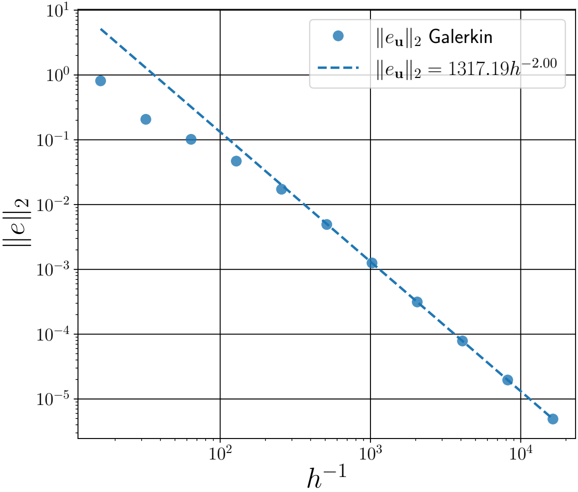


TP2: Solution as function of refinement

Refining the mesh fixes the issue. In this case, for $\mathrm{Pe} = 100$.



Convergence?



What is happening here?

A simple description

As Pe increases, we lose control of the gradients of c. For large values of Pe we have thin regions (layers) in which the solution changes rapidly. The Galerkin method has severe issues in handling this layers and tends to generate oscillations which will propagate throughout the domain. Once $\frac{1}{\mathrm{Pe}}$ becomes smaller than the mesh size, this issue occurs.

Mathematically

$$\left\| c - c^h \right\|_{H^1} \leq \left(1 + C_p^{-2}\right)\left(1 + Pe\right) C_h h$$

with C_p and C_h constants. c is the analytical solution and c^h is the numerical solution.

Idea

We will denote from now on $D = \frac{1}{\mathrm{Pe}}$. The issue we have is that when D is too small:

$$(\boldsymbol{v} \cdot \nabla c, u)_\Omega + (D \nabla c, \nabla u)_\Omega = 0$$

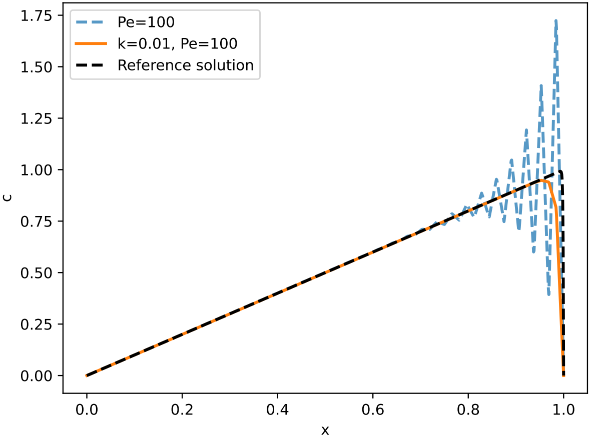
we observe oscillations in the solution. The natural solution is to add more diffusion to the problem to stabilize the solution. We do so by adding k diffusion as follows:

$$(\boldsymbol{v} \cdot \nabla c, u)_\Omega + (D \nabla c, \nabla u)_\Omega + (k \nabla c, \nabla u)_\Omega = 0$$

This will fix our issue, because layers will be allowed to diffuse. However, how do we choose k?

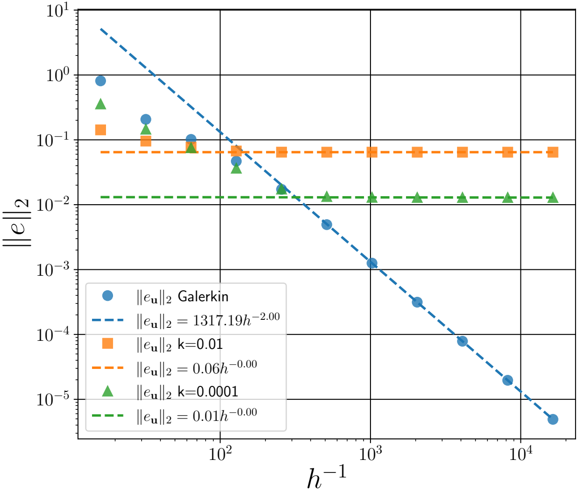
Solution obtained

Adding k allows us to recover a smooth solution:



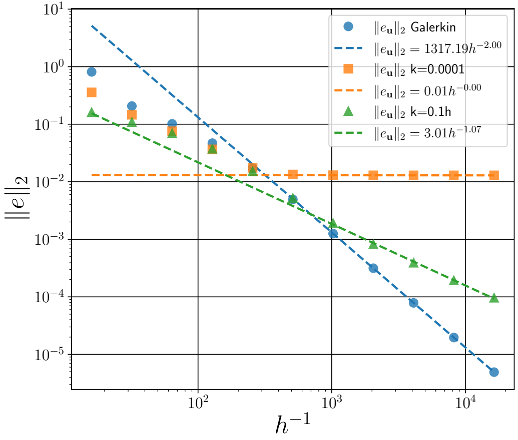
Convergence

Choosing a finite value of k creates a variational inconsistency:



Convergence

A solution is to choose k such that it depends on the element size h. This recovers a form of variational consistency, but lowers the order of the underlying scheme.



Partial conclusion

Adding artificial diffusion has the following consequences:

- Regularizes the solution to ensure that the gradients are bounded.
- Leads to a form of variational inconsistency (lowered order of convergence).
- Adds significant diffusion in the cross-wind direction (will not show up in 1D, but will in 2D and 3D) $\rightarrow$ **not shown here** .

We need a solution which adds diffusion in a more coherent way...

Streamline artificial diffusion

A solution to mitigate this problem is to add artificial diffusion in a single direction (the velocity direction).

$$\boldsymbol{v} \cdot \nabla c - \nabla \cdot \left(D\mathcal{I} \cdot \nabla c + \kappa \cdot \nabla c \right) = 0$$

where $\boldsymbol{\kappa}$ is a diffusion tensor. What does it look like?

Building it

Thus we obtain

$$\boldsymbol{v} \cdot \nabla c - \nabla \cdot \left(D\mathcal{I} \cdot \nabla c + \frac{\kappa}{\|v\|^2} \boldsymbol{v} \otimes \boldsymbol{v} \cdot \nabla c \right) = 0$$

we use this to define:

$$\tau = \frac{\kappa}{\|v\|^2}$$

Let's now do the weak form and figure things out.

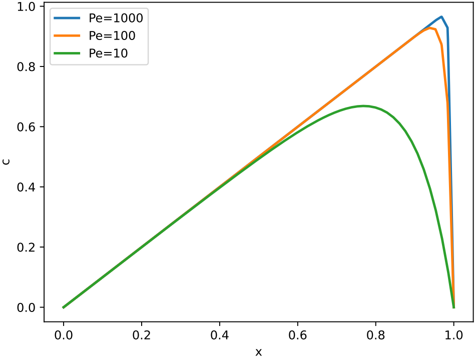
Final form

After integrating by parts we obtain:

$$(\boldsymbol{v} \cdot \nabla c, u)_\Omega + (D\nabla c, \nabla u)_\Omega + (\tau \boldsymbol{v} \cdot \nabla c, \boldsymbol{v} \cdot \nabla u)_\Omega = 0$$

The consequence of this is that now that artificial diffusion is only applied in the direction of the velocity vector. This is the **streamline artificial diffusion** method.

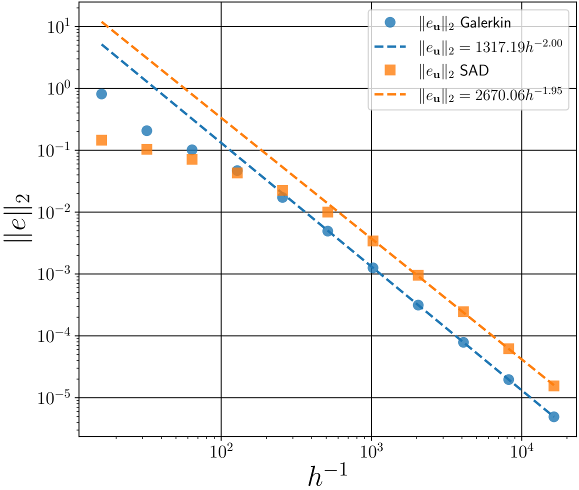
TP2: Result



No oscillations observed... what about convergence?

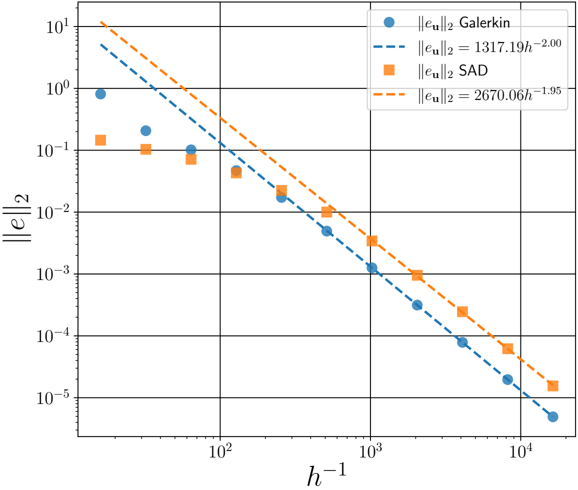
TP1: Convergence

We obtain the expected order with Q1 elements:

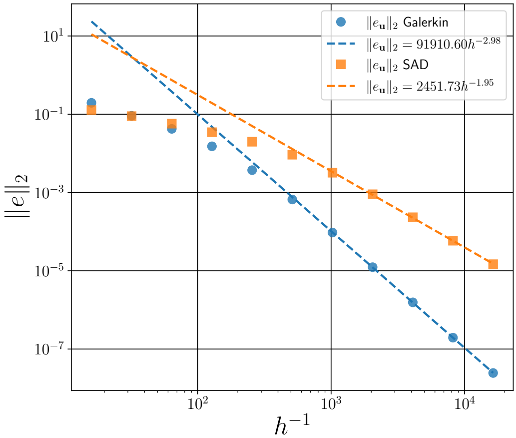


TP2: Convergence

We obtain the expected order with Q1 elements:



TP1: High-order convergence



Does not obtain the right order when using Q2 elements...

Variational consistency

Consider again TP1:

$$\boldsymbol{v} \cdot \nabla c - D\nabla^2 c = 0$$

For which the weak form is:

$$(\boldsymbol{v} \cdot \nabla c, u)_\Omega + (D\nabla c, \nabla u)_\Omega = 0$$

and with streamline artificial diffusion:

$$(\boldsymbol{v} \cdot \nabla c, u)_\Omega + (D\nabla c, \nabla u)_\Omega + (\tau \boldsymbol{v} \cdot \nabla c, \boldsymbol{v} \cdot \nabla u)_\Omega = 0$$

The main issue is that if $(\tau \boldsymbol{v} \cdot \nabla c, \boldsymbol{v} \cdot \nabla u)_\Omega$ does not vanish variational consistency is not recovered. So what happened when we moved from Q1 to Q2?

Variational consistency

Consider a generalized form of TP2:

$$\boldsymbol{v} \cdot \nabla c - D\nabla^2 c = f$$

For which the weak form is:

$$(\boldsymbol{v} \cdot \nabla c, u)_\Omega + (D\nabla c, \nabla u)_\Omega - (f, u)_\Omega = 0$$

and with streamline artificial diffusion:

$$(\boldsymbol{v} \cdot \nabla c, u)_\Omega + (D\nabla c, \nabla u)_\Omega - (f, u)_\Omega + (\tau \boldsymbol{v} \cdot \nabla c, \boldsymbol{v} \cdot \nabla u)_\Omega = 0$$

The same issue could also occur at Q1 if f is a non-trivial function... (I thought it would actually occur in the present case, it did not.)

Idea

The main idea behind SUPG (which is a brillant one) is to transform streamline artificial diffusion into something that is **variationally consistent**. This is achieved by using the residual of the equation. Starting from our PDE:

$$\boldsymbol{v} \cdot \nabla c - D\nabla^2 c = 1$$

We define the strong residual $R(c)$ as:

$$R(c) = \boldsymbol{v} \cdot \nabla c - D\nabla^2 c - 1$$

This will be used for our upwinding.

Result

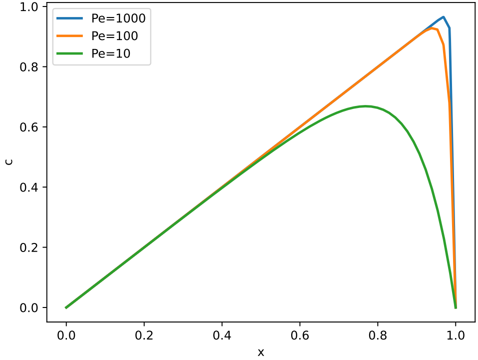
$$
\begin{aligned}
(\boldsymbol{v}\cdot\nabla c, u)_\Omega + (D\nabla c, \nabla u)_\Omega - (1,u)_\Omega +& \\
&(\tau(\boldsymbol{v}\cdot\nabla c - D\nabla^2 c - 1), \boldsymbol{v}\cdot\nabla u)_\Omega = 0
\end{aligned}
$$

This is the Streamline-Upwind / Petrov-Galerkin (SUPG) method which was first published by Brooks and Hughes in 1982. This was a revolution in the world of the finite element method.
It is a very interesting approach because it is an upwinding method that preserves the order of the underlying scheme and just adds the right about of numerical diffusion.

Results

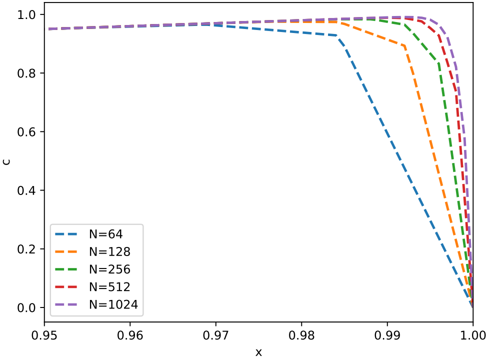
It works... (luckily for me heh?)

The solution appears less continuous as the Péclet number increases. It has more jagged edges. We will understand why in what follows...

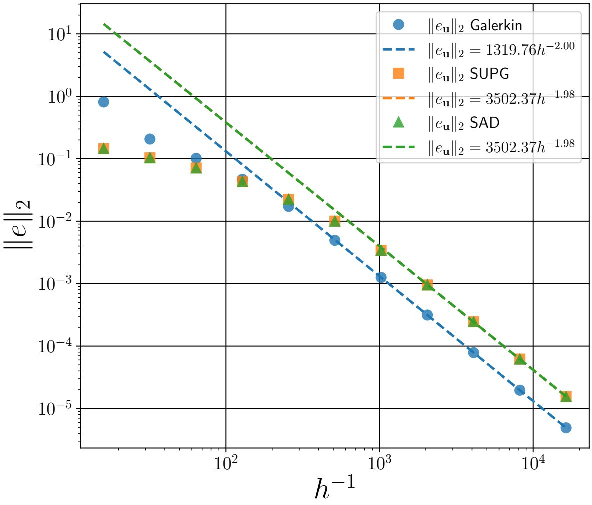


Influence of the mesh

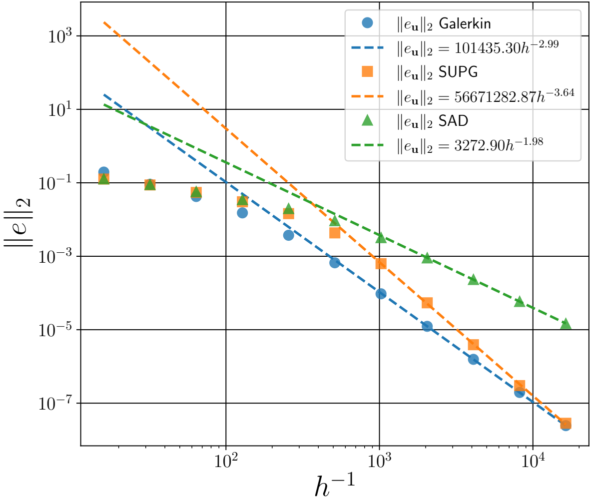
Stabilization introduces just enough numerical diffusion to ensure that the solution is adequate.



Convergence Q1

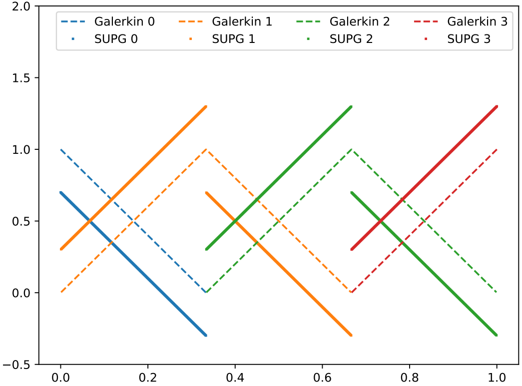


Convergence Q2



Interpretation

The Streamline Upwind Petrov-Galerkin method skews the test function of the FEM scheme to be larger *upwind* then *downwind* by using the strong form of the integral.



Outline

Two important topics

Transient problems

Transient problems are critical in engineering. The FEM is quite able to solve them easily. Extending a solver to solve a transient problem is relatively straightforward, depending on the time-stepping scheme you use.

Transport problems

Transport problems are very subtle. Solving them with FEM is quite challenging and the literature on stabilized method is very difficult to understand. FEM works correctly for transport problems, but it is less straightforward to implement than it is for the Finite Volume Method for example. Hence the latter being more common in CFD. The literature on this is huge! There are many alternatives such as **Discontinuous Galerkin** methods.