Time-dependent variational methods

MATMEK-4270

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Time dependent variational forms

In lectures 11-12 we have considered steady equations like

$$\mathcal{L}(u) = f$$

for a variety of operators $\mathcal{L}$ and a numerical solution depending only on space $u_N(\boldsymbol{x})$.

In this lecture we will add two types of time-dependency

$$\frac{\partial u}{\partial t} + \mathcal{L}(u) = f \quad \text{and} \quad \frac{\partial^2 u}{\partial t^2} + \mathcal{L}(u) = f$$

and approximations $u_N(\boldsymbol{x}, t) \in V_N = \text{span}\{\psi_j\}_{j=0}^N$:

$$u_N(\boldsymbol{x}, t) = \sum_{j=0}^{N} \hat{u}_j(t)\psi_j(\boldsymbol{x})$$

where the expansion coefficients are time dependent.

Finite difference in time, Galerkin in space

Consider the equation

$$\frac{\partial u}{\partial t} + \mathcal{L}(u) = f$$

A finite difference approximation in time, with forward Euler:

$$\frac{u^{n+1} - u^n}{\Delta t} + \mathcal{L}(u^n) = f^n$$

where

$$u^n(\boldsymbol{x}) = u(\boldsymbol{x}, t_n), f^n(\boldsymbol{x}) = f(\boldsymbol{x}, t_n)$$

and time is discretized as always for time domain $[0, T]$

$$t_n = n\Delta t, \quad n = 0, 1, \ldots, N_t, \quad N_t = T/\Delta t$$

We normally drop the spatial dependence and write only u^n or f^n.

The residual is now a function of time

$$\mathcal{R}(u^{n+1}; u^n) = \frac{u^{n+1} - u^n}{\Delta t} + \mathcal{L}(u^n) - f^n$$

> **Note**
>
> The notation $\mathcal{R}(u^{n+1}; u^n)$ is used to indicate that u^{n+1} is the unknown and u^n (right of the semicolon) is known.

Introduce the approximation to $u^n(\boldsymbol{x}) = u(\boldsymbol{x}, t_n)$

$$u(\boldsymbol{x}, t_n) \approx u_N^n(\boldsymbol{x}) = \sum_{j=0}^{N} \hat{u}_j^n \psi_j(\boldsymbol{x})$$

where $\hat{u}_j^n = \hat{u}_j(t_n)$ are the time dependent expansion coefficients (the unknowns at time t_n). Insert into the residual to get the **numerical residual**

$$\mathcal{R}_N = \mathcal{R}(u_N^{n+1}; u_N^n) = \frac{u_N^{n+1} - u_N^n}{\Delta t} + \mathcal{L}(u_N^n) - f^n$$

The method of weighted residuals

The method of weighted residuals is to find $u_N^{n+1} \in V_N$ such that

$$(\mathcal{R}_N, v) = 0, \quad \forall\, v \in W$$

and for the Galerkin method $W = V_N$.

In order to solve the time-dependent problem we need to solve this Galerkin problem many times. The procedure is

1. Initialize $u_N^0(\boldsymbol{x})$ by projecting the given initial condition $u(\boldsymbol{x}, 0)$ to V_N (function approximation, see lectures 8, 9). That is, find $u_N^0 \in V_N$ such that

$$(u_N^0 - u(\boldsymbol{x}, 0), v) = 0, \quad \forall\, v \in V_N$$

2. For $n = 0, 1, \ldots, N_t - 1$ find $u_N^{n+1} \in V_N$ such that

$$(\mathcal{R}_N, v) = 0, \quad \forall\, v \in V_N$$

Stability of time-dependent variational methods

Recap - remember the early lectures 2, 3 and 5

$$\text{Exponential decay} \quad \frac{\partial u(t)}{\partial t} = -au(t)$$

$$\text{Vibration equation} \quad \frac{\partial^2 u(t)}{\partial t^2} + \omega^2 u(t) = 0$$

$$\text{Wave equation} \quad \frac{\partial^2 u(x,t)}{\partial t^2} = c^2 \frac{\partial^2 u(x,t)}{\partial x^2}$$

In order to study stability we introduced the ansatz

$$u^{n+1} = gu^n \rightarrow u^n = g^n u^0$$

into the discretized equations. For stability we required $|g| \leq 1$.

We actually called the amplification factor A, but since then we have started using matrices that we rather have as A. Hence the amplification factor is now called g.

Recap vibration equation

$$\frac{\partial^2 u(t)}{\partial t^2} + \omega^2 u(t) = 0$$

Discretize with central finite difference

$$\frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2} + \omega^2 u^n = 0$$

Insert for ansatz $u^n = g^n u^0$

$$g^n(g - 2 + g^{-1})u^0 + (\omega\Delta t)^2 g^n u^0 = 0$$

Divide by $g^n u^0$

$$g + g^{-1} = 2 - (\omega\Delta t)^2$$

and solve quadratic equation (g may be complex) to find stability $|g| = 1$ for $\omega\Delta t \leq 2$

Recap - stability of the diffusion equation

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2}$$

Use forward Euler in time and central difference in space

$$u_j^{n+1} - u_j^n = \frac{\Delta t}{\Delta x^2}(u_{j+1}^n - 2u_j^n + u_{j-1}^n)$$

where $u_j^n = u(j\Delta x, n\Delta t)$ and $x_j = j\Delta x$ and $t_n = n\Delta t$. Make the ansatz as always

$$u_j^{n+1} = g u_j^n \rightarrow u_j^n = g^n u_j^0$$

and let the initial condition be a periodic Fourier wave with wavenumber k

$$u_j^0 = e^{\hat{\imath} k x_j}$$

where $\hat{\imath} = \sqrt{-1}$.

Write the equation in matrix form

$$u_j^{n+1} - u_j^n = \frac{\Delta t}{\Delta x^2}(u_{j+1}^n - 2u_j^n + u_{j-1}^n)$$

$$\boldsymbol{u}^n = (u_j^n)_{j=0}^N$$

$$\boldsymbol{u}^{n+1} - \boldsymbol{u}^n = \frac{\Delta t}{\Delta x^2}\tilde{D}^{(2)}\boldsymbol{u}^n$$

$$D^{(2)} = \frac{1}{\Delta x^2}\tilde{D}^{(2)} = \frac{1}{\Delta x^2}\underbrace{\begin{bmatrix} -2 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ \vdots & & & \ddots & & & & \cdots \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix}}_{\tilde{D}^{(2)}}$$

Find the amplification factor

$$\boldsymbol{u}^{n+1} - \boldsymbol{u}^n = \frac{\Delta t}{\Delta x^2}\tilde{D}^{(2)}\boldsymbol{u}^n$$

Insert for ansatz $\boldsymbol{u}^n = g^n\boldsymbol{u}^0$

$$(g-1)\boldsymbol{u}^0 = \frac{\Delta t}{\Delta x^2}\tilde{D}^{(2)}\boldsymbol{u}^0$$

Inserting for $u_j^0 = e^{\hat{\imath}kj\Delta x}$ we get

$$(g-1)e^{\hat{\imath}kj\Delta x} = \frac{\Delta t}{\Delta x^2}(e^{\hat{\imath}k(j+1)\Delta x} - 2e^{\hat{\imath}kj\Delta x} + e^{\hat{\imath}k(j-1)\Delta x})$$

Divide by $e^{\hat{\imath}kj\Delta x}$ to obtain

$$g - 1 = \frac{\Delta t}{\Delta x^2}(e^{\hat{\imath}k\Delta x} - 2 + e^{-\hat{\imath}k\Delta x})$$

Simplify $g - 1 = \frac{\Delta t}{\Delta x^2}(e^{\hat{\imath} k \Delta x} - 2 + e^{-\hat{\imath} k \Delta x})$

Use $e^{\hat{\imath} x} + e^{-\hat{\imath} x} = 2\cos x, \cos(2x) = \cos^2 x - \sin^2 x$ and $1 = \cos^2 x + \sin^2 x$

$$g = 1 - \frac{4\Delta t}{\Delta x^2}\sin^2\left(\frac{k\Delta x}{2}\right)$$

We want $|g| \leq 1$, so we need

$$\left|1 - \frac{4\Delta t}{\Delta x^2}\sin^2\left(\frac{k\Delta x}{2}\right)\right| \leq 1$$

Since $\sin^2(k\Delta x/2) \leq 1$ and positive, we get that $1 - \frac{4\Delta t}{\Delta x^2}$ is always less than 1. However, $1 - \frac{4\Delta t}{\Delta x^2}$ can be smaller than -1, and that gives us the stability limit

$$1 - \frac{4\Delta t}{\Delta x^2} \geq -1 \Rightarrow \boxed{\Delta t \leq \frac{\Delta x^2}{2}}$$

A lot of hard work to find

$$\left|1 - \frac{4\Delta t}{\Delta x^2}\right| \leq 1 \Rightarrow \Delta t \leq \frac{\Delta x^2}{2}$$

Can we find an easier approach?

We have the simple looking formula

$$(g-1)\boldsymbol{u}^0 = \frac{\Delta t}{\Delta x^2}\tilde{D}^{(2)}\boldsymbol{u}^0$$

But how can we eliminate the two $\boldsymbol{u}^0$ terms on each side when there is the matrix $\tilde{D}^{(2)}$?

Eigenvalues! The eigenvalues λ of a matrix A with associated eigenvectors $\boldsymbol{x}$ are

$$A\boldsymbol{x} = \lambda\boldsymbol{x}$$

Hence the simplification $\tilde{D}^{(2)}\boldsymbol{u}^0 = \lambda\boldsymbol{u}^0$ and

$$(g-1)\boldsymbol{u}^0 = \frac{\Delta t}{\Delta x^2}\lambda\boldsymbol{u}^0 \Rightarrow g = 1 + \frac{\lambda\Delta t}{\Delta x^2}$$

Stability limit through eigenvalues

Assume the ansatz $\boldsymbol{u}^n = g^n \boldsymbol{u}^0$:

$$(g-1)\boldsymbol{u}^0 = \frac{\Delta t}{\Delta x^2}\tilde{D}^{(2)}\boldsymbol{u}^0$$

Insert for $\tilde{D}^{(2)}\boldsymbol{u}^0 = \lambda \boldsymbol{u}^0$ to get

$$g = 1 + \frac{\lambda \Delta t}{\Delta x^2}$$

To satisfy $|g| \leq 1$

$$|g| = |1 + \frac{\lambda \Delta t}{\Delta x^2}| \leq 1$$

But we need to compute the eigenvalues..

Compute eigenvalues

```
1 import numpy as np
2 from scipy import sparse
3 N = 11
4 D2 = sparse.diags((1, 1, -2, 1, 1), (-N, -1, 0, 1, N), shape=(N+1, N+1))
5 Lambda = np.linalg.eig(D2.toarray())[0]
6 Lambda
```

```
array([ 0.        , -0.26794919, -1.        , -2.        , -3.        ,
       -4.        , -3.73205081, -0.26794919, -1.        , -3.73205081,
       -2.        , -3.        ])
```

The minimum eigenvalue is -4 (worst case). Hence we obtain again exactly the same limit

$$|1 + \frac{\lambda \Delta t}{\Delta x^2}| \leq 1 \Rightarrow |1 - \frac{4\Delta t}{\Delta x^2}| \leq 1 \Rightarrow \Delta t \leq \frac{\Delta x^2}{2}$$

But with a lot less work!

> **Note**
>
> The complex exponentials $e^{\hat{ikx}}$ are **eigenfunctions** of the Laplace operator in 1D, so we actually used eigenvalue theory also for the hard approach, we just did not mention it!

Stability of the forward Euler method for the Galerkin method

For the forward Euler method we now consider instead the Galerkin method for the discretization of space (instead of finite differences)

$$(\mathcal{R}_N, v) = 0 \Rightarrow \left(u_N^{n+1}, v\right) = (u_N^n, v) + \Delta t \, (\mathcal{L}(u_N^n), v)$$

and make the same ansatz as before

$$u_N^{n+1} = g u_N^n \quad \text{and thus} \quad u_N^n = g^n u_N^0$$

Insert into the variational form

$$\left(g^{n+1} u_N^0, v\right) = \left(g^n u_N^0, v\right) + \Delta t \left(\mathcal{L}(g^n u_N^0), v\right)$$

Divide by g^n (g is not dependent on x) to obtain

$$g \left(u_N^0, v\right) = \left(u_N^0, v\right) + \Delta t \left(\mathcal{L}(u_N^0), v\right)$$

Derive the linear algebra form

Insert for $u_N^0 = \sum_{j=0}^{N} \hat{u}_j^0 \psi_j$ and $v = \psi_i$ to obtain

$$g \sum_{j=0}^{N} (\psi_j, \psi_i) \hat{u}_j^0 = \sum_{j=0}^{N} (\psi_j, \psi_i) \hat{u}_j^0 + \Delta t \sum_{j=0}^{N} (\mathcal{L}(\psi_j), \psi_i) \hat{u}_j^0$$

In matrix form this is

$$gA\hat{\boldsymbol{u}}^0 = A\hat{\boldsymbol{u}}^0 + \Delta t M \hat{\boldsymbol{u}}^0$$

where $a_{ij} = (\psi_j, \psi_i)$ and $m_{ij} = (\mathcal{L}(\psi_j), \psi_i)$. Multiply from the left by A^{-1} to obtain

$$g\hat{\boldsymbol{u}}^0 = \hat{\boldsymbol{u}}^0 + \Delta t A^{-1} M \hat{\boldsymbol{u}}^0$$

Compute the eigenvalues λ of the matrix $H = A^{-1}M$ such that $H\hat{\boldsymbol{u}}^0 = \lambda \hat{\boldsymbol{u}}^0$ and

$$g\hat{\boldsymbol{u}}^0 = \hat{\boldsymbol{u}}^0 + \lambda \Delta t \hat{\boldsymbol{u}}^0 \Rightarrow \boxed{g = 1 + \lambda \Delta t}$$

$$\text{Stability limit:} \quad |g| = |1 + \lambda \Delta t| \leq 1$$

Complete worked example, the diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad x, t \in (0, L) \times (0, T]$$

$$u(x, 0) = \sin(\pi x/L) + \sin(10\pi x/L)$$
$$u(0, t) = 0, u(L, t) = 0$$

Forward Euler in time, Galerkin in space, and Dirichlet Legendre polynomials:

$$\text{Basis:} \qquad \psi_j(x) = P_j(X) - P_{j+2}(X) \quad V_N = \text{span}\{\psi_j\}_{j=0}^N$$
$$\text{Mapping:} \qquad x(X) = \tfrac{L}{2}(1 + X) \qquad X(x) = \tfrac{2x}{L} - 1$$

We get the variational form used on the previous slide with diffusion for $\mathcal{L}(\psi_j)$ and integration by parts (boundary terms canceled since $\psi_j(0) = \psi_j(L) = 0$):

$$\sum_{j=0}^{N} (\psi_j, \psi_i) \hat{u}_j^{n+1} = \sum_{j=0}^{N} (\psi_j, \psi_i) \hat{u}_j^n - \Delta t \left(\sum_{j=0}^{N} (\psi_j', \psi_i') \hat{u}_j^n - \cancel{[u_N^n \psi_i]_{x=0}^{x=L}} \right)$$

The stiffness matrix (ψ_j', ψ_i')

$$\begin{aligned}\int_0^L \psi_j'(x)\psi_i'(x)dx &= \int_{-1}^1 (P_j'(X) - P_{j+2}'(X))\frac{dX}{dx}(P_i'(X) - P_{i+2}'(X))\frac{dX}{dx}\frac{dx}{dX}dX \\ &= \frac{2}{L}\int_{-1}^1 (P_j'(X) - P_{j+2}'(X))(P_i'(X) - P_{i+2}'(X))dX \\ &= \frac{2}{L}(P_j' - P_{j+2}', P_i' - P_{i+2}')_{L^2(-1,1)}\end{aligned}$$

Using equality: $(2j+3)P_{j+1} = P_{j+2}' - P_j'$ and $(P_{i+1}, P_{j+1})_{L^2(-1,1)} = \|P_{i+1}\|^2\delta_{ij}$ and $\|P_i\|^2 = \frac{2}{2j+1}$

$$\begin{aligned}\int_0^L \psi_j'(x)\psi_i'(x)dx &= \frac{2}{L}(-(2j+3)P_{j+1}, -(2j+3)P_{i+1}) \\ &= \frac{2}{L}(2j+3)^2\|P_{i+1}\|^2\delta_{ij} \\ &= \frac{8j+12}{L}\delta_{ij}\end{aligned}$$

The mass matrix (ψ_j, ψ_i)

$$\begin{aligned}\int_0^L \psi_j(x)\psi_i(x)dx &= \int_{-1}^1 (P_j(X) - P_{j+2}(X))(P_i(X) - P_{i+2}(X))\frac{dx}{dX}dX \\ &= \frac{L}{2}(P_j - P_{j+2}, P_i - P_{i+2})_{L^2(-1,1)} \\ &= \frac{L}{2}((P_j, P_i) - (P_{j+2}, P_i) - (P_j, P_{i+2}) + (P_{j+2}, P_{i+2}))\end{aligned}$$

Using now $(P_j, P_i) = \|P_i\|^2\delta_{ij} = \frac{2}{2i+1}\delta_{ij}$:

$$\begin{aligned} j = i \qquad & (\psi_i, \psi_i) = \tfrac{L}{2}((P_i, P_i) + (P_{i+2}, P_{i+2})) = \tfrac{L}{2}(\|P_i\|^2 + \|P_{i+2}\|^2) \\ j = i+2 \qquad & (\psi_{i+2}, \psi_i) = -(P_{i+2}, P_{i+2}) = -\tfrac{L}{2}\|P_{i+2}\|^2 \end{aligned}$$

Since the mass matrix $a_{ij} = a_{ji} = (\psi_j, \psi_i)$ is symmetric, we get the tri-diagonal

$$a_{ij} = a_{ji} = \frac{L}{2}\begin{cases} \|P_i\|^2 + \|P_{i+2}\|^2, & i = j \\ -\|P_{i+2}\|^2, & j = i+2 \\ 0, & \text{otherwise} \end{cases}$$

Implementation

It is rather messy to work with composite basis functions. A very smart trick is thus to use a **stencil matrix** S, such that (summation on repeated j index)

$$\psi_i = P_i - P_{i+2} = s_{ij} P_j$$

This defines $S \in \mathbb{R}^{(N+1)\times(N+3)}$ for the Dirichlet problem as

$$s_{ij} = \begin{cases} 1 & i = j \\ -1 & j = i+2 \end{cases} \qquad S = \begin{bmatrix} 1 & 0 & -1 & 0 & 0 & \cdots & \\ 0 & 1 & 0 & -1 & 0 & \cdots & \\ 0 & 0 & 1 & 0 & -1 & \cdots & \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \\ 0 & 0 & 0 & \cdots & 1 & 0 & -1 \end{bmatrix}$$

With $\boldsymbol{\psi} = \{\psi_i\}_{i=0}^{N}$ and $\boldsymbol{P} = \{P_i\}_{i=0}^{N+2}$ we get all basis functions in matrix form:

$$\boldsymbol{\psi} = S\boldsymbol{P}$$

Why is the stencil matrix smart?

Consider the mass matrix

$$\begin{aligned}(\psi_j, \psi_i) &= (P_j - P_{j+2}, P_i - P_{i+2}) \\ &= (P_j, P_i) - (P_j, P_{i+2}) - (P_{j+2}, P_i) + (P_{j+2}, P_{i+2})\end{aligned}$$

You need to sort out the four (diagonal) matrices on the right.

Now use stencil matrix instead (summation on k and l):

$$\begin{aligned}(\psi_j, \psi_i) &= (s_{jk} P_k, s_{il} P_l) \\ &= s_{il} (P_l, P_k) s_{jk}\end{aligned}$$

You need only the diagonal matrix $P = ((P_l, P_k))_{k,l=0}^{N+2}$, where $(P_l, P_k) = \frac{2}{2l+1}\delta_{kl}$.

Matrix form

$$A = ((\psi_j, \psi_i))_{i,j=0}^{N} = SPS^T$$

Stiffness matrix through stencil matrix

$$
\begin{aligned}
(\psi_j'', \psi_i) &= (s_{jk} P_k'', s_{il} P_l) \\
&= s_{il} (P_l'', P_k) s_{jk}
\end{aligned}
$$

Again you need only the single matrix using orthogonal polynomials
$q_{kl} = (P_l'', P_k) = -(P_l', P_k')$

$$
M = ((\psi_j'', \psi_i))_{i,j=0}^{N} = SQS^T
$$

Implementation using shenfun

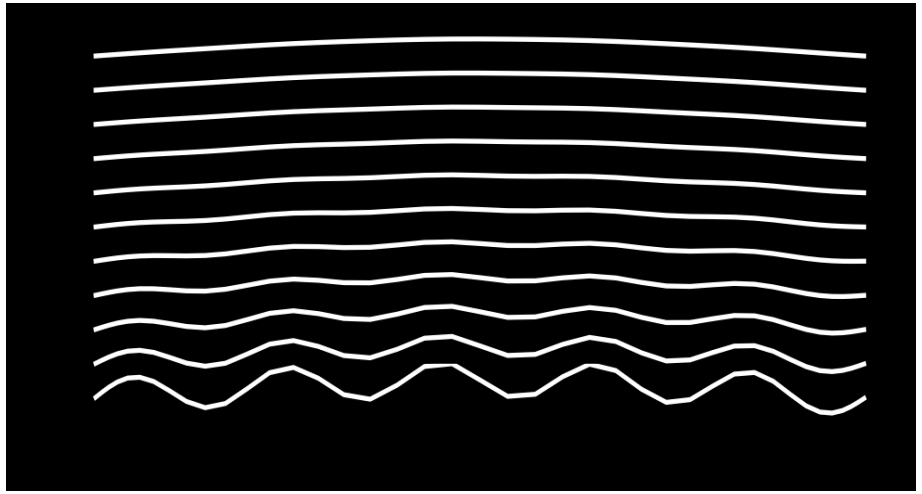
```python
import numpy as np
import sympy as sp
from scipy import sparse
from shenfun import TrialFunction, TestFunction, FunctionSpace, \
    project, inner, Dx, la, Function

x, t, c, L = sp.symbols('x,t,c,L')

class FE_Diffusion:
    def __init__(self, N, L0=1, u0=sp.sin(sp.pi*x/L)+sp.sin(10*sp.pi*x/L), family='L'):
        self.N = N
        self.L = L0
        self.u0 = u0.subs({L: L0})
        self.V = self.get_function_space(family=family)
        self.uh_np1 = Function(self.V)
        self.uh_n = Function(self.V)
        self.A, self.S = self.get_mats()
        self.sol = la.Solver(self.A)
        self.A = self.A.diags()
        self.S = self.S.diags()

    def get_function_space(self, family='L'):
        return FunctionSpace(self.N+1, family, bc=(0, 0), domain=(0, self.L))

    def get_mats(self):
```

Run solver

Use longest stable time step

$dt = 2/\max(\lambda)$

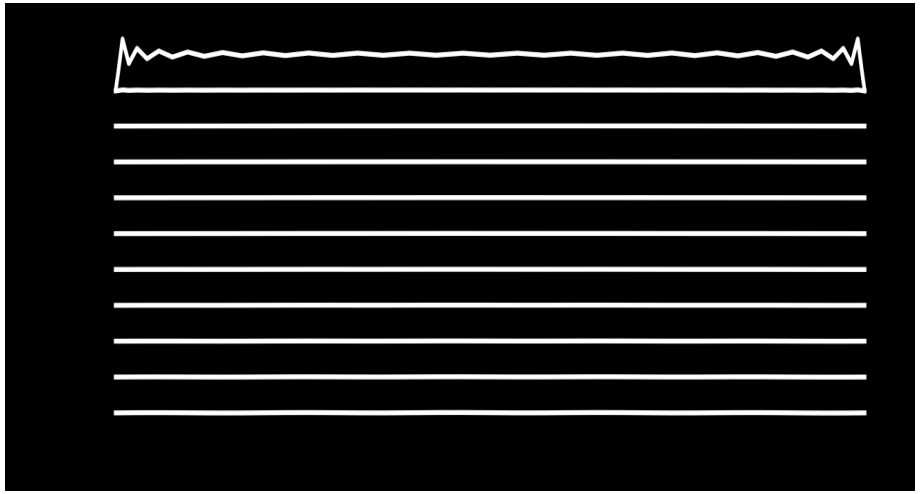
```
from utilities import plot_with_offset
sol = FE_Diffusion(42, L0=2)
dt = 2/max(sol.get_eigenvalues())
data = sol(1000, dt=dt, save_step=100)
plot_with_offset(data, sol.V.mesh(), figsize=(8, 3)
```



Use slightly too large time step

$dt = 2.04/\max(\lambda)$

```
#
#
#
data = sol(1000, dt=dt*1.02, save_step=100)
plot_with_offset(data, sol.V.mesh(), figsize=(8, 3)
```



Backward Euler for diffusion equation

The forward Euler method requires a very short time step for the diffusion equation. How about the backward Euler method

$$\left(u_N^{n+1}, v\right) = \left(u_N^n, v\right) + \Delta t \left(\frac{\partial^2 u_N^{n+1}}{\partial x^2}, v\right)$$

The linear algebra problem is now

$$\sum_{j=0}^{N} \left((\psi_j, \psi_i) + \Delta t(\psi_j', \psi_i')\right)\hat{u}_j^{n+1} = \sum_{j=0}^{N}(\psi_j, \psi_i)\hat{u}_j^n$$

Insert the ansatz $u_N^{n+1} = g u_N^n$

$$\sum_{j=0}^{N} g\left((\psi_j, \psi_i) + \Delta t(\psi_j', \psi_i')\right)\hat{u}_j^{0} = \sum_{j=0}^{N}(\psi_j, \psi_i)\hat{u}_j^0$$

Backward Euler on matrix form

$$\sum_{j=0}^{N} g\left((\psi_j, \psi_i) + \Delta t(\psi_j', \psi_i')\right)\hat{u}_j^0 = \sum_{j=0}^{N}(\psi_j, \psi_i)\hat{u}_j^0$$

becomes

$$g(A + \Delta t S)\hat{\boldsymbol{u}}^0 = A\hat{\boldsymbol{u}}^0$$

If we multiply from left to right by A^{-1} we get

$$g(I + \Delta t A^{-1} S)\hat{\boldsymbol{u}}^0 = \hat{\boldsymbol{u}}^0$$

Here we can once again use $H = A^{-1}S$ and $H\hat{\boldsymbol{u}}^0 = \lambda\hat{\boldsymbol{u}}^0$ and thus we find

$$g = \frac{1}{1 + \Delta t\lambda}$$

Since all time steps and eigenvalues are real numbers larger than 0, g is always less than 1 and positive and the backward Euler method is as such *unconditionally* stable.

The wave equation as a variational problem

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}, \quad (x,t) \in (0,L) \times (0,T]$$

$$u(x,0) = f(x) \quad \frac{\partial u}{\partial t}(x,0) = 0$$

We will consider both Dirichlet and Neumann boundary conditions in space and use finite differences in time such that

$$\frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2} = c^2 \frac{\partial^2 u^n}{\partial x^2}$$

A numerical residual $\mathcal{R}_N = \mathcal{R}(u_N^{n+1}; u_N^n, u_N^{n-1})$ can now be defined as

$$\mathcal{R}_N = u_N^{n+1} - 2u_N^n + u_N^{n-1} - \alpha^2 (u_N^n)''$$

with $\alpha = c\Delta t$ and $u' = \frac{\partial u}{\partial x}$.

The Galerkin methods for the wave equation

Initialize u_N^0 and u_N^1. The Galerkin method is to find $u_N^{n+1} \in V_N$ such that

$$\left(u_N^{n+1} - 2u_N^n + u_N^{n-1} - \alpha^2 (u_N^n)'', v\right) = 0, \quad \forall\, v \in V_N$$

for $n = 1, \ldots, N_t - 1$. We can also integrate the last term by parts

$$(u_N^{n+1} - 2u_N^n + u_N^{n-1}, v) + \alpha^2 \left(((u_N^n)', v') - \left[(u_N^n)' v\right]_{x=0}^{x=L} \right) = 0, \quad \forall\, v \in V_N$$

Insert for $u_N^{n-1}, u_N^n, u_N^{n+1} \in V_N$ and use $v = \psi_i$ to get the linear algebra problem

$$\sum_{j=0}^{N} (\psi_j, \psi_i) \left(\hat{u}_j^{n+1} - 2\hat{u}_j^n + \hat{u}_j^{n-1} \right) + \alpha^2 \left(\sum_{j=0}^{N} (\psi_j', \psi_i') \hat{u}_j^n - \left[(u_N^n)' \psi_i\right]_{x=0}^{x=L} \right) = 0$$

> **Note**
>
> All time dependency is in the expansion coefficients $\hat{u}_j^{n+1}, \hat{u}_j^n, \hat{u}_j^{n-1}$.

Matrix form

Rearrange such that the unknown $\hat{u}_j^{n+1}$ is on the left hand side and the rest of the known terms are on the right hand side

$$\sum_{j=0}^{N} (\psi_j, \psi_i)\hat{u}_j^{n+1} = \sum_{j=0}^{N} (\psi_j, \psi_i)(2\hat{u}_j^n - \hat{u}_j^{n-1}) - \alpha^2 \left(\sum_{j=0}^{N} \left(\psi_j', \psi_i'\right)\hat{u}_j^n - \left[(u_N^n)'\psi_i\right]_{x=0}^{x=L} \right)$$

With matrix notation, $a_{ij} = (\psi_j, \psi_i)$ and $s_{ij} = (\psi_j', \psi_i')$, we get

$$A\hat{\boldsymbol{u}}^{n+1} = A(2\hat{\boldsymbol{u}}^n - \hat{\boldsymbol{u}}^{n-1}) - \alpha^2 \left(S\hat{\boldsymbol{u}}^n - \boldsymbol{b}^n\right)$$

where $\boldsymbol{b}^n = ((u_N^n)'(L)\psi_i(L) - (u_N^n)'(0)\psi_i(0))_{i=0}^N$.

We can write this as

$$A\hat{\boldsymbol{u}}^{n+1} = \boldsymbol{f}^n$$

where the vector $\boldsymbol{f}^n = A(2\hat{\boldsymbol{u}}^n - \hat{\boldsymbol{u}}^{n-1}) - \alpha^2 \left(S\hat{\boldsymbol{u}}^n - \boldsymbol{b}^n\right)$.

Dirichlet boundary conditions $u(0,t) = a$ and $u(L,t) = b$

$$b_i^n = (u_N^n)'(L)\psi_i(L) - (u_N^n)'(0)\psi_i(0), \quad i = 0, 1, \ldots, N$$

Global variational methods

$$\psi_i(0) = \psi_i(L) = 0, \quad i = 0, 1, \ldots, N$$

$$\Rightarrow \boldsymbol{b}^n = 0, \quad \forall\, n = 1, 2, \ldots, N_t - 1$$

Use a boundary function (with reference coordinate $X \in [-1, 1]$)

$$B(x) = \tilde{B}(X) = \frac{b}{2}(1 + X) + \frac{a}{2}(1 - X)$$

and solve for $\tilde{u}_N^n \in V_N = \text{span}\{\psi_j\}_{j=0}^N$. Final solution is then

$$u_N^n = \tilde{u}_N^n + B(x)$$

Dirichlet with the finite element method

Makes use of Lagrange polynomials and $\psi_i(0) = 1$ for $i = 0$ and zero otherwise. Similarly, $\psi_i(L) = 1$ for $i = N$ and zero otherwise. Hence it is only b_0^n and b_N^n that potentially are different from zero. However,

$$u(0,t) = a = \hat{u}_0^{n+1} \quad \text{and} \quad u(L,t) = b = \hat{u}_N^{n+1}$$

> **Note**
>
> Since $\hat{u}_0$ and $\hat{u}_N$ are known we do not solve the linear PDE for $i = 0$ or $i = N$. Simply ident the coefficient matrix A and set $f_0^n = a$ and $f_N^n = b$.

$$\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ a_{10} & a_{11} & a_{12} & \cdots & a_{1N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{N-1,0} & a_{N-1,1} & a_{N-1,2} & \cdots & a_{N-1,N} \\ 0 & \cdots & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \hat{u}_0^{n+1} \\ \hat{u}_1^{n+1} \\ \vdots \\ \hat{u}_{N-1}^{n+1} \\ \hat{u}_N^{n+1} \end{bmatrix} = \begin{bmatrix} a \\ f_1^n \\ \vdots \\ f_{N-1}^n \\ b \end{bmatrix}$$

Neumann boundary conditions

$$u'(0,t) = g_0 \quad \text{and} \quad u'(L,t) = g_L$$

$$b_i^n = (u_N^n)'(L)\psi_i(L) - (u_N^n)'(0)\psi_i(0), \quad i = 0, 1, \ldots, N$$

Apply Neumann strongly through basis

Use basis functions that eliminates b_i^n and ensures $(\tilde{u}_N^n)'(0) = (\tilde{u}_N^n)'(L) = 0$

$$\psi_j'(0) = \psi_j'(L) = 0, \quad j = 0, 1, \ldots, N$$

Add a boundary function $u_N^n = \tilde{u}_N^n + B(x)$ that satisfied $B'(0) = g_0$ and $B'(L) = g_L$

$$B(x) = \tilde{B}(X) = \frac{L}{8}\left(g_L(1+X)^2 - g_0(1-X)^2\right)$$

The L is there since $X = -1 + \frac{2x}{L}$ and $\frac{\partial X}{\partial x} = \frac{2}{L}$ and thus

$$\frac{\partial B}{\partial x} = \frac{\partial \tilde{B}}{\partial X}\frac{\partial X}{\partial x} = \frac{2}{L}\frac{\partial \tilde{B}}{\partial X}$$

Neumann boundary conditions weakly

Apply boundary condition weakly through variational form

$$b_i^n = (u_N^n)'(L)\psi_i(L) - (u_N^n)'(0)\psi_i(0), \quad i = 0, 1, \ldots, N$$

Insert for $(u_N^n)'(0) = g_0$ and $(u_N^n)'(L) = g_L$

$$b_i^n = g_L\psi_i(L) - g_0\psi_i(0)$$

Use any basis function, except those where all $\psi_i(0) = 0$ and $\psi_i(L) = 0$, for all $i = 0, 1, \ldots, N$.

- This works for the finite element method, where $\psi_0(0) = 1$ and $\psi_N(L) = 1$. Nothing else is required
- Also works for the global Galerkin method, e.g., Legendre polynomials $\psi_i(x) = P_i(X)$
- Does not work for Chebyshev because the method relies on integration by parts, which does not work with the Chebyshev weights $\omega(x) = 1/\sqrt{1 - X^2}$.

Stability of the wave equation in variational form

We have derived the linear algebra problem

$$A(\hat{\boldsymbol{u}}^{n+1} - 2\hat{\boldsymbol{u}}^{n} + \hat{\boldsymbol{u}}^{n-1}) = -\alpha^2 \left(S\hat{\boldsymbol{u}}^{n} - \boldsymbol{b}^{n}\right)$$

The ansatz $u_N^{n+1} = gu_N^n = g^{n+1}u_N^0$ also implies that

$$\hat{\boldsymbol{u}}^{n+1} = g\hat{\boldsymbol{u}}^{n} = g^{n+1}\hat{\boldsymbol{u}}^{0} \tag{1}$$

since

$$u_N^{n+1} = gu_N^n \Rightarrow \sum_{j=0}^{N} \hat{u}_j^{n+1}\psi_j = g\sum_{j=0}^{N} \hat{u}_j^{n}\psi_j = \sum_{j=0}^{N} (g\hat{u}_j^{n})\psi_j$$

Hence $\hat{u}_j^{n+1} = g\hat{u}_j^n$. Recursively, we get (1).

Find amplification factor

$$A(\hat{\boldsymbol{u}}^{n+1} - 2\hat{\boldsymbol{u}}^{n} + \hat{\boldsymbol{u}}^{n-1}) = -\alpha^2 \left(S\hat{\boldsymbol{u}}^{n} - \boldsymbol{b}^{n}\right)$$

Insert for $\hat{\boldsymbol{u}}^{n} = g^{n}\hat{\boldsymbol{u}}^{0}$ and assume that $\boldsymbol{b}^{n} = \boldsymbol{0}$

$$(g^{n+1} - 2g^{n} + g^{n-1})A\hat{\boldsymbol{u}}^{0} = -\alpha^2 g^{n} S\hat{\boldsymbol{u}}^{0}$$

Divide by g^{n} and multiply by A^{-1} from the left

$$(g - 2 + g^{-1})I\hat{\boldsymbol{u}}^{0} = -\alpha^2 A^{-1} S\hat{\boldsymbol{u}}^{0}$$

> **Note**
>
> The identity matrix I on the left is optional and can be removed.

Find amplification factor 2

$$(g - 2 + g^{-1})I\hat{\boldsymbol{u}}^0 = -\alpha^2 A^{-1} S\hat{\boldsymbol{u}}^0$$

Use $H = A^{-1}S$ and the eigenvalues $H\hat{\boldsymbol{u}}^0 = \lambda I\hat{\boldsymbol{u}}^0$ to get

$$(g - 2 + g^{-1})I\hat{\boldsymbol{u}}^0 = -\alpha^2 \lambda I\hat{\boldsymbol{u}}^0$$

and after eliminating the equal terms on both sides

$$g + g^{-1} = \beta \tag{1}$$

where $\beta = -\alpha^2\lambda + 2$.

For stability we need $|g| \leq 1$.

> **Note**
>
> If $g < 1$ is a root of (1), then $g^{-1} > 1$ is also a root, which is unstable. All roots must be ≤ 1. Hence $|g| = 1$ is the only possible solution.

Find the longest stable time step

$$g + g^{-1} = \beta$$

Solve quadratic equation for g

$$g = \frac{\beta \pm \sqrt{\beta^2 - 4}}{2}$$

Assume $-2 \leq \beta \leq 2$ such that $\beta^2 - 4 \leq 0$ and $\sqrt{\beta^2 - 4} = a\hat{\imath}$, with $a = \sqrt{4 - \beta^2}$ real

$$2|g| = \left|\beta \pm \sqrt{\beta^2 - 4}\right| = |\beta \pm a\hat{\imath}| = \sqrt{\beta^2 + a^2} = \sqrt{\beta^2 + 4 - \beta^2} = 2$$

For $-2 \leq \beta \leq 2$ we get that $|g| = 1$ and the numerical solution is stable!

Using $\beta = -\alpha^2\lambda + 2 = -(c\Delta t)^2\lambda + 2 = -2$ the longest possible time step is

$$\Delta t \leq \frac{1}{c}\sqrt{\frac{4}{\max(\lambda)}}$$

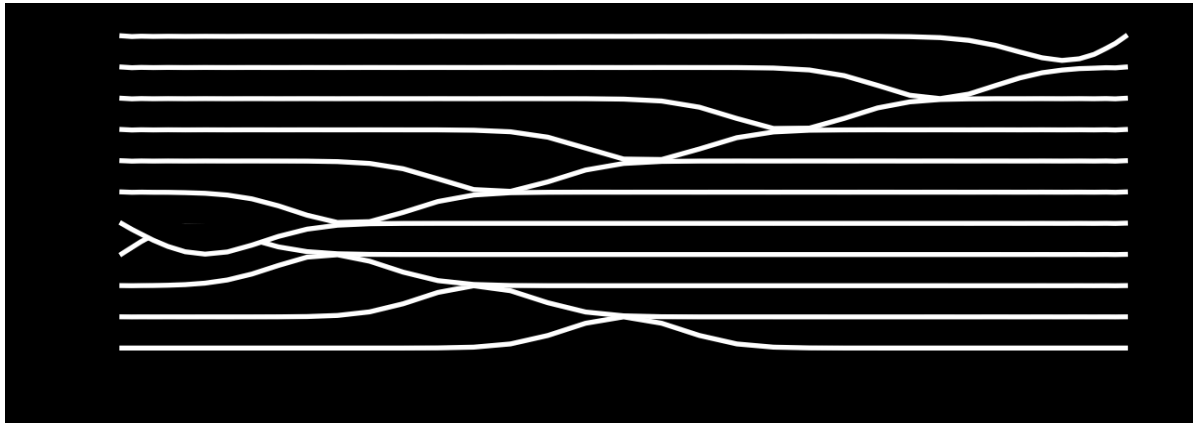
Implementation - Overload diffusion solver

We are using the same function space and thus the same matrices A and S as the diffusion equation. We only need to reimplement the time stepper in `__call__`.

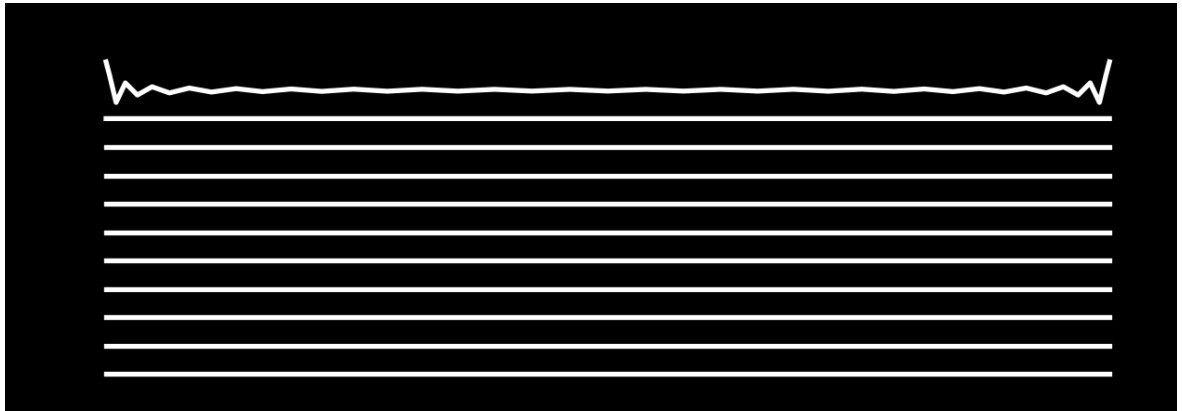
```
class Wave(FE_Diffusion):
    def __init__(self, N, L0=1, c0=1, u0=sp.sin(sp.pi*x/L)):
        u0 = u0.subs({c: c0})
        FE_Diffusion.__init__(self, N, L0=L0, u0=u0)
        self.c = c0
        self.uh_nm1 = np.zeros_like(self.uh_n)

    def __call__(self, Nt, dt=0.1, save_step=100):
        self.uh_nm1[:] = project(self.u0.subs(t, 0), self.V)
        xj = self.V.mesh()
        plotdata = {0: self.uh_nm1(xj)}
        self.uh_n[:] = project(self.u0.subs(t, dt), self.V)
        if save_step == 1: plotdata[1] = self.uh_n(xj)

        f = np.zeros(self.N+1)
        alfa = self.c*dt
        for n in range(2, Nt+1):
            f[:-2] = self.A @ (2*self.uh_n[:-2]-self.uh_nm1[:-2]) \
              - alfa**2*(self.S @ self.uh_n[:-2])
            self.uh_np1[:] = self.sol(f)
            self.uh_nm1[:] = self.uh_n
            self.uh_n[:] = self.uh_np1
            if n % save_step == 0: # save every save_step timestep
                plotdata[n] = self.uh_np1(xj)
        return plotdata
```

Check stability

```
sol = Wave(40, L0=2, c0=1, u0=sp.exp(-40*(x-L/2+c*t)**2))
dt = 1/sol.c*np.sqrt(4/max(sol.get_eigenvalues()))
data = sol(400, dt=dt, save_step=40)
plot_with_offset(data, sol.V.mesh(), figsize=(8, 2.5))
```



```
data = sol(400, dt=dt*1.01, save_step=40)
plot_with_offset(data, sol.V.mesh(), figsize=(8, 2.5))
```



Summary of lecture

- We have solved time-dependent PDEs using finite differences in time and the Galerkin method in space.
- In order to compute stability limits we have made use of the common marching ansatz

$$u_N^{n+1} = g u_N^n$$

and used eigenvalues λ and eigenfunctions $\hat{\boldsymbol{u}}^0$ to find the amplification factor g

$$\begin{aligned} g\hat{\boldsymbol{u}}^0 &= \hat{\boldsymbol{u}}^0 + \Delta t A^{-1} M \hat{\boldsymbol{u}}^0 \\ g\hat{\boldsymbol{u}}^0 &= \hat{\boldsymbol{u}}^0 + \lambda \Delta t \hat{\boldsymbol{u}}^0 \\ \Rightarrow g &= 1 + \lambda \Delta t \end{aligned}$$

- We have described how to apply Neumann boundary conditions both strongly (through basis functions) or weakly (through integration by parts of the variational form)
- We have described how to utilize a stencil matrix for the implementation of composite basis functions.