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# **AMCS 394E: FEM**

***Release 0.1.1***

**A.J.J. Lagerweij**

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## HOMework ASSIGNMENTS

<b>1</b>	<b>AMCS 394E: FEM</b>	<b>3</b>
1.1	Homework 1 . . . . .	3
1.2	About . . . . .	11
1.3	Poisson Equation . . . . .	12
1.4	Derivatives . . . . .	13
1.5	Partial Differential Equations . . . . .	14
1.6	Time Integration . . . . .	16
1.7	Mozilla Public License Version 2.0 . . . . .	17
1.8	Indices and Tables . . . . .	22
	<b>Python Module Index</b>	<b>23</b>
	<b>Index</b>	<b>25</b>







## AMCS 394E: FEM

In this repository you can find my homework for Contemporary Topics in Computational Science: Computing with the Finite Element Method. The course is hosted from [AMCS 394E: Computing with the Finite Element Method Git](#).

The folder `/src/` contains the actual functions wherase the homework functions contain the homework assignments and the scripts that are used to run tha problems.

*physics \* argmin*

### 1.1 Homework 1

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#### Topic

Homework regarding the first week. The goal is to work with basic numerical approximation of PDE's' and functions.

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#### 1.1.1 1 Method of Lines

Consider the one-dimensional advection diffusion equation:

$$u_t + cu_x - \mu u_{xx} = 0 \quad \forall x \in \Omega = [0, 1] \quad \& \quad t > 0$$

where  $\mu > 0$  is the diffusion coefficient and  $c$  the wave speed. Consider periodic boundary conditions and the following initial condition:

$$u(x, 0) = \sin(2\pi x)$$

What do we expect the exact solution to do? Due to the advective part, the initial condition travels at constant speed to the right. At the same time, due to the diffusive term, the initial condition is dissipated at a rate that depends on  $\mu$ .

Consider the following discretization. Use second-order central finite differences to approximate  $u_x$  and  $u_{xx}$ . Use forward and backward Euler to obtain full discretization (write down the schemes). Consider a fixed mesh with of  $\Delta x$ .

## 1.1 Advective Diffusive PDE

Consider a final time of  $t = 1$ ,  $c = 1$  and  $\mu = 0.01$ . For each full discretization proceed as follows:

1. Experiment using the following time step sizes:  $\Delta t = 10^4$ ,  $10^3$  and  $10^2$ .
2. How do the explicit and implicit methods behave for these time steps?

Fig. 1.1: : The forward difference scheme is unstable for  $dt = 10^{-3}$ , the backward scheme behaves as expected. [Click here for an animated version.](#)

Fig. 1.2: : With a timestep of  $dt = 10^{-3}$  both the forward and backward Euler scheme are stable. [Click here for an animated version.](#)

Fig. 1.3: : As expected with a timestep of  $dt = 10^{-4}$  both time integrations behave stable. [Click here for an animated version.](#)

```

1  r"""
2  Solving an Advective and Diffusive PDE with finite differences.
3
4  The PDE described by
5
6  .. math::
7      u_t + u_x = \mu u_{xx} \quad \text{forall } x \in \Omega = [0, 1] \quad \& \quad t > 0
8      \rightarrow 0
9
10 With a periodic boundary condition. It will show a combination of diffusive
11 and advective behaviour. The approximation used is a second order finite
12 difference scheme in space with both a forward and backward Euler method of
13 lines implementation to handle the time direction.
14
15 The goal is to implement the code in python and not rely on existing solvers.
16
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19 2021
20 """
21
22 # Importing External modules
23 import sys
24 import matplotlib.pyplot as plt
25 import numpy as np
26
27 # Importing my own scripts
28 sys.path.insert(1, '../src')
29 from pde import advectivediffusive
30 from time_integral import forwardEuler, backwardEuler
31
32 if __name__ == '__main__':
33     # Define properties
34     dx = 1e-2
35     dt = 1e-4
36     t_end = 1

```

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```

37 mu = 0.01 # Diffusive term
38 c = 1 # Advective term
39
40 # Define discrete ranges
41 dof = int(1 / dx) + 1
42 x, dx = np.linspace(0, 1, dof, retstep=True)
43 t = np.arange(0, t_end + dt, step=dt)
44
45 # Prepare solver
46 u0 = np.sin(2 * np.pi * x) # Initial condition
47
48 # Solve the problem using method of lines.
49 u_forw = forwardEuler(advectivediffusive, u0, dt, t_end, args=(dof, dx, mu, c))
50 u_back = backwardEuler(advectivediffusive, u0, dt, t_end, args=(dof, dx, mu, c))
51
52 # Plotting plotting statically
53 plt.xlim(0, 1)
54 plt.ylim(-1, 1)
55 plt.xlabel('$x$ location')
56 plt.ylabel('$u(x)$')
57 plt.annotate('time t={}'.format(t[-1]), xy=(0.5, 0.9), ha='center')
58 plt.tight_layout()
59
60 plt.plot(x, u_forw, label='forward')
61 plt.plot(x, u_back, label='backward')
62
63 plt.legend()
64 plt.show()

```

## 1.2 Advective PDE

Consider  $\mu = 0$  and  $c = 2$  and solve the PDE using the explicit and the implicit methods. Use  $\Delta t = 10^4$  and solve the problem for the following final times  $t = 1, 5, 10, 15$  and  $20$ . Comment on the behaviour of each full discretization as the final time increases.

Fig. 1.4: : Even with small time steps this type of hyperbolic like equation can become unstable when using a forward Euler method. [Click here for an animated version.](#)

There is a so called Courant-Friedrichs-Lewy condition that formulates a condition of stability on the model:

$$C = \frac{c\Delta t}{\Delta x} \leq C_{\max}$$

Where  $C_{\max}$  is a constant, which for explicit schemes, such as forward Euler, is around 1. If the condition is violated the method becomes unstable, that does not mean that the results are unstable from the first iteration. In the animation the instabilities become only clear after 14 seconds. Nevertheless, even at  $t = 1$  the method should be considered unstable. Similarly the backward Euler is inaccurate as well, it is too dissipative, after 20 seconds around 20% of our wave magnitude has disappeared.

```

1 r"""
2 Solving an Advective PDE with finite differences.
3
4 The PDE described by
5

```

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(continued from previous page)

```

6  .. math::
7      u_{t} + u_{x} = 0 \quad \text{forall } x \in \Omega = [0, 1] \quad ; ; \& ; ; t > 0
8
9  With a periodic boundary condition. The approximation used is a second order
10 finite difference scheme in space with both a forward and backward Euler method
11 of lines implementation to handle the time direction.
12
13 The goal is to implement the code in python and not rely on existing solvers.
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18 """
19
20 # Importing External modules
21 import sys
22 import matplotlib.pyplot as plt
23 import numpy as np
24
25 # Importing my own scripts
26 sys.path.insert(1, '../src')
27 from pde import advective
28 from time_integral import forwardEuler, backwardEuler
29
30
31 if __name__ == '__main__':
32     # Define properties
33     dx = 1e-2
34     dt = 1e-4
35     t_end = 20
36     c = 2 # Advective term
37
38     # Define discrete ranges
39     dof = int(1 / dx) + 1
40     x, dx = np.linspace(0, 1, dof, retstep=True)
41     t = np.arange(0, t_end + dt, step=dt)
42
43     # Prepare solver
44     u0 = np.sin(2 * np.pi * x) # Initial condition
45
46     # Solve the problem using method of lines.
47     u_forw = forwardEuler(advective, u0, dt, t_end, args=(dof, dx, c))
48     u_back = backwardEuler(advective, u0, dt, t_end, args=(dof, dx, c))
49
50     # Plotting plotting statically
51     plt.xlim(0, 1)
52     plt.ylim(-1, 1)
53     plt.annotate('time t={}'.format(t[-1]), xy=(0.5, 0.9), ha='center')
54     plt.tight_layout()
55
56     plt.plot(x, u_forw, label='forward')
57     plt.plot(x, u_back, label='backward')
58
59     plt.legend()
60     plt.show()

```

## 1.1.2 2 Approximation of functions

Consider the function:

$$f(x) = \sin^4(2\pi x) \quad \forall x \in \Omega = [0, 1]$$

for which we have to find multiple global and local approximations. Let  $f_h(x)$  be such an approximation for a given grid. We consider the following errors:

$$E_1 := \int_{\Omega} |f(x) - f_h(x)| dx \quad \text{and} \quad E_2 := \int_{\Omega} (f(x) - f_h(x))^2 dx$$

### 2.1 Global Approximations

Consider the following approximations all with  $N$  terms:

1. the Taylor series around  $x = 0.5$ ,
2. the Fourier series,
3. a global polynomial interpolation on the closed interval given by:

$$f_h(x) = a_0 + a_1x + a_2x^2 + \dots + a_{N-1}x^{N-1}$$

Consider different levels of refinement,  $N = 4, 5, 6, \dots, 10$  and for each approximation report both  $E_1$  and  $E_2$ .

#### 2.1.1 Taylor series

The Taylor series till the order  $N$  is defined through:

$$f_h(x) = \sum_{n=0}^N \frac{f^{(n)}(x_0)}{n!} (x - x_0)^n$$

Which immediately got me into problems, analyzing the  $n$ -th derivative of a function is a numerically a pain. Quickly the round off errors become significant, and from the 5th derivative onward the basic *scipy* Taylor series function became useless. As a result I decided to hardcode the weighting constants in our expansion, these are obtained from manual derivatives.

Fig. 1.5: : Approximating  $f(x)$  with a Taylor series centered around  $x_0 = 0.5$  till order 10.

From Fig. 1.5 it can be observed that the Taylor series is not a very efficient approximation. At the boundary of our domain the error is very high.

#### 2.1.2 Fourier series

The Fourier series, which we assume to be real, approximates the equation with:

$$f_h(x) = \sum_{n=0}^N c_n \exp \frac{2\pi n x}{P} i + \bar{c}_n \exp -\frac{2\pi n x}{P} i$$

where  $P$  is the period of the function  $f(x)$  and  $c_n$  are complex valued coefficients that can be found through a Fourier Transform. In our case I used a FFT algorithm to find these coefficients from our discrete dataset, essentially the real-FFH tries to solve:

$$c_n = \sum_{k=0}^K x_k \exp \frac{2\pi k n}{K-1} \quad n = 0, \dots, N$$

in a highly efficient manner. Notice that for each unknown  $c_n$  consists of a real and imaginary part. This does mean that this approximation for any given  $N$  is more complex. The resulting approximation is shown in Fig. 1.6. Which show that this series is highly efficient in the approximation of our function. This is not to surprising, after all we are approximation a trigonometric functions with a series of trigonometric functions it is likely that we find the exact function somewhere in our series.

Fig. 1.6: : Approximating  $f(x)$  with a Fourier series seems to be exact from the fourth order.

### 2.1.3 Polynomial series

The polynomial series

$$f_h(x) = a_0 + a_1x + a_2x^2 + \dots + a_{N-1}x^{N-1}$$

was to be found with a fitting through  $N$  evenly spaced points  $x_i$  throughout this interval. It should be noted that this type of fitting can be rewritten as an minimization:

$$a_0, \dots, a_{N-1} \sum_{i=0}^N (f(x_i) - f_h(x_i))^2$$

$$that means : find a_0, \dots, a_{N-1} such that f(x_i) - f_h(x_i) = 0 \quad \forall x_i$$

This minimization can efficiently be casted to a system of equations and subsequently be solved. This system of equations has  $N$  unknowns and  $N$  functions, and because each of these functions is linearly independent a solution exists. Simply said we construct a polynomial that goes exactly through these  $N$  points.

Fig. 1.7: : Approximating  $f(x)$  with a polynomials of order  $N - 1$  using  $N$  sample points.

One can also choose to use more sample points to evaluate the minimization problem, lets consider that we use  $M$  sample points. It is not generally possible to find a  $N - 1$  order polynomial to fit exactly through more then  $N$  points. But we can find the best polynomial, to be specific one that minimizes:

$$a_0, \dots, a_{N-1} \sum_{i=0}^M (f(x_i) - f_h(x_i))^2$$

Which is as if we are minimizing our error  $E_2$  at only discrete points, instead of solving the integral itself. Anyway, Fig. 1.8 shows this fit would look like. The results seems closer, because we're not just minimizing the error at  $N$  points but at  $5N$  points.

Fig. 1.8: : Approximating  $f(x)$  with a polynomials of order  $N - 1$  using  $M = 5N$  sample points.

### 2.1.4 Comparison

For the comparison of these different approximations I've plotted the errors on a log scale. Please do note that the Fourier series has 2 times as many unknowns for the  $N$  compared to the other methods.

Fig. 1.9: : The error  $E_1$  for our different approximations where the approximation order ranges from 1 to 20.

Fig. 1.10: : The error  $E_2$  for our different approximations where the approximation order ranges from 1 to 20.

I assume that the error of the Taylor series is increasing because the higher order terms will cause higher errors at the boundaries of our domain. But all in all it is my opinion that the Taylor series is a bad approximation for this purpose, it is difficult to calculate due to the derivatives and the result is inaccurate. This is not so surprising however, Taylor series are meant to approximate the behaviour of a function around a given point  $x_0$  to characterize the local behaviour. We are here using it on a relatively large domain.

The script used for these computations can be found at [3 LocalApproximation.py](#).

## 2.2 Local Approximations

Split the domain  $\Omega$  into  $N$  cells. For each cell  $K$ , compute linear and quadratic approximations  $f_K(x)$  where  $f_K(x_i) = f(x_i)$  where  $x_i$  are evenly spaced gridpoints, including the boundaries of the cell. Compute and report both  $E_1$  and  $E_2$  for a different numbers of cells  $N = 4, 5, 6, \dots, 10$ .

The approximation by linear elements is created by scaling hat (shape) functions appropriately. These functions are chosen in such a way that:

- 1) The sum of all the shape functions together equals one,  $\sum_{n=1}^N \varphi_n(x) = 1$  This is called the Partition of Unity Method.
- 2) There where a single function reaches its maximum all the other functions equal zero.

Then our approximation is defined by:

$$f_h(x) = \sum_{n=1}^N w_n \varphi_n(x)$$

where the weights  $w_n$  are unknown. But because the shape function where chosen smartly these weights are independent. After all at the point where a single shape function reaches its maximum (1) the other functions are zero. As a result the weight of this shape function equals the value of the function we are trying to approximate at the center point of the shape:

$$w_n = f(X_n)$$

where  $X_n$  denotes the point where shape function  $\varphi_n(x)$  reaches its maximum.

## 2.2.1 Linear Elements

In the case of linear elements these shape functions are defined as:

$$\varphi_n(x) = \begin{cases} 0 & \forall \quad 0 \\ \leq x \leq & X_{n-1} \\ \frac{x-X_{n-1}}{X_n-X_{n-1}} & \forall \quad X_{n-1} \\ \leq x \leq & X_n \\ 1 - \frac{x-X_n}{X_{n+1}-X_n} & \forall \quad X_n \\ \leq x \leq & X_{n+1} \\ 0 & \forall \quad X_{n+1} \\ \leq x \leq & L \end{cases}$$

where  $X_n$  is the node of this shape function,  $X_{n-1}$  and  $X_{n+1}$  the nodes surrounding ours.

A more efficient formulation includes the creation of a unit function that is rescaled depending on the locations of the nodes. But I haven't yet implemented such a function yet.

Fig. 1.11: : The function  $4 \sin(\pi x) + 1$  approximated with four elements. The first element contain the orange and half of the green shape function.

Fig. 1.12: : The function  $4 \sin(\pi x) + 1$  approximated more and more linear elements.

Fig. 1.13: : The approximation of  $f(x)$  with linear elements.

## 2.2.2 Quadratic Elements

In the case of quadratic elements there are two different types of shape function. One of these function extents into two elements, similar to what the linear element does. The second shape function is only inside a single element, and on an interior node. This node is placed exactly in the middle between the start and end of the element. I'll give these nodes the subscripts  $n - \frac{1}{2}$  and  $n + \frac{1}{2}$ . Now the shape functions are defined by:

$$\varphi_n(x) = \begin{cases} 0 & \forall \quad 0 \\ \leq x \leq & X_{n-1} \\ \frac{2}{(X_n-X_{n-1})^2}(x-X_{n-1})(x-X_{n-\frac{1}{2}}) & \forall \quad X_{n-1} \\ \leq x \leq & X_n \\ \frac{2}{(X_{n+1}-X_n)^2}(x-X_{n+1})(x-X_{n+\frac{1}{2}}) & \forall \quad X_n \\ \leq x \leq & X_{n+1} \\ 0 & \forall \quad X_{n+1} \\ \leq x \leq & L \end{cases}$$

$$\varphi_{n-\frac{1}{2}}(x) = \begin{cases} 0 & \forall \quad 0 \\ \leq x \leq & X_{n-1} \\ -\frac{4}{(X_n-X_{n-1})^2}(x-X_{n-1})(x-X_n) & \forall \quad X_{n-1} \\ \leq x \leq & X_n \\ 0 & \forall \quad X_{n+1} \\ \leq x \leq & L \end{cases}$$

Again a more efficient formulation includes the creation of a unit function that is rescaled depending on the locations of the nodes. But I haven't yet implemented such a function yet.

Fig. 1.14: : The function  $4 \sin(\pi x) + 1$  approximated with four elements. The first element contain the orange and half of the green shape function.

Fig. 1.15: : The function  $4 \sin(\pi x) + 1$  approximated more and more quadratic elements.

Fig. 1.16: : The approximation of  $f(x)$  with quadratic elements.

It is important to notice from Fig. 1.16 that the resulting curve is not smooth. for example at  $x = 0.5$  one can see that the red approximation (6 elements) is non-smooth.

## 2.2.3 Comparison

For the comparison of these different approximations I've plotted the errors on a log scale. Please do note that the quadratic elements have  $(N + 1)N$  unknowns where the linear elements have  $N + 1$  weights to be determined. Nevertheless there is no interdependency between these weights, which as mentioned before means that these can be determined independently.

The script used for these computations can be found at [4 GlobalApproximation.py](#).

*physics*

## 1.2 About

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### Toppic

The reason for me is to solve classical problems in Solid Mechanics. This section, and those below will introduce the typical equations that are encountered in solid mechanics. This section is not exhaustive and it might be extended in the future to discuss more details.

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The examples will become gradually more complex. It starts with the simplest problem, the Laplace equation:

$$\Delta u(\vec{m}) = 0 \quad \forall \vec{m} \in \Omega$$

In here one can imagine various levels of complication:

1. With a simple geometry, no sharp corners, and a combination of Neuman and Diriclet boundary conditions.
2. With a more complex geometry, sharp corners, cracks and inclusions.
3. With a 'non-linear' stiffness,  $(\vec{C} u(\vec{m}))$  adding a non-constant variable  $\vec{C}$  which is a function depending somehow on  $u$ .
4. Where  $\vec{C}$  is non-linear and history dependent, aka  $\vec{C}^{(n+1)}$  is a function af all previous timesteps.
5. With softening in the non-linear stiffness  $C$ , that is the tangent of  $\vec{C} u$  will become negative at some point.

Fig. 1.17: : The error  $E_1$  for our element based approximations with 1 to 20 elements.

Fig. 1.18: : The error  $E_1$  for our element based approximations with 1 to 20 elements.

## 6. Versions in 3D

Moving on to solids where we solve elasticity and plasticity equations:

$$\begin{aligned}\sigma + \vec{b} &= 0 \quad \forall \vec{m} \in \Omega \\ \text{where } \sigma &= C : \varepsilon \\ \varepsilon &= \frac{1}{2}(\vec{u} + (\vec{u})^T)\end{aligned}$$

The simplest problem would be linear elasticity, but more complicated versions can be build as well.

1. With a simple geometry, no sharp corners, and a combination of Neuman and Diriclet boundary conditions.
2. With a more complex geometry, sharp corners, cracks and inclusions.
3. Large displacements (geometrically non-linear) and deformations (this might require a different strain measure).
4. Softening and possbily fracture.
5. Self Contact.

*physics*

## 1.3 Poisson Equation

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### Toppic

The Poisson equation is the simplest example of the PDE's considerd in Solid Mechanics. It is an elliptical PDE, and is simplified compared to linear elasticity in the sense that its solution is a scalar field, instead fo the vector field found in elasticity problems. This makes Poisson's equation a good start to explore numerical solving strategies for Solid Mechanics problems.

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### 1.3.1 Laplace Equation

The most basic description of the Laplace equation is given by:

$$\begin{aligned}\Delta u(\vec{m}) &= [2]ux + [2]uy = 0 \\ \forall \vec{m} &\in \Omega \\ \text{s.t.: } u(\vec{m}) &= \tilde{u}(\vec{m}) \\ \forall \vec{m} &\in \mathcal{S}_u \\ u(\vec{m}) &= \tilde{t}(\vec{m}) \\ \forall \vec{m} &\in \mathcal{S}_t\end{aligned}$$



Where the entirety of the boundary  $\partial\Omega$  is the union of these two boundary conditions that do not intersect.

$$\begin{aligned}\partial\Omega &= \mathcal{S}_u \cup \mathcal{S}_t \\ 0 &= \mathcal{S}_u \cap \mathcal{S}_t\end{aligned}$$

The following images summarize this.

Fig. 1.19: A domain  $\Omega$  subjected to the Laplace equation with combined boundary conditions.

### 1.3.2 Poisson equation

In case of nonhomogeneous formulations the Laplace equation is called the Poisson equation.

$$\begin{aligned}{}^2u(\vec{m}) &= [2]ux + [2]uy = \vec{b}(\vec{m}) \\ \forall \vec{m} &\in \Omega \\ \text{s.t.: } u(\vec{m}) &= \vec{u}(\vec{m}) \\ \forall \vec{m} &\in \mathcal{S}_u \\ u(\vec{m}) &= \vec{t}(\vec{m}) \\ \forall \vec{m} &\in \mathcal{S}_t\end{aligned}$$

The boundary condition is still defined in the same way as in the Laplace equation.

### 1.3.3 Weak form

## 1.4 Derivatives

Storing various derivatives for the purpose of importing them into the partial derivative equations in another script.

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`derivative.Dx(dof, dx, bc='periodic')`

Return the central differences matrix for the first derivative. That is the matrix  $D_x$  represents the central difference approximation of  $\partial_x$  in 1D axis systems.

#### Parameters

- **dof** (*int*) – Number of spatial degrees of freedom.
- **dx** (*float*) – Spatial step size.
- **bc** (*string, optional*) – The type of boundary condition to be used. The default is 'periodic'.

**Raises ValueError** – Is raised when the requested boundary condition is not implemented.

**Returns** The central difference approximation of the first derivative.

**Return type** matrix (sparse csr format)

`derivative.Dxx(dof, dx, bc='periodic')`

Return the central differences matrix for the second derivative. That is the matrix  $D_{xx}$  represents the central difference approximation of  $\partial_{xx}$  in 1D axis systems.

#### Parameters

- **dof** (*int*) – Number of spacial degrees of freedom.
- **dx** (*float*) – Spacial step size.
- **bc** (*string*, *optional*) – The type of boundary condition to be used. The default is 'periodic'.

**Raises** **ValueError** – Is raised when the requested boundary condition is not implemented.

**Returns** The central difference approximation of the first derivative.

**Return type** matrix (sparse csr format)

## 1.5 Partial Differential Equations

Storing varios PDE's that can be will be solved in this course. This includes:

- Diffusive 1D

$$u_t = \mu u_{xx} \quad \forall x \in \Omega = [0, 1] \quad \& \quad t > 0$$

- Advective 1D

$$u_t + cu_x = 0 \quad \forall x \in \Omega = [0, 1] \quad \& \quad t > 0$$

- Diffusive-Advective 1D

$$u_t + cu_x = \mu u_{xx} \quad \forall x \in \Omega = [0, 1] \quad \& \quad t > 0$$

The goal is to implement the code in python and not rely on existing methods.

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`pde.advective` (*dof*, *dx*, *c*)

Time derivative of the PDE for advective diffusive problems.

$$u_t + cu_x = 0 \quad \forall x \in \Omega = [0, 1] \quad \& \quad t > 0$$

Thus this returns:

$$u_t = -cu_x$$

Because we use finite difference based matrix products we can convert this into a matrix vector product, where  $D_x$  is the central difference approximation of  $\partial_x$ :

$$u_t = -cD_x u = Ku$$

This function calculates the matrix  $K$ . Because it should be compatible with general, non-homogeneous formulation, a part that is independent of  $u$  is also included.

### Parameters

- **dof** (*int*) – Number of degrees of freedom.
- **dx** (*float*) – Stepsize in the of spatial discretisation.
- **c** (*float*) – The avective coefficient.

### Returns

- **K** (*matrix (sparse csr format)*) – The time derivative part of the pde obtained from the spatial part.

- **b** (*vector (dense array)*) – The remaining term, in this homeneous case it is a zero array.

pde.**advectivediffusive** (*dof, dx, mu, c*)

Time derivative of the PDE for advective diffusive problems.

$$u_t + cu_x = \mu u_{xx} \quad \forall x \in \Omega = [0, 1] \quad \& \quad t > 0$$

Thus this returns:

$$u_t = -cu_x + \mu u_{xx}$$

Because we use finite difference based matrix products we can convert this into a matrix vector product, where  $D_x$  is the central difference approximation of  $\partial_x$  and similarly  $D_{xx}$  the central difference apprximation of  $\partial_{xx}$ :

$$u_t = -cD_x u + \mu D_{xx} u = (-cD_x + \mu D_{xx}) u = Ku$$

This function calculates the matrix  $K$ . Because it should be compatible with general, non-homogeneous formulation, a part that is independent of  $u$  is also included.

#### Parameters

- **dof** (*int*) – Number of degrees of freedom.
- **dx** (*float*) – Stepsize in the of spatial discretisation.
- **mu** (*float*) – The diffusive coefficient.
- **c** (*float*) – The avective coefficient.

#### Returns

- **K** (*matrix (sparse csr format)*) – The time derivative part of the pde obtained from the spatial part.
- **b** (*vector (dense array)*) – The remaining term, in this homeneous case it is a zero array.

pde.**diffusive** (*dof, dx, mu*)

Time derivative of the PDE for advective diffusive problems.

$$u_t = \mu u_{xx} \quad \forall x \in \Omega = [0, 1] \quad \& \quad t > 0$$

Thus this returns:

$$u_t = \mu u_{xx}$$

Because we use finite difference based matrix products we can convert this into a matrix vector product, where  $D_{xx}$  is the central difference approximation of  $\partial_{xx}$ :

$$u_t = \mu D_{xx} u = Ku$$

This function calculates the matrix  $K$ . Because it should be compatible with general, non-homogeneous formulation, a part that is independent of  $u$  is also included.

#### Parameters

- **dof** (*int*) – Number of degrees of freedom.
- **dx** (*float*) – Stepsize in the of spatial discretisation.
- **mu** (*float*) – The defusive coefficient.

#### Returns

- **K** (*matrix (sparse csr format)*) – The time derivative part of the pde obtained from the spatial part.
- **b** (*vector (dense array)*) – The remaining term, in this homeneous case it is a zero array.

## 1.6 Time Integration

Various implementations of the method of lines to progress through time. The goal is to implement the code in python and not rely on existing solvers.

Bram Lagerweij COHMAS Mechanical Engineering KAUST 2021

`time_integral.backwardEuler` (*func*, *u*, *dt*, *t\_end*, *args*=())

Iterate a through time with the backward Euler method.

The backward Euler method predicts the field of our function based upon information of the previous timestep only. Imagine that we are at timestep  $n$  and want to predict our field at timestep  $u^{(n+1)}$ . Now a backward finite difference approximation used the time derivative of the next timestep, which is not yet known:

$$u_t^{(n+1)} = \frac{-u^{(n)} + u^{(n+1)}}{dt}$$

That is we can predict our field in the future timestep as:

$$u^{(n+1)} = u^{(n)} + dt u_t^{(n+1)}$$

It is important to notice that there is a term with an unknown, as that is at time step  $n+1$  on both sides of the equation. Our time derivative is obtained with an approximation equation:

$$u_t = Ku + b$$

where matrix  $K$  and vector  $b$  stem from approximations of our spatial derivatives defined by the function provided to *func*. This results in:

$$u^{(n+1)} = u^{(n)} + dt (Ku^{(n+1)} + b)$$

Now we rewrite it into a system of equations where we find all unknowns on the left hand side and all known on the right hand side.

$$(I - dt K) u^{(n+1)} = u^{(n)} + dt b$$

### Parameters

- **func** (*callable*) – The time derivative of the pde to be solved such that  $u_t = Ku + b$ .
- **u** (*array\_like*) – The field at the start  $u(t = 0)$ .
- **dt** (*float*) – The size of the time step.
- **t\_end** (*float*) – Time at termination.
- **args** (*tuple, optional*) – The parameters into the PDE approximation. Defaults to an empty tuple.

**Returns** The function for all time steps.

**Return type** `array_like`

`time_integral.forwardEuler` (*func*, *u*, *dt*, *t\_end*, *args*=())

Iterate a through time with the forward Euler method.

The backward Euler method predicts the field of our function based upon information of the previous timestep only. Imagine that we are at timestep  $n$  and want to predict our field at timestep  $u^{(n+1)}$ . Now a forward finite difference approximation is used:

$$u_t^{(n)} = \frac{-u^{(n)} + u^{(n+1)}}{dt}$$

That is we can predict our field in the future timestep as:

$$u^{(n+1)} = u^{(n)} + dt u_t^{(n)}$$

Our time derivative at the current timestep,  $u_t^{(n)}$  is obtained with:

$$u_t = Ku + b$$

where matrix  $K$  and vector  $b$  stem from approximations of our spatial derivatives defined by the function provided to *func*. Resulting in the following update scheme:

$$u^{(n+1)} = u^{(n)} + dt (Ku^{(n)} + b)$$

most important of all is to see that everything on the right hand side is exactly known. Thus the updated field can be calculated directly.

#### Parameters

- **func** (*callable*) – The time derivative of the pde to be solved such that  $u_t = Ku + b$ .
- **u** (*array\_like*) – The field at the start  $u(t = 0)$ .
- **dt** (*float*) – The size of the step.
- **t\_end** (*float*) – Time at termination.
- **args** (*tuple, optional*) – The parameters into the PDE approximation. Defaults to an empty tuple.

**Returns** The function for all time steps.

**Return type** *array\_like*

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## 1.8 Indices and Tables

- [genindex](#)
- [modindex](#)
- [search](#)

## PYTHON MODULE INDEX

### d

`derivative`, [13](#)

### p

`pde`, [14](#)

### t

`time_integral`, [16](#)



## INDEX

### A

`advective()` (*in module `pde`*), [14](#)  
`advectivediffusive()` (*in module `pde`*), [15](#)

### B

`backwardEuler()` (*in module `time_integral`*), [16](#)

### D

`derivative`  
    module, [13](#)  
`diffusive()` (*in module `pde`*), [15](#)  
`Dx()` (*in module `derivative`*), [13](#)  
`Dxx()` (*in module `derivative`*), [13](#)

### F

`forwardEuler()` (*in module `time_integral`*), [16](#)

### M

module  
    `derivative`, [13](#)  
    `pde`, [14](#)  
    `time_integral`, [16](#)

### P

`pde`  
    module, [14](#)

### T

`time_integral`  
    module, [16](#)