Project



Computational Methods for Engineering Applications Last edited: November 3, 2023

Due date: December 01 at 23:59

Template codes are available on the course's webpage at https://moodle-app2.let.ethz.ch/course/view.php?id=20880.

This project contains some tasks marked as **Core problems**. If you hand them in before the deadline above, these tasks will be corrected and graded. After a successful interview with the assistants (to be scheduled after the deadline), extra points will be awarded. Full marks for the all core problems in all assignments will give a 25% bonus on the total points in the final exam. This is really a bonus, which means that at the exam you can still get the highest grade without having the bonus points (of course then you need to score more points at the exam).

You only need to hand in your solution for tasks marked as core problems for full points, and the interview will only have questions about core problems. However, in order to do them, you may need to solve the previous non-core tasks.

The total number of points for the Core problems of this project is **100 points**.

Important note: please avoid handing in your binary files. Ideally, what you upload to Moodle should be exactly the same files in the same folder structure from the template, with your code in the labeled spots of the code files – nothing less, nothing more.

Exercise 1 Finite Differences for the Porous Media Equation in 2D

In this problem we consider the finite differences (FD) discretization of the equation of porous media on the unit square:

$$-\nabla \cdot (\sigma \nabla u) = f \quad \text{in } \Omega := (0, 1)^2,$$

$$u = 0 \quad \text{on } \partial \Omega,$$
(1)

for a bounded and continuous function $f \in \mathcal{C}^0(\overline{\Omega})$. In a general formulation of the problem σ is a smooth function of u; for simplicity, here we take $\sigma : \Omega \longrightarrow \mathbb{R}$, $\sigma \in \mathcal{C}^1(\Omega)$. Note that for $\sigma \equiv 1$, one recovers Poisson's equation.

We consider a regular tensor product grid with meshwidth $h := (N+1)^{-1}$ and we assume a lexicographic numbering of the interior vertices of the mesh as depicted in Fig.1.

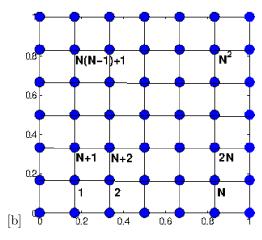


Figure 1: Lexicographic numbering of vertices of the equidistant tensor product mesh.

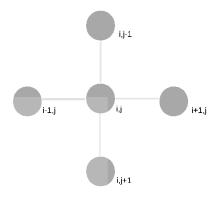


Figure 2: 5-point stencil used in this problem.

We consider the 5-point finite difference scheme described by the stencil shown in Fig. 2.

1a)

Write the system

$$\mathbf{A}\mathbf{u} = \mathbf{F} \tag{2}$$

corresponding to the discretization of (1) using the stencil in Fig. 2, specifying the matrix \mathbf{A} and the vectors \mathbf{F} and \mathbf{u} .

Hint: Consider starting the discretization as $\frac{\partial}{\partial x}(\sigma \frac{\partial u}{\partial x}) \approx \frac{1}{h}((\sigma \frac{\partial u}{\partial x})_{i+\frac{1}{2},j} - (\sigma \frac{\partial u}{\partial x})_{i-\frac{1}{2},j})$

1b)

(Core problem) In the template file finite_difference.cpp, implement the function

void createPorousMediaMatrix2D(SparseMatrix& A, FunctionPointer sigma, int N, double dx),

to construct the matrix A in (2), where N denotes the number of interior grid points along one dimension, with typedef Eigen::SparseMatrix<double> SparseMatrix. Assume the matrix A to have an uninitialized size at the beginning.

1c)

(Core problem) In the template file finite_difference.cpp, implement the function

 $\label{thm:poissonSolve} Vector\ poissonSolve(FunctionPointer\ f,\ FunctionPointer\ sigma,\ {\tt int}\ N),$

to solve the system (2), which returns u the vector containing the values of the approximate solution at all the grid points, *including those on the boundary*, and the other arguments as in the previous subproblems.

Hint: You may use the function void createRHS(Vector& rhs, FunctionPointer f, int N, double → dx) provided in the same file.

1d)

Plot the discrete solution that you get from subproblem 1c) when $f(x,y) = 4\pi^2 \sin(2\pi x) \sin(2\pi y) (4\cos(2\pi x)\cos(2\pi y) + \pi), \quad \sigma(x,y) = \frac{\pi}{2} + \cos(2\pi x)\cos(2\pi y)$

and N = 500. Use the provided script plot_2dfd. Note that the exact solution in this case is $u(x,y) := \sin(2\pi x)\sin(2\pi y)$.

1e)

(Core problem) In the template file finite_difference.cpp, implement the function

void convergeStudy(FunctionPointer F, FunctionPointer sigma),

that uses the infinity norm, i.e.

for
$$\mathbf{a} \in \mathbb{R}^d$$
, $\|\mathbf{a}\|_{\infty} := \max_{0 \le i \le d} |\mathbf{a}_i|$, (3)

to compute the error between your discrete solution obtained with

$$f(x,y) = 4\pi^2 \sin(2\pi x) \sin(2\pi y) (4\cos(2\pi x)\cos(2\pi y) + \pi), \quad \sigma(x,y) = \frac{\pi}{2} + \cos(2\pi x)\cos(2\pi y)$$

for $N=2^k, k=3...8$ and the exact solution $u(x,y)=\sin(2\pi x)\sin(2\pi y)$. You can use the provided script plot_convergence.

Hint: Use your code from 1c).

Exercise 2 Linear Finite Elements for stationary reactiondiffusion equation in 2D

We consider the problem

$$-\nabla \cdot (\sigma \nabla u) + ru = f(\boldsymbol{x}) \quad \text{in } \Omega \subset \mathbb{R}^2$$
 (4)

$$u(\mathbf{x}) = g(\mathbf{x}) \quad \text{on } \partial\Omega$$
 (5)

where $f \in L^2(\Omega)$, $r \in \mathbb{R}_+$ is some positive constant and $\sigma : \Omega \longrightarrow \mathbb{R}_+$, $\sigma \in \mathcal{C}^1(\Omega)$.

In the folder unittest you can find routines to test your implementation tasks for this problem.

2a)

Write the variational formulation for (4)-(5).

We solve (4)-(5) by means of linear finite elements on triangular meshes of Ω . Let us denote by φ_i^N , $i=0,\ldots,N-1$ the finite element basis functions (hat functions) associated to the vertices of

a given mesh, with $N = N_V$ the total number of vertices. The finite element solution u_N to (4) can thus be expressed as

$$u_N(\boldsymbol{x}) = \sum_{i=0}^{N-1} \mu_i \varphi_i^N(\boldsymbol{x}), \tag{6}$$

where $\boldsymbol{\mu} = \{\mu_i\}_{i=0}^{N-1}$ is the vector of coefficients. Notice that we don't know μ_i if i corresponds to an interior vertex, but we know that $\mu_i = g(x_i)$ if x_i is a vertex on the boundary $\partial\Omega$.

Hint: Here and in the following, we use zero-based indices in contrast to the lecture notes.

Inserting φ_i^N , i = 0, ..., N-1 as test functions in the variational formulation from subproblem **2a**) we obtain the linear system of equations

$$\mathbf{A}\boldsymbol{\mu} = \mathbf{F},\tag{7}$$

with $\mathbf{A} \in \mathbb{R}^{N \times N}$ and $\mathbf{F} \in \mathbb{R}^N$.

2b)

Write an expression for the entries of \mathbf{A} and \mathbf{F} in (7).

2c)

(Core problem) Complete the template file shape.hpp implementing the function

inline double lambda(int i, double x, double y)

which computes the the value a local shape function $\lambda_i(\mathbf{x})$, with i that can assume the values 0, 1 or 2, on the reference element depicted in Fig. 3 at the point $\mathbf{x} = (x, y)$.

The convention for the local numbering of the shape functions is that $\lambda_i(\boldsymbol{x}_j) = \delta_{i,j}$, i, j = 0, 1, 2, with $\delta_{i,j}$ denoting the Kronecker delta.

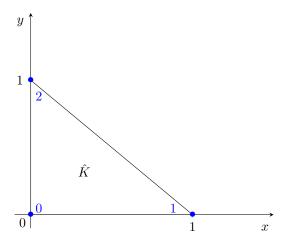


Figure 3: Reference element \hat{K} for 2D linear finite elements.

2d)

(Core problem) Complete the template file grad_shape.hpp implementing the function

```
inline Eigen::Vector2d gradientLambda(const int i, double x, double y)
```

which returns the value of the derivatives (i.e. the gradient) of a local shape functions $\lambda_i(\boldsymbol{x})$, with i that can assume the values 0,1 or 2, on the reference element depicted in Fig. 3 at the point $\boldsymbol{x}=(x,y)$.

The routine makeCoordinateTransform contained in the file coordinate_transform.hpp computes the Jacobian matrix of the linear map $\Phi_l : \mathbb{R}^2 \to \mathbb{R}^2$ such that

$$\Phi_l egin{pmatrix} 1 \ 0 \end{pmatrix} = egin{pmatrix} a_{11} \ a_{12} \end{pmatrix} = oldsymbol{a}_1, \quad \Phi_l egin{pmatrix} 0 \ 1 \end{pmatrix} = egin{pmatrix} a_{21} \ a_{22} \end{pmatrix} = oldsymbol{a}_2,$$

where $a_1, a_2 \in \mathbb{R}^2$ are the two input arguments.

2e)

(Core problem) Complete the template file stiffness_matrix.hpp implementing the routine

that returns the *element stiffness matrix* for the bilinear form associated to (4) and for the triangle with vertices a, b and c.

Use the provided function integrate. It takes a function f(x,y) as a parameter, and it returns the value of $\int_K f(x,y)dV$, where K is the triangle with vertices in (0,0), (1,0) and (0,1).

Hint: Do not forget to take into account the proper coordinate transformations!

Hint: Use the routine gradientLambda from subproblem 2d) to compute the gradients and the routine makeCoordinateTransform to transform the gradients and to obtain the area of a triangle.

The routine integrate in the file integrate.hpp uses a quadrature rule to compute the approximate value of $\int_{\hat{K}} f(\hat{x}) d\hat{x}$, where f is a function, passed as input argument.

2f)

(Core problem) Complete the template file load_vector.hpp implementing the routine

that returns the element load vector for the linear form associated to (4), for the triangle with vertices a, b and c, and where f is a function handler to the right-hand side of (4).

Hint: Use the routine lambda from subproblem 2c) to compute values of the shape functions on the reference element, and the routines makeCoordinateTransform and integrate from the handout to map the points to the physical triangle and to compute the integrals.

2g)

(Core problem) Complete the template file stiffness_matrix_assembly.hpp implementing the routine

to compute the finite element matrix **A** as in (7). The input argument vertices is a $N_V \times 3$ matrix of which the *i*-th row contains the coordinates of the *i*-th mesh vertex, $i = 0, ..., N_V - 1$, with N_V the number of vertices. The input argument triangles is a $N_T \times 3$ matrix where the *i*-th row contains the *indices* of the vertices of the *i*-th triangle, $i = 0, ..., N_T - 1$, with N_T the number of triangles in the mesh.

Hint: Use the routine computeStiffnessMatrix from subproblem 2e) to compute the local stiffness matrix associated to each element.

Hint: Use the sparse format to store the matrix A.

2h)

(Core problem) Complete the template file load_vector_assembly.hpp implementing the routine

to compute the right-hand side vector \mathbf{F} as in (7). The input arguments vertices and triangles are as in subproblem $2\mathbf{g}$), and f is as in subproblem $2\mathbf{f}$).

Hint: Proceed in a similar way as for assembleStiffnessMatrix and use the routine computeLoadVector from subproblem **2f**).

The routine

implemented in the file dirichlet_boundary.hpp provided in the handout does the following:

- it gets in input the matrices vertices and triangles as defined in subproblem 2g) and the function handle g to the boundary data, i.e. to g such that u = g on $\partial\Omega$;
- it returns in the vector interior VertexIndices the indices of the interior vertices, that is of the vertices that are not on the boundary $\partial\Omega$;
- if x_i is a vertex on the boundary, then it sets $u(i)=g(x_i)$.

2i)

(Core problem) Complete the template file fem_solve.hpp with the implementation of the function

This function takes in input the matrices vertices, triangles as defined in the previous subproblems, the function handle f to the right-hand side f, the function handle sigma as σ in (4), and the function handle g to the boundary data. The output argument u has to contain, at the end of the function, the finite element solution u_N to (4). The function returns the number of degrees of freedom (namely, the number of interior vertices).

Hint: Use the routines assembleStiffnessMatrix and assembleLoadVector from subproblems 2g) and 2h), respectively, to obtain the matrix A and the vector F as in (7), and then use the provided routine setDirichletBoundary to set the boundary values of g and to select the free degrees of freedom. The function $gl::slice_into$ may be useful for writing the result for the interior vertices into the full solution array.

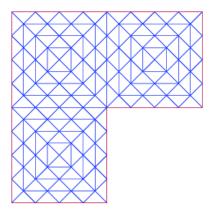


Figure 4: Domain for subproblem 2j).

2j)

Run the routine solveL contained in the file Lshape.hpp to compute the finite element solution to (4)-(5) when Ω is the L-shaped domain $\Omega=(-1,1)^2\setminus((0,1)\times(-1,0))$, as depicted in Fig. 4, and r=0.5. The forcing term is given by $f(\boldsymbol{x})=0$, $\sigma\equiv 1$, the boundary condition by $g=u_{|\partial\Omega}$, with u the exact solution, which, in polar coordinates, is given by $u(r,\vartheta)=r^{\frac{2}{3}}\sin(\frac{2}{3}\vartheta)$, for $r\geq 0$ and $\vartheta\in[0,\frac{3}{2}\pi]$. This is already coded in file Lshape.hpp, comment and uncomment as appropriate. The mesh used is Lshape_5.mesh. Use then the script plot_on_mesh.py to produce a plot of the solution.

2k)

In the same Ω as above, and using the same mesh Lshape_5.mesh, approximate the solution when

$$\sigma(x,y) = 0.01(x+2)^2$$
, $f(x,y) = \sin(\pi y)^2$, $r = 0.5$, $g(x,y) = x^3 + y$

21)

To test your code, we provide you with a sample test case. This is commented out in file fem2d.cpp. Uncomment the block of code around line 45, and run fem2d again. Verify with the script plot_convergence that the order of convergence of your code is correct, in L^2 - and H^1 -norm.

The following information is included for your own knowledge; the exercise is over. Often one comes across a problem, as in this exercise, where it is not easy to find a single non-trivial test for which the solution is known. How can one then test one's implementation and its order of convergence? The idea we have used here is often referred as manufactured solutions. It is a very simple idea: instead of finding a solution for a fixed set of parameters, decide a solution, and set parameters that match it.

In this case, we have arbitrarily chosen to have $u(x,y) := \sin(2\pi x)\sin(2\pi y)$ as solution, so clearly we must have $g \equiv 0$. We keep the non-trivial parameters we used before; that is, r = 0.5 and $\sigma = 0.01(x+2)^2$. And now, all we have to do is pick an appropriate f so that the equation is verified.

Finding such f is as simple as setting $f := -\nabla \cdot (\sigma \nabla u) + ru$; this is how one arrives to the (somewhat complicated) expresion in function f_square in fem2d.cpp.

Heat equation in 1D with variable coefficient Exercise 3

We consider the following one-dimensional, time dependent heat equation:

$$\frac{\partial u}{\partial t}(x,t) - a(x)\frac{\partial^2 u}{\partial x^2}(x,t) = 0, \qquad (x,t) \in (0,1) \times (0,T), \qquad (8)$$

$$u(0,t) = a_1(t) \qquad u(1,t) = a_2(t) \qquad t \in [0,T] \qquad (9)$$

$$u(0,t) = g_L(t), \quad u(1,t) = g_R(t), \qquad t \in [0,T], \tag{9}$$

$$u(x,0) = u_0(x), x \in [0,1], (10)$$

where T > 0 is the final time, and $g_L, g_R : [0, T] \longrightarrow \mathbb{R}$ are Dirichlet boundary conditions¹, and $a:[0,1]\to\mathbb{R}$ is a given function modeling a spatially varying heat conductivity.

We first discretize the above equation with respect to the spatial variable, using centered finite differences.

¹The problem is only well-defined if $g_L(0) = u_0(0)$, $g_R(0) = u_0(1)$.

To this aim, we subdivide the interval [0,1] in N+1 subintervals of equal length, where N is the number of interior grid points x_1, \ldots, x_N , and $x_0 = 0$, $x_{N+1} = 1$.

The space discretization leads to a semidiscrete system of equations associated to (8):

$$\frac{\partial \boldsymbol{u}}{\partial t}(t) + \mathbf{A}\boldsymbol{u}(t) = \boldsymbol{G}(t),\tag{11}$$

where $\mathbf{A} \in \mathbb{R}^{N \times N}$ and $\mathbf{u} = \{u_i\}_{i=1}^N$ denotes the approximate values of the solution at the interior grid points, and

 $G:[0,T]\longrightarrow \mathbb{R}^N$ is a source term coming from the boundary conditions.

Hint: G appears from the fact that the discretization for u_1 and u_N includes respectively $u_0 = g_L(t)$ and $u_{N+1} = g_R(t)$

Hint: This exercise has *unit tests* which can be used to test your solution. To run the unit tests, run the executable unittest. Note that correct unit tests are *not* a guarantee for a correct solution. In some rare cases, the solution can be correct even though the unit tests do not pass (always check the output values, and if in doubt, ask the teaching assistant!)

Hint: The template of this exercise has a lot of files, but you only need to edit the following files:

- create_poisson_matrix.cpp
- forward_euler.cpp
- crank_nicolson.cpp

all other files should not be edited.

Hint: If you are running from the command line, all executables are located in build/bin, so from your build-folder, you should run

- ./bin/unittest
- ./bin/run_boundaries_forward_euler
- ./bin/run_stability_forward_euler
- ./bin/run_boundaries_crank_nicolson
- ./bin/run_stability_crank_nicolson

If you are using Visual Studio, Xcode, QtCreator or any similar IDE, the projects have the same names as the executable (unittest, run_boundaries_forward_euler, run_stability_forward_euler, run_stability_crank_nicolson, run_boundaries_crank_nicolson).

3a)

Denote by h the mesh width, that is $h = \frac{1}{N+1}$. Write down the matrix **A** and the vector $\mathbf{G}(t)$ explicitly.

Hint: Both A and G will depend on a.

To fully discretize (8), we still need to apply a time discretization to (11).

3b)

Apply the forward Euler scheme to (11), denoting by $\mathbf{u}^k = \{u_i^k\}_{i=1}^N$ the approximate value of the vector \mathbf{u} at time k, for $k = 0, \dots, K$, and by $\Delta t = \frac{T}{K}$ the time step. How does the update formula at each time step look like?

3c)

(Core problem) In the template file create_poisson_matrix.cpp, implement the function

```
SparseMatrix createPoissonMatrix(int N, const std::functional<double(double)>& a),
```

where using SparseMatrix = Eigen::SparseMatrix<double>. This function computes the matrix A from (11). Here the input parameter N denotes the number of *interior* grid points. Assume that the size of the input matrix A has not been initialized.

Hint: You can copy the routine directly from the solution to an old assignment and do very small modifications to obtain the desired matrix!

Hint: You can test your code by running the unit tests (./bin/unittest from the command line). The relevant unit tests are those marked as TestCreatePoissonMatrix.

3d)

(Core problem) In the template file forward_euler.cpp, implement the function

```
std::pair<Eigen::MatrixXd, Eigen::VectorXd> forwardEuler(
    const Eigen::VectorXd& u0,
    double dt,
    double T,
    int N,
    const std::function<double(double)>& gL,
```

```
const std::function<double(double)>& gR,
const std::function<double(double)>& a);
```

The input and output parameters are specified in the template file.

Hint: You can test your code by running the unit tests (./bin/unittest from the command line). The relevant unit tests are those marked as TestForwardEuler.

Hint: Eigen's function **segment** to access part of a vector can be very useful here. If **a**, **b** are two vectors, one can do e.g. **a.segment(3,5)** = **b.segment(0,2)**;

3e)

Assume a is constant, that is

$$a(x) = \bar{a} > 0$$
 for all $x \in [0, 1]$,

and assume zero boundary conditions $(g_L = g_R = 0)$. Show that if

$$\Delta t \le \frac{h^2}{2\bar{a}},$$

then the maximum is obeyed for the Forward Euler scheme in exercise 3c).

3f)

Run the executable run_boundaries_forward_euler, which will run the following configurations:

- N = 63
- T = 0.25
- $\Delta t = \frac{1}{2.64.64}$
- Boundary and initial conditions:
 - 1. $g_L^1(x) = g_R^1(x) = 0$; $u_0^1(x) = \min(2x, 2 2x)$.
 - 2. $g_L^2(x) = 0$, $g_R^2(x) = 1$; $u_0^2(x) = x + \min(2x, 2 2x)$.
 - 3. $g_L^3(x) = g_R^3(x) = \exp(-10t); u_0^3(x) = 1 + \min(2x, 2 2x)$

With the help of the script sol_movie.m or sol_movie.py provided in the handout, observe a movie of the approximate solution to (8) when using the forward Euler scheme. What happens to the energy of the system for each of the boundary conditions?

Hint: To run the script, on Matlab, you can use sol_movie("forward_euler"); on Python, use python sol_movie.py forward_euler (resp. crank_nicolson).

3g)

For this exercise, we will test the following coefficients:

```
a_1(x) = 0.1 a_2(x) = 1 a_3(x) = 0.5 + 0.25\sin(4\pi x) for x \in [0, 1].
```

Run the executable run_stability_forward_euler, which will run the following configurations:

- N = 127
- T = 0.25
- $\Delta t_1 = \frac{128}{2 \cdot 128^2}$, $\Delta t_2 = \frac{8}{2 \cdot 128^2}$, $\Delta t_3 = \frac{1}{2 \cdot 128^2}$
- Boundary and initial conditions: $g_L(x) = g_R(x) = 0$, $u_0(x) = \min(2x, 2-2x)$

With the help of the script plot_stability.m or plot_stability.py provided in the handout, study the plot of the solution with the different values of a and Δt to (8) when using the forward Euler scheme. Which combinations are stable?

3h)

We now consider an implicit timestepping. Namely, we derive the Crank-Nicolson scheme. Start with the semidiscrete formulation (11) and integrate over $[t^k, t^{k+1}]$. Use the trapezoidal rule for the integrals involving $\mathbf{A}\boldsymbol{u}$ and G(t), and the approximation $\boldsymbol{u}^k \approx \boldsymbol{u}(t^k)$. Write down the system of equations to be solved at each timestep (this should agree with the Crank-Nicolson scheme stated in the script).

3i)

(Core problem) In the template file crank_nicolson.cpp, implement the function

```
std::pair<Eigen::MatrixXd, Eigen::VectorXd> crankNicolson(
    const Eigen::VectorXd& u0,
    double dt, double T, int N,
    const std::function<double(double)>& gL,
    const std::function<double(double)>& gR,
    const std::function<double(double)>& a);
```

The input and output parameters are specified in the template file.

Hint: You can test your code by running the unit tests (./bin/unittest from the command line). The relevant unit tests are those marked as TestCrankNicolson.

Hint: In this exercise, you may want to compute I - M, where M is a certain sparse matrix and I is the identity. Due to Eigen typecasting, if I is not explicitly defined as a sparse matrix (e.g. it is generated with Eigen::MatrixXd::Identity), I - M will not be a sparse matrix, and sparse solvers will not work. There are several ways to go around this; a simple one is to define I as sparse too with:

```
SparseMatrix I(N,N);
I.setIdentity();
```

3j)

Run the executable run_boundaries_crank_nicolson, which will run the following configurations:

- N = 63
- T = 0.25
- $\Delta t = \frac{1}{2.64.64}$
- Boundary and initial conditions:
 - 1. $g_L^1(x) = g_R^1(x) = 0$; $u_0^1(x) = \min(2x, 2 2x)$.
 - 2. $g_L^2(x) = 0$, $g_R^2(x) = 1$; $u_0^2(x) = x + \min(2x, 2 2x)$.
 - 3. $g_L^3(x) = g_R^3(x) = \exp(-10t); u_0^3(x) = 1 + \min(2x, 2 2x)$

With the help of the script sol_movie.m or sol_movie.py provided in the handout, observe a movie of the approximate solution to (8) when using the Crank-Nicolson scheme. What happens to the energy of the system for each of the boundary conditions?

Hint: You should observe the same as in exercise **3j**)

3k)

For this exercise, we will test the following coefficients:

$$a_1(x) = 0.1$$
 $a_2(x) = 1$ $a_3(x) = 0.5 + 0.25\sin(4\pi x)$ for $x \in [0, 1]$.

Run the executable run_stability_crank_nicolson, which will run the following configurations:

- N = 127
- T = 0.25

- $\Delta t_1 = \frac{128}{2 \cdot 128^2}$, $\Delta t_2 = \frac{8}{2 \cdot 128^2}$, $\Delta t_3 = \frac{1}{2 \cdot 128^2}$
- Boundary and initial conditions: $g_L(x) = g_R(x) = 0$, $u_0^1(x) = \min(2x, 2-2x)$

With the help of the script plot_stability.m or plot_stability.py provided in the handout, study the plot of the solution with the different values of a and Δt to (8) when using the forward Euler scheme. Which combinations are stable?