



Discrete-Space Analysis of Partial Differential Equations

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There are numerous examples that arise and benefit from the reachability analysis problem. In cyber-physical systems (CPS), most dynamic phenomena are described as systems of ordinary differential equations (ODEs). Previous work has been done using zonotopes, support functions, and other geometric data structures to represent subsets of the reachable set and have been shown to be efficient. Meanwhile, a wide range of important control problems are more precisely modeled by partial differential equations (PDEs), even though not much attention has been paid to their reachability analyses. This reason motivates us to investigate the properties of these equations, especially from the reachability analysis and verification perspectives. In contrast to ODEs, PDEs have other space variables that also affect their behaviors and are more complex. In this paper, we study the discrete-space analysis of PDEs. Our ultimate goal is to propose a set of PDE reachability analysis benchmarks, and present preliminary analysis of different dimensional heat equations and wave equations. Finite difference methods (FDMs) are utilized to approximate the derivative at each mesh point with explicit order of errors. FDM will convert the PDE to a system of ODEs depending on the type of boundary conditions and discretization scheme chosen. After that, the problem can be treated as a common reachability problem and relevant conceptions and approaches can be applied and evaluated directly. We used SpaceEx to generate the plots and reachable regions for these equations given inputs and the series of results are shown and analyzed.

1 Context and Origin

Reachability analysis for Cyber-Physical Systems (CPS) involving ODE dynamics has been explicitly investigated in the last two decades which leads to the innovation of numerous efficient techniques and tools. CPS with linear ODE dynamics can be analyzed efficiently using support function-based method implemented in SpaceEx [1] or zonotope-based method utilized in CORA [2]. Notably, the most recent tool called Hylaa using simulation-based method [3, 4] can analyze linear systems with up to 10000 dimensions [5]. In addition to linear ODEs, the analysis of CPS with nonlinear ODE dynamics has been solved for small-scale systems. Notable techniques are Taylor models [6] and the δ -reachability analysis [7].

Although most of CPS applications involve ODE dynamics, there are many practical applications utilizing sensing and control of PDEs, such as fluid dynamics control, quantum mechanics, heat flow control, electrostatics and electrodynamics [8]. These applications require new verification methodologies and tools to deal with PDE dynamics in which the state vector depends

not only on time but also on space. A notable work in this direction is controller synthesis for safety specifications for hybrid systems with Hamilton-Jacobi PDE dynamics which is proposed in [9]. Analyzing a system with PDE dynamics for the whole space in which the dynamics are defined is challenging [10]. However, a cheaper analysis can be done if we only consider the system properties at some discrete points in the space. To do that, an *approximate discrete-space model* of a PDE needs to be obtained. This can be done efficiently using the Finite Different Method (FDM), a fundamental approach for solving PDEs in the field of numerical methods [11].

Using semi-explicit FDM, an approximate discrete-space model of a PDE can be obtained in the form of ODEs which then can be analyzed using existing verification tools. Generally, the obtained discrete-space model has finite dimensions, and approximates the behavior of the original PDE at specific *mesh points*. It is noted that increasing the number of mesh points in discretization grows the size of the obtained ODEs.

In this paper, we study the discrete-space analysis of some popular PDEs including the parabolic and hyperbolic equations. The derivation of ODE models from those equations is presented in detail. Our ultimate objective is to introduce PDE benchmarks to the verification community. Since we can obtain arbitrarily large ODEs by increasing the number of mesh points in discretization, e.g, ODEs with billions of dimensions, our benchmarks are suitable for evaluating the scalability of the existing or new verification approaches. The SpaceEx and Flow* models of all benchmarks introduced in this paper can be generated automatically using the PDE-to-ODE printer provided in the *pdev* prototype [10] which is written in Python and available at: <https://github.com/verivital/pdev>.

The paper is organized as follows. Section 2 presents in detail the derivation of the discrete-space models of all introduced benchmarks. The corresponding algorithms to generate these models are given in Appendix. Section 3 provides the analysis results of some small models of the benchmarks using SpaceEx. Section 4 discusses some open questions and concludes the paper.

2 Discrete-space Model Derivation

In this section, we present, in detail, how to derive the discrete-space models of PDEs using the semi-explicit FDM. All benchmarks considered in our paper are linear PDEs. We particularly focus on parabolic and hyperbolic PDEs in which heat and wave equations are two well-known representatives. Several types of boundary conditions for PDEs are addressed in this paper.

2.1 Parabolic Equation

The heat-flow and diffusion-type problems are fundamental physical processes which can be modeled as parabolic PDEs. These problems can happen in 1-dimensional, 2-dimensional or 3-dimensional physical objects. One simple example is that of heat flow on a 2-dimensional metal plate. The boundaries of the plate may be *insulated* or connected to a *heat source* or free to exchange the heat with the environment. To analyze such a physical process, the initial condition (IC) and boundary conditions (BCs) are essential concerns.

2.1.1 One-dimensional Heat Equation [12]

This benchmark is depicted in Figure 1. As shown in the figure, we have a copper rod with $L = 200cm$ of length. The top and two sides of the rod are insulated while the bottom is

immersed in moving water having a constant temperature of $20^\circ C$. The initial temperature of the rod is $0^\circ C$. The mathematical model of this heat-flow problem is as follows:

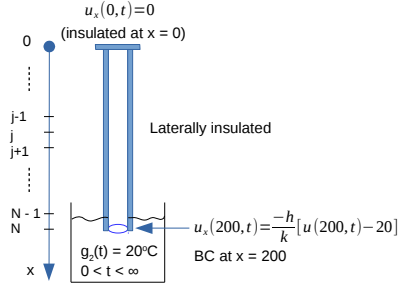


Figure 1: One-dimensional heat equation

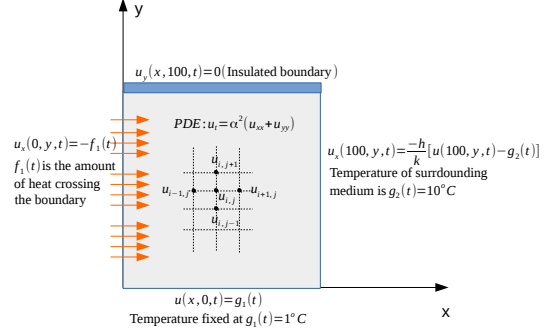


Figure 2: Two-dimensional heat equation

$$\begin{aligned}
 &PDE : u_t = \alpha^2 u_{xx}, \quad 0 < x < 200, \quad 0 < t < \infty \\
 &BCs : \begin{cases} u_x(0,t) = 0 \\ u_x(200,t) = -\frac{h}{k} [u(200,t) - g_2(t)] \end{cases}, \quad 0 < t < \infty \\
 &IC : u(x,0) = 0^\circ C, \quad 0 \leq x \leq 200
 \end{aligned} \tag{1}$$

where:

- $u(x,t)$ is the temperature of the rod at the position x and time t ,
- u_x is the partial derivative of the temperature.
- $\alpha^2 = 1.16 \text{cm}^2/\text{sec}$ is the diffusivity constant for copper,
- $k = 0.93 \text{cal}/\text{cm} \cdot \text{sec} \cdot ^\circ C$ is the thermal conductivity of copper,
- $h = 1$ is the heat exchange coefficient.

By discretizing the length of the rod into N segments and then using the semi-explicit FDM, we can obtain a discrete-space model in the form of linear ODEs with $N - 1$ state variables representing the temperatures at the discretized points of the rod. Let u_j be the temperature at the point j on the x -axis as shown in Figure 1. From the first boundary condition, we have $u_0 = 0$. Approximating the right hand side of the PDE using *central-difference approximation* leads to:

$$\frac{du_j}{dt} = \alpha^2 u_{xx} = \alpha^2 \frac{u_{j-1} - 2u_j + u_{j+1}}{\Delta x^2}, \tag{2}$$

where $\Delta x = L/N$ is the discretization step.

To obtain the discrete-space model, one more step that needs to be done is to approximate the boundary conditions at $x = 200$ and $x = 0$. Using the *backward-difference approximation* scheme for the boundary condition at $x = 200$, we have:

$$u_x^N = \frac{u_N - u_{N-1}}{\Delta x} = -\frac{h}{k} [u_N - g_2(t)]. \tag{3}$$

Consequently, the formula for the point N 's temperature is:

$$u_N = \frac{k}{k + \Delta x \times h} u_{N-1} + \frac{\Delta x \times h}{k + \Delta x \times h} g_2(t). \quad (4)$$

Similarly, using the *forward-difference approximation* scheme for the boundary condition at $x = 0$, we have:

$$u_x^0 = \frac{u_1 - u_0}{\Delta x} = 0 \Rightarrow u_1 = u_0. \quad (5)$$

Using Equations (2), (4) and (5), the discrete-space model of the heat-flow problem is obtained in the form $\dot{x} = Ax + Bv$ with following characteristics:

$$x = [u_1, u_2 \dots u_{N-1}]^T, v = g_2(t) = 20,$$

$$A = \frac{\alpha^2}{\Delta^2} \begin{bmatrix} -1 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 1 & -2 & 1 \\ 0 & \cdots & 0 & 0 & 1 & -2 + \frac{k}{k + \Delta x \times h} \end{bmatrix}, \quad B = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ \frac{\alpha^2 h}{\Delta x (k + \Delta x \times h)} \end{bmatrix}.$$

2.1.2 Two-dimensional Heat Equation [12]

This benchmark is depicted in Figure 2. The related constants (α^2, k, h) are the same as in the one-dimensional benchmark. The square copper plate has the width and height of $W = H = 1m = 100cm$. The mathematical model of this problem is as follows.

$$\begin{aligned} PDE : u_t &= \alpha^2(u_{xx} + u_{yy}) \\ BCs : \begin{cases} u_x(0, y, t) = -f_1(t) = -1 \\ u_x(100, y, t) = -\frac{h}{k}[u(100, y, t) - g_2(t)] \\ u(x, 0, t) = g_1(t) = 1^\circ C \\ u_y(x, 100, t) = 0 \end{cases}, & 0 < t < \infty \\ IC : u(x, y, 0) &= \sin(\pi x/100), \quad 0 \leq x \leq 100 \end{aligned} \quad (6)$$

where:

$u(x, y, t)$ is the temperature of at the position (x, y) and time t ,

u_{xx}, u_{yy} are the second order partial derivatives of the temperature along the x- and y-axes.

Similar to the one-dimensional heat-flow benchmark, we can obtain a discrete-space model of this two-dimensional heat-flow benchmark by discretizing the square copper plate by a number of mesh points and then using the semi-explicit. Assume that we discretize the width and the height of the plate by N and M segments along the x-axis and y-axis respectively. Totally, we have a $N \times M$ grid of mesh points and then the corresponding linear model of this benchmark has $(N - 1) \times (M - 1)$ state variables. The discretization steps along the x-axis and y-axis are $\Delta x = W/N$ and $\Delta y = H/M$ respectively.

Let $u_{i,j}$ be the temperature at the mesh point (i, j) as depicted in Figure 2. Using the

central-difference approximation scheme for the right hand side of the PDE leads to:

$$\begin{aligned} u_{xx}^{i,j} &= \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{\Delta x^2}, \\ u_{yy}^{i,j} &= \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{\Delta y^2}, \\ \frac{du_{i,j}}{dt} &= \alpha^2 \left[\frac{u_{i-1,j} + u_{i+1,j}}{\Delta x^2} + \frac{u_{i,j-1} + u_{i,j+1}}{\Delta y^2} - \left(\frac{2}{\Delta x^2} + \frac{2}{\Delta y^2} \right) u_{i,j} \right] \end{aligned} \quad (7)$$

Using *forward-approximation* for the first boundary condition, we have:

$$u_x(0, j) = \frac{u_{1,j} - u_{0,j}}{\Delta x} = -f_1(t) \Rightarrow u_{0,j} = u_{1,j} + \Delta x f_1(t). \quad (8)$$

Using the *backward-approximation* scheme for the second boundary condition yields:

$$u_x(N, j) = \frac{u_{N,j} - u_{N-1,j}}{\Delta x} = -\frac{h}{k} [u(N, j) - g_2(t)].$$

Consequently, we have:

$$u_{N,j} = \frac{k}{k + \Delta x \times h} u_{N-1,j} + \frac{\Delta x \times h}{k + \Delta x \times h} g_2(t). \quad (9)$$

The third boundary condition for the discretized mesh points is:

$$u_{i,0} = g_1(t). \quad (10)$$

Using the *back-ward approximation* scheme for the last boundary condition, we get:

$$u_y(i, M) = \frac{u_{i,M} - u_{i,M-1}}{\Delta y} = 0 \Rightarrow u_{i,M} = u_{i,M-1}. \quad (11)$$

Combining Equations (7)-(11), a linear model with $(N-1) \times (M-1)$ -dimensions of the form $\dot{x} = Ax + Bv$ of the two-dimensional heat-flow problem can be obtained, where:

$$u = \left[\underbrace{u_{1,1}, \dots, u_{N-1,1}}_{1^{st} \text{ column of MPs}}, \underbrace{u_{1,2}, \dots, u_{N-1,2}}_{2^{nd} \text{ column of MPs}}, \dots, \underbrace{u_{1,M-1}, \dots, u_{N-1,M-1}}_{(M-1)^{th} \text{ column of MPs}} \right]^T,$$

The input vector v is defined by $v = [f_1(t) \ g_1(t) \ g_2(t)]$.

Let $n = (N-1) \times (M-1)$, then the matrices $A \in \mathbb{R}^{n \times n}$ and $B \in \mathbb{R}^{n \times 3}$ can be obtained by Algorithm 1.1.

2.2 Hyperbolic Equation

Wave equations are used to model a large collection of phenomena such as the flow of fluids through a porous media and atmospheric flows. In this paper, we consider the one- and two-dimensional wave equations with the Dirichlet boundary condition and periodic boundary condition [13]. It should be noted that we can only obtain a discrete-space model in the form of ODEs for a first-order derivative wave equation while the second-order derivative wave equation is also usual in practice.

2.2.1 One-dimensional Wave Equation

$$\begin{aligned}
PDE : u_t + \alpha u_x &= 0, 0 < x < 30, 0 < t < \infty \\
BCs : u(0, t) &= u(30, t), \text{ (periodic BCs)} \\
ICs : \begin{cases} u(x, 0) = 1, & 14 \leq x \leq 18 \\ u(x, 0) = 0, & \text{otherwise,} \end{cases}
\end{aligned} \tag{12}$$

where α is the wave propagation speed.

By discretizing the space of interest with N uniform steps $\Delta x = 30/N$ and using the forward scheme, the spacial derivative u_x at the i^{th} mesh point is approximated as:

$$u_x^i = \frac{u_{i+1} - u_i}{\Delta x}, \quad u_i \equiv u(i \times \Delta x, t).$$

This leads to:

$$\frac{du_i}{dt} = \frac{\alpha}{\Delta x} (u_{i+1} - u_i) \tag{13}$$

At the boundary, we have the following constraints:

$$\frac{du_{N-1}}{dt} = \frac{\alpha}{\Delta x} (u_N - u_{N-1}), \quad u_N = u_0 \tag{14}$$

From (13) and (14), the discrete-space model of this wave equation is obtained in the form $\dot{x} = Ax$, where:

$$x = [u_0, \dots, u_{N-1}]^T, \quad A = \frac{\alpha}{\Delta x} \begin{bmatrix} -1 & 1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 1 & 0 & \dots & 0 \\ 0 & 0 & -1 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & -1 & 1 \\ 1 & 0 & 0 & \dots & 0 & -1 \end{bmatrix}$$

2.2.2 Two-dimensional Wave Equation

$$\begin{aligned}
PDE : u_t + \alpha u_x + \beta u_y &= 0, 0 < x < 6, 0 < y < 6, 0 < t < \infty \\
BCs : \begin{cases} u(0, y, t) = 0, \text{ (Dirichlet BC)} \\ u(x, 0, t) = u(x, 6, t), \text{ (periodic BC)} \end{cases} \\
ICs : \begin{cases} u(x, y, 0) = 1, & 0 \leq x \leq 1, 0 \leq y \leq 1 \\ u(x, y, 0) = 0, & \text{otherwise} \end{cases}
\end{aligned} \tag{15}$$

where $\alpha = 1cm/sec$ and $\beta = 1cm/sec$ are velocities of the wave in x and y directions respectively.

Discretizing the space of interest by $N \times M$ mesh points as in the case of the two-dimensional heat equation and using the backward-difference approximation scheme, we have:

$$\begin{aligned}
u_x^{i,j} &= \frac{u_{i,j} - u_{i-1,j}}{\Delta x}, \\
u_y^{i,j} &= \frac{u_{i,j} - u_{i,j-1}}{\Delta y}, \\
u_{i,j} &\equiv u(i \times \Delta x, j \times \Delta y), \quad \Delta x = \frac{30}{N}, \quad \Delta y = \frac{30}{M}.
\end{aligned} \tag{16}$$

At the boundary, we have the following constraints:

$$\begin{aligned} w_x^{1,j} &= \frac{u_{1,j} - u_{0,j}}{\Delta x} = \frac{u_{1,j}}{\Delta x}, \\ w_y^{i,1} &= \frac{u_{i,1} - u_{i,0}}{\Delta x} = \frac{u_{i,1} - u_{i,M}}{\Delta x}. \end{aligned} \quad (17)$$

Using (16) and (17), the discrete-space model of the two dimensional wave equation can be obtained in the form of $\dot{x} = Ax$, where $x = [u_{1,1}, \dots, u_{N,1}, u_{1,2}, \dots, u_{N,2}, \dots, u_{1,M}, \dots, u_{N,M}]^T$. The matrix $A \in \mathbb{R}^{NM \times NM}$ can be generated from Algorithm 1.2.

3 Reachability analysis

All discrete-space models of the PDE benchmarks studied in this paper can be analyzed by existing verification tools such as SpaceEx, Flow*, CORA and Hylaa which support ODE dynamics. It is worth noting that the traditional over-approximation tools such as SpaceEx, Flow* and CORA can analyze those models with small and medium sizes, i.e., from several to hundreds of state variables while the simulation-based tool Hylaa can analyze large models with thousands of state variables. We refer the reader to the generated SpaceEx/Flow* models for the detailed information of the initial conditions and safety requirements of all benchmarks.

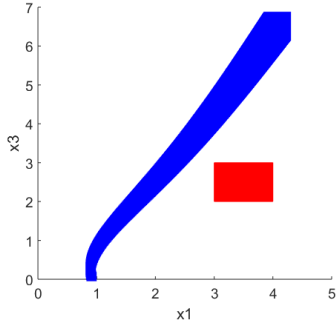


Figure 3: A reachable set of (x_1, x_3) of the discrete-model of the two dimensional heat equation using 3×3 grid of mesh points.

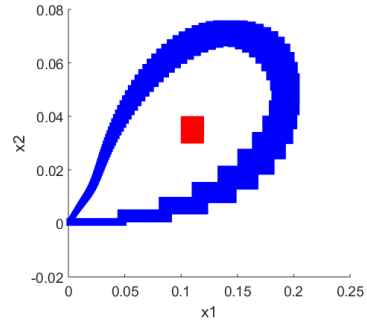


Figure 4: A reachable set of (x_1, x_2) of the discrete-model of the two dimensional wave equation using 3×3 grid of mesh points.

Figure 3 describes the reachable set of the pair (x_1, x_3) state variables of the discrete-space model of the two dimensional heat equation using SpaceEx. To obtain the discrete-space model, the space of interest is discretized by 3×3 grid of mesh points. The reachability analysis is done with an assumption that the input functions are constant in some bounded ranges. The unsafe region is the red square region defined by $3 \leq x_1 \leq 4$ and $2 \leq x_3 \leq 3$. The analysis shows that the discrete-space model satisfies its safety requirement.

Similarly, Figure 4 shows the reachable set of the pair (x_1, x_2) state variables of the discrete-space model of the two dimensional wave equation using SpaceEx. The discrete-space model is obtained by discretizing the space of interest using 3×3 grid of mesh points. The reachable set is computed with an assumption that the initial conditions are constant in some bounded ranges. The unsafe region (red square) is defined by $0.1 \leq x_1 \leq 0.12$ and $0.03 \leq x_2 \leq 0.04$. From the figure, one can conclude that the discrete-space model of the wave equation is safe.

4 Outlook

We have studied the discrete-space analysis for parabolic and hyperbolic PDEs by leveraging the well-known semi-explicit FDM and the existing verification tools supporting ODE dynamics. By doing that, we can verify the *safety of the discrete-space model* of PDEs at specific mesh points in the space. However, achieving a formal guarantee for a CPS with PDE dynamics is still a big challenge because of two reasons. Firstly, the FDM used in this paper is only an approximation method that does not give a *formal measurement* about the distance between the approximate behavior of the discrete-space model at a specific mesh point and the actual behavior of the original PDEs at that point. Secondly, suppose we have a completely formal discrete-space analysis approach, we still cannot answer anything about the safety of the system between two mesh points. From this observation and the fact that there are many CPSs involving PDEs dynamics, there is an urgent need of novel formal methodologies to analyze the safety of PDEs, not only at specific mesh points, but also for a whole continuous region in the space.

The SpaceEx/Flow* models generated from the considered PDEs benchmarks are useful for testing the scalability of verification techniques and tools. A billion dimensional discrete-space model of the two-dimensional heat equation has been used to evaluate the recent simulation-based reachability analysis approach leveraging Krylov subspace method [14]. In the future, we are going to explore some new types of PDEs such as elliptic and, more importantly, some real safety-critical applications related to PDE dynamics.

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Appendix A Algorithms for Two-dimensional Heat and Wave Equations

Algorithm 1.1 Discrete-space model of 2-dimensional heat-flow equation

Input: (N, M) % number of discretization steps along x and y-axis

Output: (A, B) % matrix of the linear ODE: $\dot{x} = Ax + Bv$

```

1: procedure INITIALIZATION
2:   n = (N - 1) × (M - 1) % number of state variables
3:   A ← (n × n) sparse matrix
4:   B ← (n × 3) sparse matrix
5:   α2 ← diffusivity constant
6:   q ←  $\frac{h}{k}$  % heat loss constant
7:   Δx ←  $\frac{W}{N} = \frac{100}{N}$  % discretization step along x-axis
8:   Δy ←  $\frac{H}{M} = \frac{100}{M}$  % discretization step along y-axis
9: procedure FILLING A AND B
10: loop for i = 0 to n:
11:   A[i, i] ←  $-2(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2})$ 
12:   posx ← i % (N - 1) % x-position of i-th state variable
13:   posy ← int( $\frac{i - pos_x}{N - 1}$ ) % y-position of i-th state variable
14:   if posx - 1 ≥ 0:
15:     A[i, i - 1] ←  $\frac{1}{\Delta x^2}$ 
16:   else:
17:     A[i, i] ← A[i, i] +  $\frac{1}{\Delta x^2}$ 
18:     B[i, 0] ←  $\frac{1}{\Delta x}$ 
19:   if posx + 1 ≤ N - 2:
20:     A[i, i + 1] ←  $\frac{1}{\Delta x^2}$ 
21:   else:
22:     A[i, i] ← A[i, i] +  $\frac{1}{\Delta x^2(1 + q\Delta x)}$ 
23:     B[i, 2] ←  $\frac{q}{\Delta x(1 + q\Delta x)}$ 
24:   if posy - 1 ≥ 0:
25:     A[i, (posy - 1)(N - 1) + posx] ←  $\frac{1}{\Delta y^2}$ 
26:   else:
27:     B[i, 1] ←  $\frac{1}{\Delta y^2}$ 
28:   if posy + 1 ≤ M - 2:
29:     A[i, (posy + 1)(N - 1) + posx] ←  $\frac{1}{\Delta y^2}$ 
30:   else:
31:     A[i, i] ← A[i, i] +  $\frac{1}{\Delta y^2}$ 
32: end loop: A ← α2A, B ← α2B
33: return (A, B)

```

Algorithm 1.2 Discrete-space model of 2-dimensional wave equation

Input: (N, M) % number of discretization steps along x and y-axis

Output: A % matrix of the linear ODE: $\dot{x} = Ax$

```

1: procedure INITIALIZATION
2:    $n = N \times M$ 
3:    $A \leftarrow (n \times n)$  sparse matrix
4:    $\alpha \leftarrow$  wave propagation speed in x direction
5:    $\beta \leftarrow$  wave propagation speed in y direction
6:    $\Delta x \leftarrow$  discretization step along x-axis
7:    $\Delta y \leftarrow$  discretization step along y-axis
8:    $a \leftarrow \alpha / \Delta x$ 
9:    $b \leftarrow \beta / \Delta y$ 
10: procedure FILLING  $A$ 
11: loop for  $i = 0$  to  $n$ :
12:    $A[i, i] \leftarrow a + b$ 
13:    $pos_x = i \bmod N$  % x-position corresponding to i-th state variable
14:    $pos_y = \text{int}((i - pos_x) / N)$  % y-position corresponding to i-th state variable
15:   if  $pos_y == 0$  then:
16:      $A[i, i - 1] \leftarrow -a$ 
17:      $A[i, i] \leftarrow b + a$ 
18:   else:
19:      $A[i, i - 1] \leftarrow -a$ 
20:      $A[i, i] \leftarrow b + a$ 
21:      $A[i, i - N] \leftarrow -b$ 
22:   if  $pos_y == M - 1$  then:
23:      $A[pos_x, i] \leftarrow -b$ 
24: end loop
25: Return( $A$ )

```
