Geometric Time Integration with Absorbing Boundary conditions. A case study for the wave equation

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1. Evolutionary Initial Value Problems: preliminaries

Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^n$ be a smooth enough function and let y_0 be a point in Ω, the phase space.

We are concerned with the first order in time initial value problem

$$\left.\begin{array}{rcll} y' & = & f(y), & t \geq 0, \\ y(0) & = & \alpha \in \Omega & \end{array}\right\} \tag{1}$$

From suitable hypotheses of regularity, there is a unique solution $y(t) = y(t, \alpha)$ of (1). Let t be a time value such that the solution $y(t)$ of (1) is well defined. The flow ϕ_t is the map

$$\begin{array}{rcl} \phi_t : \Omega & \to & \Omega \\ \alpha & \to & y(t, \alpha) \end{array}$$

Example We take $\Omega = \mathbb{R}^2$, $\lambda > 0$, and we consider the second order in time initial value problem

$$\left.\begin{array}{rcll} y'' & = & -\lambda^2 y, & t \geq 0, \\ y(0) & = & \alpha_1, & \\ y'(0) & = & \alpha_2. & \end{array}\right\} \tag{2}$$

Making the change of variables $y_1 = y, y_2 = y'$, we obtain an equivalent first order in time initial value problem

$$\left.\begin{array}{rcl} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}' & = & \begin{bmatrix} 0 & 1 \\ -\lambda^2 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}, \\ \begin{bmatrix} y_1(0) \\ y_2(0) \end{bmatrix} & = & \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} = \alpha \end{array}\right\} \tag{3}$$

The solution of (3) is given by

$$\begin{aligned}
\begin{bmatrix} y_1(t) \\ y_2(t) \end{bmatrix} &= \begin{bmatrix} \cos(t\lambda) & \lambda^{-1}\operatorname{sen}(t\lambda) \\ -\lambda\operatorname{sen}(t\lambda) & \cos t \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} \\
&= \exp\left(t \begin{bmatrix} 0 & 1 \\ -\lambda^2 & 0 \end{bmatrix}\right) \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} \\
&= \begin{bmatrix} -i & i \\ \lambda & \lambda \end{bmatrix} \exp\left(t \begin{bmatrix} -i\lambda & 0 \\ 0 & i\lambda \end{bmatrix}\right) \begin{bmatrix} -i & i \\ \lambda & \lambda \end{bmatrix}^{-1} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix}
\end{aligned}$$

2. Evolutionary Initial Value Problems: Hamiltonian problems (Hamilton 1834)

An initial value problem is Hamiltonian if $n = 2d$, and, with the notation $y = (p, q) \in \mathbb{R}^d \times \mathbb{R}^d$, there exists $H : \Omega \to \mathbb{R}$, such that

$$f^i = -\frac{\partial H}{\partial q_i}, \qquad f^{i+d} = \frac{\partial H}{\partial p_i}, \qquad i = 1, \ldots, d.$$

- H is the Hamiltonian function.

- d is the number of degrees of freedom.

or, alternatively,

$$\frac{dy}{dt} = J^{-1} \nabla H(y), \qquad J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$$

where 0 and I respectively represent the zero and unit $d \times d$ matrices.

A relevant property of the solution of a Hamiltonian initial value problem is the conservation of the energy which can be deduced from

$$\frac{dH(y(t))}{dt} = \nabla H(y(t))^T \frac{dy(t)}{dt} = \nabla H(y(t))^T J^{-1} \nabla H(y(t)) = 0.$$

Therefore, if $y(t)$ is the solution of the Initial Value Problem, then

$$H(y(t)) = H(y(0)), \quad t \geq 0.$$

Hamiltonian problems are suitable as model for situations where dissipation is absent or may be ignored.

Example We take the Hamiltonian function ($d = 1$),

$$H(p, q) = \frac{p^2}{2} + \frac{\lambda^2 q^2}{2}$$

which is the sum of the kinetic an potential energies of a material point of mass equals to 1 attached to a spring with stiffness constant λ^2.

The corresponding differential equation is

$$\dot{p} = -\lambda^2 q, \quad \dot{q} = p,$$

which is, with the notation $y(t) = (q(t), p(t))$, the same one we introduced in (2).

The general solution is given by the oscillations

$$\begin{aligned} q(t) &= c_1 \operatorname{sen}(\lambda t + c_2), \\ p(t) &= \lambda c_1 \cos(\lambda t + c_2), \end{aligned}$$

and in the (p, q)-phase space $\Omega = \mathbb{R}^2$, the parametric curves $(p(t), q(t)$ correspond to the ellipses

$$\frac{p^2}{2} + \frac{\lambda^2 q}{2} = constant,$$

which are circles when $\lambda = 1$. These curves are the orbits of the diagram phase. They are closed curves corresponding to periodic solutions of the differential system.

Symplecticness

Definition: A differentiable transformation $y^* = \Psi(y)$, $y^* = (p^*, q^*)$, $y = (p, q)$, $\Psi : \Omega \to \mathbb{R}^d \times \mathbb{R}^d$ is called symplectic (canonical) if its Jacobian matrix $\Psi'(y)$ satisfies, for each $y = (p, q) \in \Omega$,

$$\Psi'(y)^T J \Psi'(y) = J$$

The flow Φ_t of a Hamiltonian system is symplectic (canonical) for each fixed t.

Geometric interpretation: For $d = 1$, the symplecticness is equivalent to the relation

$$\Delta = \det\left(\frac{\partial(p^*, q^*)}{\partial(p, q)}\right) = \frac{\partial p^*}{\partial p}\frac{\partial q^*}{\partial q} - \frac{\partial p^*}{\partial q}\frac{\partial q^*}{\partial p} \equiv 1$$

Therefore, the transformation is canonical if and only if it preserves oriented areas.

For $d > 1$, let $D \subset \Omega$ be an oriented two-dimensional bounded surface. Let $\Pi_i(D)$ be the projection of D onto each of the d two-dimensional planes of the variables (p_i, q_i), $i = 1, \ldots, d$. Now we compute

$$S(D) = \sum_i \pm Area(\Pi_i(D)),$$

where the signs depend on the orientation of each $\Pi_i(D)$. Then a transformation Ψ is canonical if and only if $S(D) = S(\Psi(D))$ for each D.

3. Evolutionary Initial Value Problems: numerical methods

We want to obtain an approximation to the solution of (1) in the interval $[0, T]$, where $T > 0$ is fixed.

For this, we take $M > 0$ integer, $k = T/M$ (the step-size), and we consider the grid $t_n = nk$, $n = 0, 1, \ldots M$. Then, we look for approximations $y_n \approx y(t_n)$. The simplest method is Euler's scheme given by

$$\left.\begin{array}{rcl} y_0 & = & \alpha \\ y_{n+1} & = & y_n + kf(y_n) \end{array}\right\}$$

Euler's scheme is a particular case of one step methods given by

$$\left.\begin{array}{rcl} y_0 & = & \alpha \\ y_{n+1} & = & \psi_k(y_n),\ n \geq 0 \end{array}\right\}$$

With this notation, the mapping

$$\psi_k : \Omega \to \mathbb{R}^d$$

is an approximation to the flow Φ_k defined from the exact solution.

The Runge Kutta methods are a well known class of one step methods. They are given by the equations

$$\left\{\begin{array}{rcl} Y_i & = & y_n + k\sum_{j=1}^{s} a_{ij} f(t_n + c_j k, Y_j) \\ y_{n+1} & = & y_n + k\sum_{i=1}^{s} b_i f(t_n + c_i k, Y_i), \end{array}\right. \tag{4}$$

where Y_i, $i = 1, \cdots, s$ are the intermediate stages. Each choice of the parameters $\mathbf{b} = [b_j]_{j=1}^{s}, \mathbf{c} = [c_j]_{j=1}^{s} \in \mathbb{R}^s$, $\mathcal{A} = [a_{ij}]_{i,j=1}^{s} \in \mathbb{R}^{s\times s}$, gives rise to a different Runge-Kutta method

Euler's method is an example of Runge-Kutta method with 1 stage given by the equations

$$\begin{cases} Y_1 &= y_n \\ y_{n+1} &= y_n + kf(t_n, Y_1), \end{cases} \tag{5}$$

Another example with 1 stage is the implicit midpoint rule

$$\begin{cases} Y_1 &= y_n + kf(t_n + k/2, Y_1) \\ y_{n+1} &= y_n + (k/2)Y_1, \end{cases} \tag{6}$$

Notice that in this last case, the equation for the stage is implicit.

4. Evolutionary Initial Value Problems: the error

The global error in the interval $[0, T]$ committed by the numerical method is

$$e_M = \max_{0 \leq n \leq M} | \, y_n - y(t_n)|,$$

where we recall that $Mh = T$, and therefore $y_M = \psi_k^M(y_0)$ and $y(T) = \phi_k^M(y_0)$.

The numerical scheme is convergent of order p when

$$e_M = O(k^p), \quad k \to 0.$$

For example, Euler's method is convergent of first order and the mid-point rule is convergent of second order. It is possible to find Runge Kutta methods with any order $p > 0$ integer.

5. Evolutionary Initial Value Problems: absolute stability

We consider the linear autonomous equation

$$y' = Ly, \tag{7}$$

where L is a normal complex constant matrix such that $\{\Re(\lambda) \leq 0 \, : \, \lambda \in \sigma(L)\}$

The solution of (7) is given by

$$y(t) = \exp(tL)\alpha,$$

where α is the vector of initial conditions and, from the hypotheses, the bound

$$\begin{aligned} \|y(t)\| &= \|\exp(tL)\alpha\|_2 \leq \|\exp(tL)\|_2 \|\alpha\|_2 \\ &= \rho(\exp((tL))\|\alpha\|_2 \leq C, \end{aligned}$$

holds for C a constant independent of $t \geq 0$.

If we use a Runge-Kutta method to approximate the solution of (7), we obtain

$$y_{n+1} = r(kL)y_n, \tag{8}$$

where $r(z) = 1 + z\mathbf{b}^T(\mathcal{I} - z\mathcal{A})^{-1}\mathbf{1}$, the absolute stability function of the Runge-Kutta method. ($\mathbf{1} = [1, \ldots, 1]^T \in \mathbb{R}^s$)

Examples:

- Euler's method: $r(z) = 1 + z$.
- Implicit midpoint rule: $r(z) = (1 + z/2)(1 - z/2)^{-1}$.

$r(z)$ is always a rational function.

Suppose that we start the computation with the initial condition $y_0 = \alpha$ and let y_n, $0 \leq n \leq N$ be the numerical solution obtained in this way. Then

$$y_n = r(kL)y_{n-1} = r^n(kL)y_0.$$

Since the solution is bounded for $t \geq 0$, it is reasonable to wish that the bound

$$||r^n(kL)|| \leq C, \tag{9}$$

holds for a constant C independent of $0 \leq n \leq N$.

From now on,

$$\mathcal{R}_A = \{z \in \mathbb{C} : |r(z)| \leq 1\},$$

is the absolute stability region and the Runge-Kutta method is absolutely stable for $z \in \mathbb{C}$ if $z \in \mathcal{R}_A$.

Suppose that L is a normal matrix with $\{\Re(\lambda) \leq 0 : \lambda \in \sigma(L)\}$ and consider the Euclidean norm. Then

$$||r^n(kL)||_2 = \rho(r^n(kL)) = \rho^n(r(kL)).$$

Therefore, the stability bound (9) is satisfied with the Euclidean norm when $|r(k\lambda_i)| \leq 1$ for each $\lambda_i \in \sigma(L)$ or, equivalently, when

$$k\lambda_i \in \mathcal{R}_A \,\text{for each}\, \lambda_i \in \sigma(L).$$

- Since L is arbitrary, it is convenient that the absolute stability region is as wide as possible. In this way, it is possible to use big values of h without losing the stability.

- In general, when the eigenvalues are very big (stiff problems), then $\mathcal{R}_A$ has to be unbounded.

- The most favorable case is an A-stable method, when

$$\{z \in \mathbb{C} : \Re(z) \leq 0\} \subset \mathcal{R}_A.$$

- If the system to be solved (7) is Hamiltonian, then $\sigma(L) \subset i\mathbb{R}$. Now, the best situation is $i\mathbb{R} \subset \mathcal{R}_A$.

6. Geometric Integration: preliminaries When we approximate numerically an initial value problem:

- Look for numerical methods for specific classes of problems
- Design methods taking in account geometric properties of the flow.

Examples:

- Hamiltonian problems,
- Problems with symmetries,
- Volume preserving flows,
- etc.

7. Geometric Integration: symplectic methods Let Φ_t^H be the flow associated to a Hamiltonian system with Hamiltonian function $H(p,q)$. Then

$$(p(t_{n+1}), q(t_{n+1})) = \Phi_k^H(p(t_n), q(t_n))$$

We approximate this solution operator by means of a one-step method given by

$$(p_{n+1}, q_{n+1}) = \Psi_k^H(p_n, q_n),$$

Since the mapping Φ_t^H is a symplectic transformation, it is reasonable to insist on Ψ^H also being a symplectic transformation.

A Runge-Kutta method is symplectic if the coefficients of the method satisfy

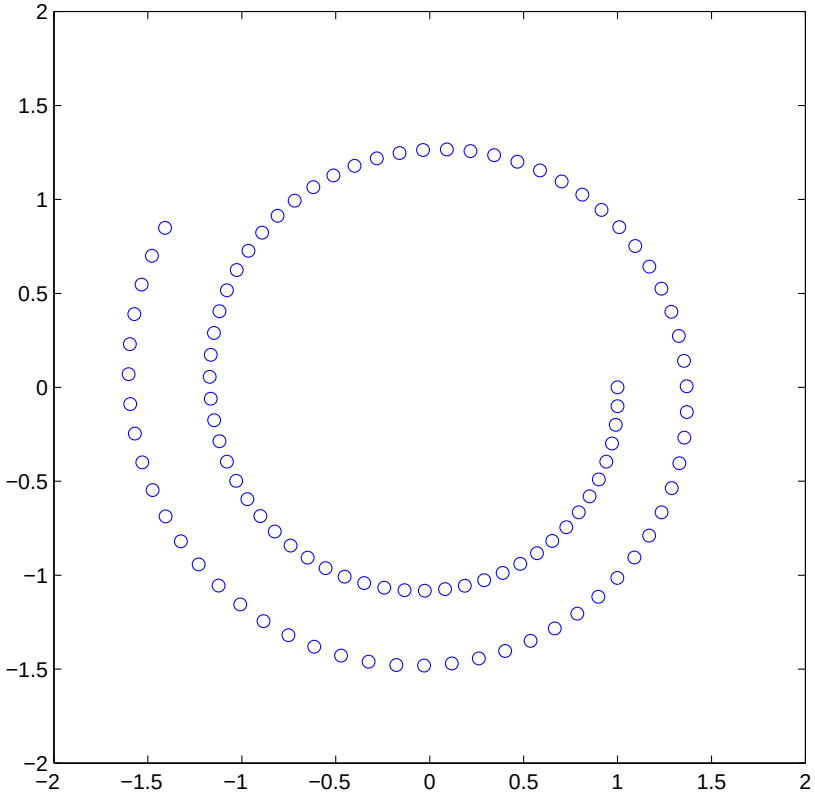
$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad i,j = 1,\ldots,s$$

- Euler's method is not symplectic.

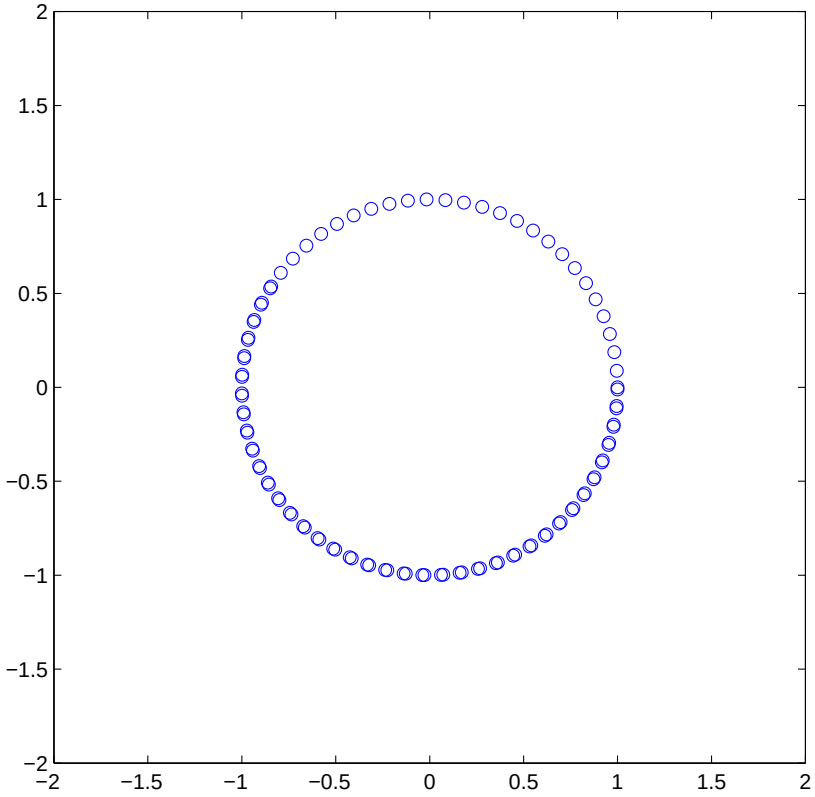
  In fact, for $b \in \mathbb{R}$, $|r(ib)| = |1 + ib| = \sqrt{1 + b^2} > 1$ and we deduce that $i\mathbb{R} \cap \mathcal{R}_A = \emptyset$.

- The midpoint rule is symplectic.

  In fact, for $b \in \mathbb{R}$, $|r(ib)| = |(1 - ib/2)^{-1}(1 + ib/2)| = 1$ and we deduce that $i\mathbb{R} \subset \mathcal{R}_A$. Notice that $r(z)$ has a singularity at $z = 2$.



The harmonic oscillator with initial condition $y0 = [1, 0]^T$ integrated by the non symplectic explicit Euler method.



The harmonic oscillator with initial condition $y0 = [1, 0]^T$ integrated by the symplectic midpoint rule.

8. Geometric Integration: Diagonally Implicit Symplectic Runge-Kutta methods

Diagonally implicit: $a_{ij} = 0, \quad j > i$ or, equivalently, $A = [a_{ij}]_{i,j=1}^{s}$ is lower triangular. This condition leads to the solution of s $2d$ dimensional systems per time step (in the general case, we solve a $2sd$-system).

The symplecticness conditions lead to $a_{ij} = b_i$ for $i < j$ and $a_{ii} = b_i/2$.

The resulting method is a concatenation of s steps of midpoint rules with steplengths $b_1 h, b_2 h, \ldots, b_s h$.

Example: With $s = 3$ stages, and taking

$$b_1 = b_3 = \frac{1}{3}(2 + 2^{1/3} + 2^{-1/3}),$$
$$b_2 = 1 - 2b_1 < 0,$$

the resulting method has order $p = 4$.

The corresponding stability function is

$$r(z) = (1 - zb_1/2)^{-1}(1 + zb_1/2)(1 - zb_2/2)^{-1}(1 + zb_2/2)(1 - zb_3/2)^{-1}(1 + zb_3/2)$$

which has a singularity in $z = 2/b_2 < 0$ and its stability region includes the left half plane $\Re(z) \leq 0$, except for a little island almost circular which intersections with the real axis are $-1.1344\cdots$ and $-1.2006\cdots$.

This method is not A-stable. However, if it is used to integrate a Hamiltonian problem, we do not have any trouble because $i\mathbb{R} \subset \mathcal{R}_A$.

9. Absorbing and transparent Boundary conditions

Subject: Numerical solution of a PDE defined in an unbounded domain.

Solution: to choose a finite computational domain and to use

- Transparent Boundary conditions (TBCs)

- Absorbing Boundary Conditions (ABCs)

10. Discretization of a pure initial value problem for the one dimensional wave equation

We consider the one dimensional wave equation

$$u_{tt} = u_{xx}, \quad x \in \mathbb{R}, t \geq 0. \tag{10}$$

Spatial discretization.

Let $h > 0$ be a positive parameter, $x_j = a + jh$ para $j \in \mathbb{Z}$. We define

$$\frac{d^2U_j}{dt^2} = \frac{U_{j+1} - 2U_j + U_{j-1}}{h^2}, \quad j \in \mathbb{Z}, t \geq 0. \tag{11}$$

where $U_j(t) \approx u(x_j, t)$.

Dirichlet boundary conditions.

We consider the interval $[a, b]$ and we add the boundary conditions $u(a, t) = u(b, t) = 0$, $t \geq 0$ to the problem (10).

We now denote $[a, b] = [x_0, x_N] = [a, a + Nh]$, $h = (b - a)/N$, $N \in \mathbb{N}$.

At the boundary, the spatial discretization if given by $U_0 = U_N = 0$ and we obtain the ordinary differential system

$$\frac{d^2 u_h}{dt^2}(t) = A_h u_h, \tag{12}$$

where $u_h = [u_1, \ldots, u_{N_1}]^T$, $A_h = \frac{1}{h^2} A_{N-1}$, and

$$A_{N+1}^{(4)} = \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix},$$

We rewrite (12) as the first order differential system

$$\frac{d}{dt}\begin{bmatrix} u_h \\ v_h \end{bmatrix} = \mathcal{A}_h \begin{bmatrix} u_h \\ v_h \end{bmatrix} = \begin{bmatrix} 0 & I \\ A_h & 0 \end{bmatrix}\begin{bmatrix} u_h \\ v_h \end{bmatrix}, \tag{13}$$

where $v_h = du_h/dt$.

A_h is symmetric a negative definite and $\mathcal{A}_h$ is a normal matrix with purely imaginary eigenvalues ($\sigma(\mathcal{A}_h) \subset [-i/(2h), i/(2h)]$).

In fact, (13) is a Hamiltonian system and the time integration can be achieved with a Symplectic Runge Kutta method such that $i\mathbb{R} \subset \mathcal{R}_A$ without any stability difficulty.

Absorbing boundary conditions.

We denote the computational window by $[a,b]=[x_0,x_N]=[a,a+Nh]$, $h=(b-a)/N$, $N\in\mathbb{N}$. The TBCs are given, in Fourier variables, by

$$\left.\begin{array}{rcl}\widehat{u}_0(\omega) & = & r_1(\omega h)\,\widehat{u}_1(\omega),\\ \widehat{u}_N(\omega) & = & r_1(\omega h)\,\widehat{u}_{N-1}(\omega),\end{array}\right\} \tag{14}$$

at $x=x_0$ and $x=x_N$ respectively, where

$$\widehat{u}_j(\omega)=\frac{1}{2\pi}\int_{\mathbb{R}}\exp(-i\omega t)u_j(t)dt,\quad 0\le j\le N,$$

and the kernel function is $r_1(z)=1-\dfrac{z^2}{2}-iz\left(1-(\dfrac{z}{2})^2\right)^{1/2}$.

The ABCs are obtained by approximating the kernel function $r_1(\omega h)$ for small frequencies ω with Taylor or Padé expansions and taking the inverse Fourier transform in order to deduce the ABCs in the original variables.

The formulas for ABC(2,2) To achieve ABC(2,2) we consider the fourth order Padé expansion of r_1, given by

$$r_1(z) = \frac{1 - \frac{i}{2}z - \frac{1}{8}z^2}{1 + \frac{i}{2}z - \frac{1}{8}z^2} + O(z^5).$$

From (14), where r_1 is replaced with this Padé expansion, and taking inverse Fourier transform

$$\begin{aligned} u_0 + \tfrac{h}{2}u_0' + \tfrac{h^2}{8}u_0'' &= u_1 - \tfrac{h}{2}u_1' + \tfrac{h^2}{8}u_1'', \\ u_N + \tfrac{h}{2}u_N' + \tfrac{h^2}{8}u_N'' &= u_{N-1} - \tfrac{h}{2}u_{N-1}' + \tfrac{h^2}{8}u_{N-1}''. \end{aligned}$$

We now replace u_1'' and u_{N-1}'' with its value at the inside the interval and we have

$$u_0'' = \frac{1}{h^2}(-7u_0 + 6u_1 + u_2) - \frac{4}{h}(u_0' + u_1'),$$

$$u_N'' = \frac{1}{h^2}(-7u_N + 6u_{N-1} + u_{N-2}) - \frac{4}{h}(u_N' + u_{N-1}').$$

We obtain the ordinary differential system

$$\frac{d^2u_h}{dt^2}(t) = A_h^{(4)}u_h + B_h^{(4)}\frac{du_h}{dt}, \tag{15}$$

where $u_h = [u_0, \ldots, u_N]^T$, $A_h^{(4)} = \frac{1}{h^2}A_{N+1}^{(4)}$, $B_h^{(4)} = \frac{1}{h}B_{N+1}^{(4)}$, and

$$A_{N+1}^{(4)} = \begin{bmatrix} -7 & 6 & 1 & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & 1 & 6 & -7 \end{bmatrix}, \quad B_{N+1}^{(4)} = \begin{bmatrix} -4 & -4 & & & \\ 0 & 0 & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & 0 & 0 \\ & & & -4 & -4 \end{bmatrix}.$$

We rewrite (15) as the first order in time differential system

$$\frac{d}{dt}\begin{bmatrix} u_h \\ v_h \end{bmatrix} = \mathcal{A}_h^{(4)}\begin{bmatrix} u_h \\ v_h \end{bmatrix} = \begin{bmatrix} 0 & I \\ A_h^{(4)} & B_h^{(4)} \end{bmatrix}\begin{bmatrix} u_h \\ v_h \end{bmatrix}, \tag{16}$$

- Since the solution is absorbed at the boundary, there exist $\mu \in \sigma(\mathcal{A}_h^{(i)})$ with $\Re(\mu) < 0$

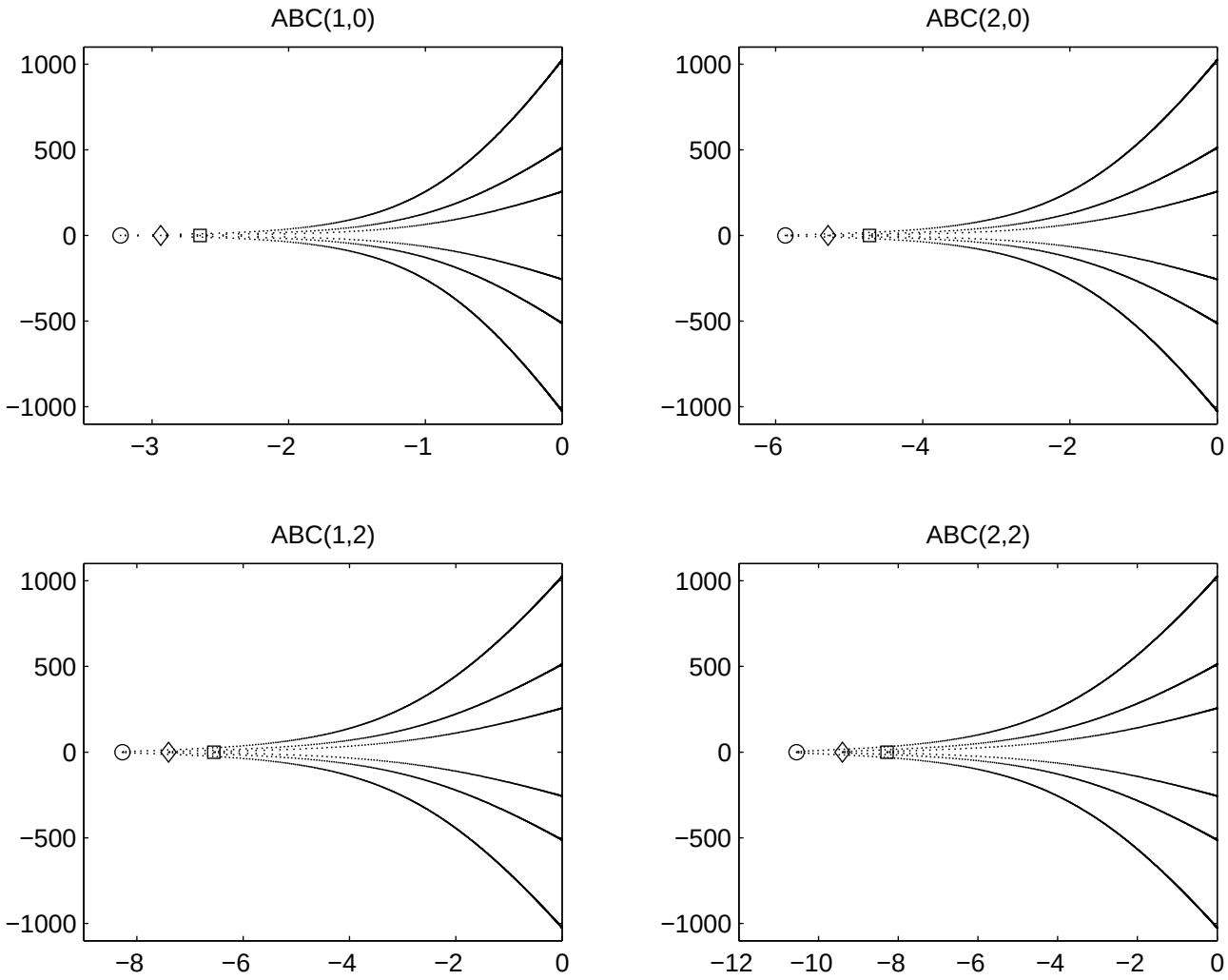
- If $\Re(\mu) > 0$ for some $\mu \in \sigma(\mathcal{A}_h^{(i)})$, the problem (16) is ill posed.

Theorem 1 *Let* $\mathcal{A}_h^{(4)}$ *be the coefficient matrix of the differential system (16). Then,* $\Re(\mu) \leq 0$ *for all* $\mu \in \sigma(\mathcal{A}_h^{(4)})$.

Behaviour of the eigenvalues: numerical computation

- when N increases, the sizes of the real and imaginary parts of the eigenvalues grow with N.

- the real parts of the eigenvalues also grow when the order of absorption increases.



Eigenvalues μ, for ABC(1,0), ABC(2,0), ABC(1,2) and ABC(2,2).
$N = 256$ (in), $N = 512$ (medium), $N = 1024$ (out)

Full discretization, absorbing boundary conditions and time stability

We discretize in time the system (16) by means of a Runge-Kutta method.

If the stability function of the Runge-Kutta method is $r(z)$, we obtain the numerical approximation

$$\begin{bmatrix} u_{h,n+1} \\ v_{h,n+1} \end{bmatrix} = r\left(k\mathcal{A}_h^{(i)}\right) \begin{bmatrix} u_{h,n} \\ v_{h,n} \end{bmatrix} \tag{17}$$

To avoid stability problems, it is suitable that the Runge-Kutta method is A-stable, i.e.

$$\{z \in \mathbb{C} : \Re(z) \leq 0\} \subset \mathcal{R}_A.$$

Full discretization, absorbing boundary conditions, geometric integration and time stability

- the problem must be conservative in order to use geometric integrators.

- the incorporation of ABCs converts the original problem into a strongly dissipative system.

A paradox?

No, the geometric properties of the solution are still relevant inside the computational domain.

However, A-stable symplectic Runge-Kutta methods (Gauss methods) are very expensive when they are used to solve systems of high dimension.

Then the time integrator is not A-stable, and the sizes of $\Re(\mu), \mu \in \sigma(\mathcal{A}_h^{(i)})$, must not increase too fast when the spatial discretization is refined.

For our case study, we can observe numerically that the sizes of the real parts of the eigenvalues grow slower than the ones of imaginary parts.

Theorem 2 *The eigenvalues* μ *of the matrices* $\mathcal{A}_h^{(4)}$ *satisfy*

$$\Re(\mu) = O(N^{1-\alpha}),$$
$$\Im(\mu) = O(N),$$

as $N \to \infty$, *for every* $\alpha \in (0, 1)$.

Taking $N = 128, 256, 512, 1024$, which are in a useful range, the value of α observed in practice is $\alpha = 0.8$. Therefore, $\Re(\mu) = O(N^{0.2})$.

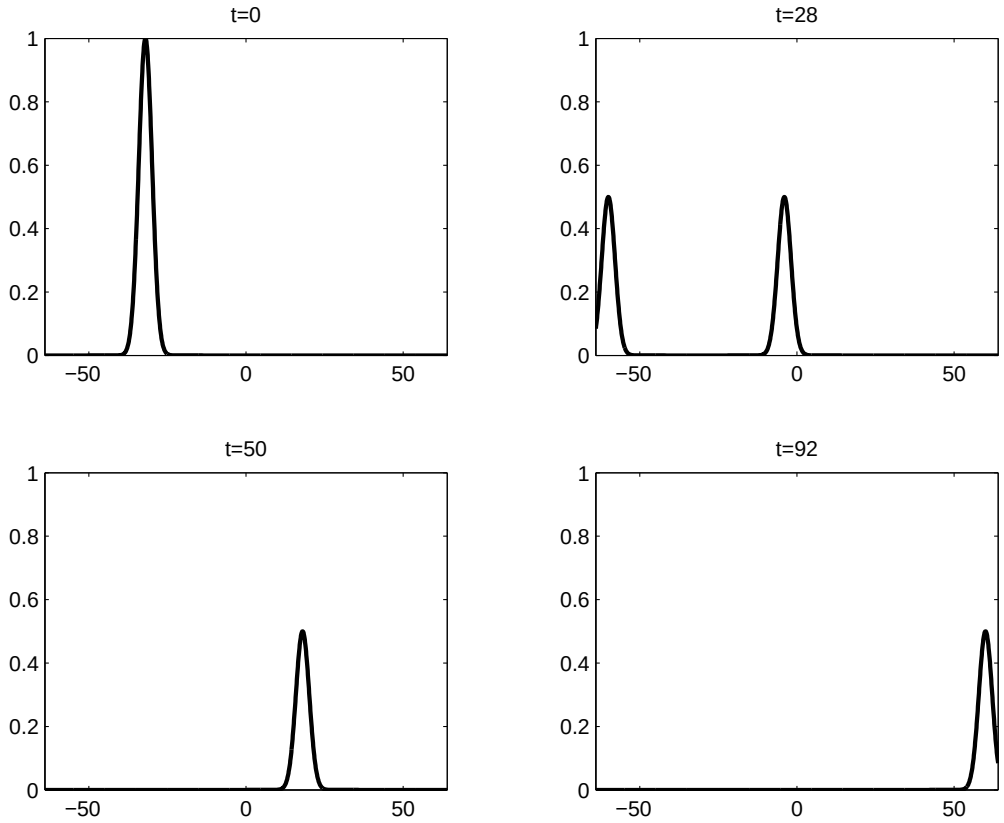
11. A numerical experiment

We consider the problem (10) and the computational window $[-64, 64]$ with absorbing boundary conditions in the boundary. We take $L = 64$ and the initial conditions $u(x, 0) = e^{-B(x+32)^2}$ and $u_t(x, 0) = 0$. We choose $B = (22 \times \log(10))/(L/3)^2$ to achieve $e^{-B(L/3)^2} < 10^{-20}$ and, in practice, we can consider the support of $u(x, 0)$ contained in $[-32 - L/3, -32 + L/3]$.

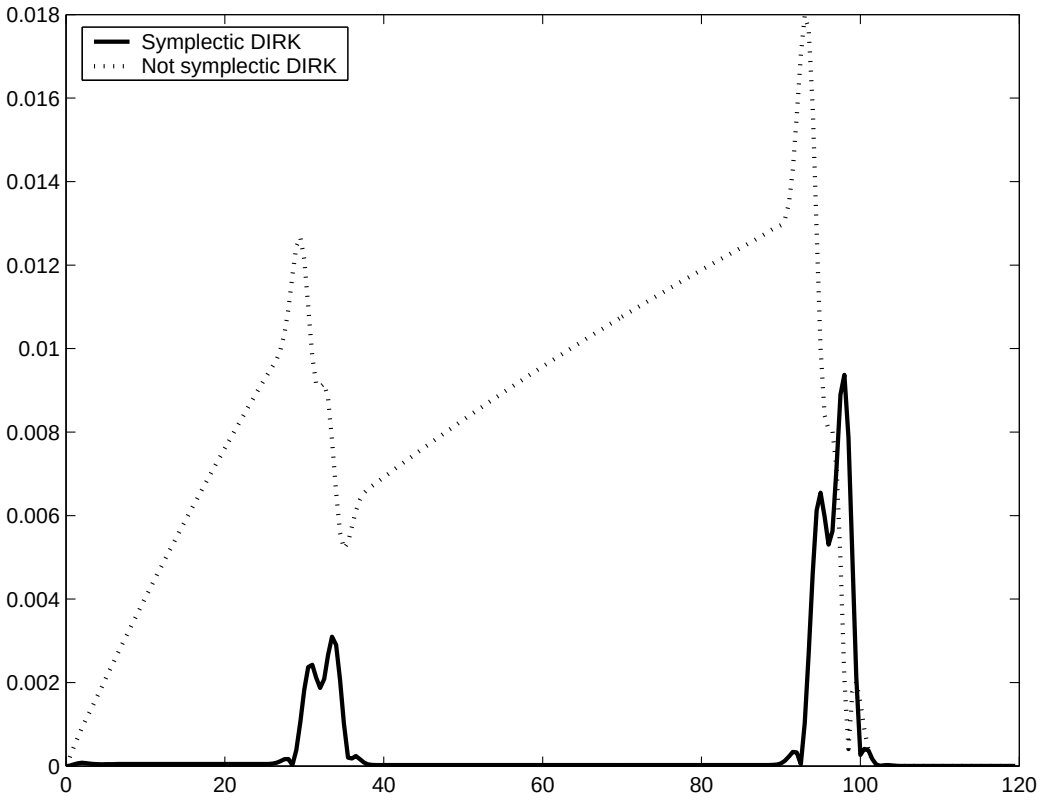
We select as symplectic method the 3-stage fourth order symmetric DIRK method previously introduced and we choose a non symplectic method, the 3-stage singly DIRK method of fourth order given by

$$\begin{array}{c|ccc} \frac{1+\nu}{2} & \frac{1+\nu}{2} & 0 & 0 \\ \frac{1}{2} & -\frac{\nu}{2} & \frac{1+\nu}{2} & 0 \\ \frac{1-\nu}{2} & 1+\nu & -1-2\nu & \frac{1+\nu}{2} \\ \hline & \frac{1}{6\nu^2} & 1-\frac{1}{3\nu^2} & \frac{1}{6\nu^2} \end{array} \tag{18}$$

where $\nu = (2/\sqrt{3})\cos(\pi/18)$. This method is A-stable.

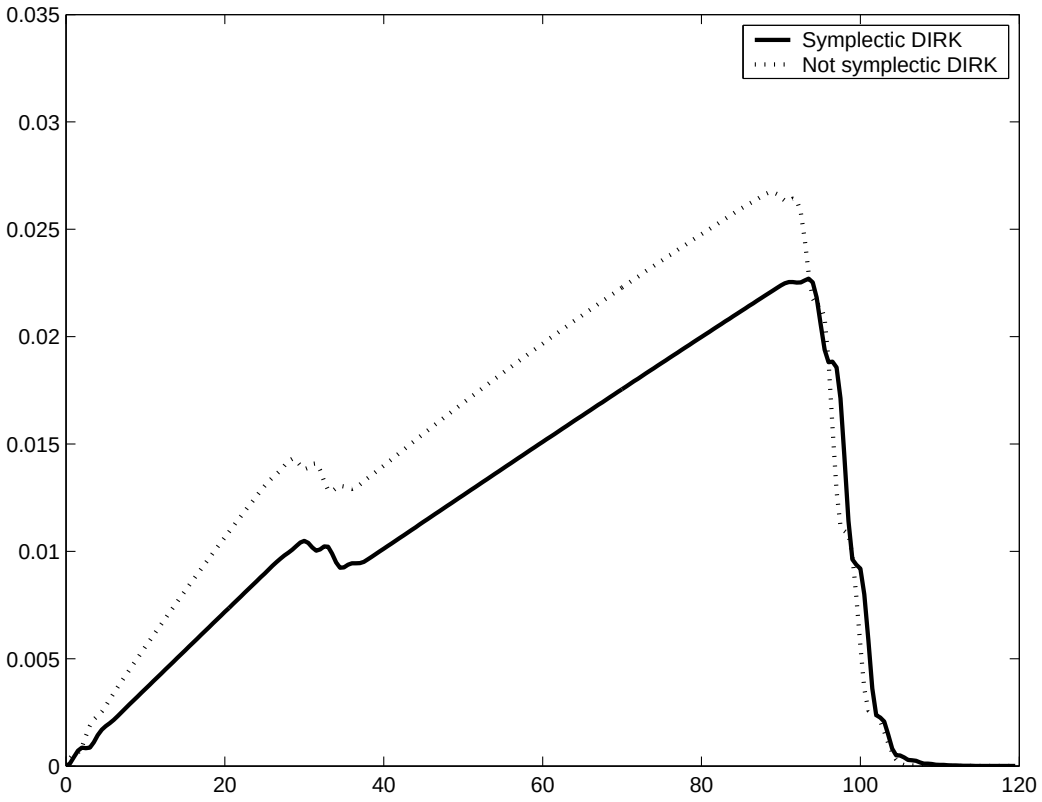


Solution of the problem test for $t = 0$, $t = 28$, $t = 50$ and $t = 92$.



Energy error versus time. $N = 1000,\ \Delta t = 0.5$

In previous Figure we show the absolute error of the energy for the two considered DIRK methods. The size of the energy error for the symplectic method can not be distinguished in Figure when the solution is not being absorbed. In fact, in the first part it is approximately 4×10^{-5} and between $t = 40$ and $t = 90$ it is 2.4×10^{-5} roughly. Since the remaining energy after the first absorption is a half of the initial energy, the absorption error does not transmit inside the computational window.



Relative errors in Euclidean norm versus time. $N = 1000$, $\Delta t = 0.5$

In previous figure we show the relative errors in Euclidean norm. It can be observed, as a consequence of the better behaviour of the first one inside the spatial interval, that the errors produced by the geometric method are lower than the errors of the non geometric one and the difference between both errors grows with the time.

12. Conclusions

- When geometric integration and absorbing boundary conditions are used simultaneously, the stability analysis must be revisited.

- We can not expect that the geometric time integrator is A-stable, even when its imaginary interval stability is the whole imaginary axis.

- Apart from being negative, the size of the real parts of the eigenvalues of the discretized differential operator must be in control to avoid possible instabilities.

- For a case study, the 1D wave equation discretized by means of finite differences, we are able to prove that the eigenvalues of the semidiscrete operator behave properly.