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Scientific Computing II

Exercise C

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Tutorial: Time Discretisation

In the following, we consider the differential equation

$$\frac{d^2}{dt^2}\vec{r}(t) = -\vec{r}(t).$$

a) Discuss possible solutions of this differential equation. How many initial conditions need to be given to make the solution unique? Do the solutions differ for the 1D-, 2D- or 3D-case?

Answer:

From the detailed vector notation

$$\frac{d^2}{dt^2}\begin{pmatrix} r_1(t) \\ \vdots \\ r_n(t) \end{pmatrix} = -\begin{pmatrix} r_1(t) \\ \vdots \\ r_n(t) \end{pmatrix}$$

one can see that the system of differential equations can be solved component-wise:

$$\frac{d^2}{dt^2}\vec{r_i}(t) = -\vec{r_i}(t).$$

Thus we can restrict ourselves to the 1D case. In this case, all linear combinations $A\sin(t) + B\cos(t)$ are solution to the ODE:

$$\frac{d^2}{dt^2}\left(A\sin(t) + B\cos(t)\right) = -A\sin(t) - B\cos(t).$$

Consequently, we need – per dimension – two initial conditions to fix the coefficients A and B. In general, these are the conditions for $\vec{r}(t_0)$ and $\frac{d}{dt}\vec{r}(t_0)$.

Note: In our equation, we are using Hooke's Law (with $k = 1$): the force is equivalent to the deflection.

b) Transform the 1D-equations in a system of 1st order differential equations and apply the numerical methods known to you: explicit and implicit Euler, trapezoidal rule (Crank-Nicholson), mid-point rule, Störmer-Verlet and its Leapfrog variant.

Answer:

According to the lecture we formulate the following system of two 1st order ODEs:

$$\begin{aligned} \frac{d}{dt} r(t) &= p(t) \\ \frac{d}{dt} p(t) &= -r(t) \end{aligned}$$

For the known time stepping methods we get the following schemas:

- Explicit Euler method

$$\begin{aligned} r^{(n+1)} &= r^{(n)} + \tau p^{(n)} \\ p^{(n+1)} &= p^{(n)} - \tau r^{(n)} \end{aligned}$$

- Implicit Euler method

$$\begin{aligned} r^{(n+1)} &= r^{(n)} + \tau p^{(n+1)} \\ p^{(n+1)} &= p^{(n)} - \tau r^{(n+1)} \end{aligned} \quad \Leftrightarrow \quad \begin{aligned} r^{(n+1)} - \tau p^{(n+1)} &= r^{(n)} \\ \tau r^{(n+1)} + p^{(n+1)} &= p^{(n)} \end{aligned}$$

  (Solve 2×2 systems of linear equations in every time step).

- Trapezoidal rule:

$$\begin{aligned} r^{(n+1)} &= r^{(n)} + \tau \left(p^{(n)} + p^{(n+1)} \right) /2 \\ p^{(n+1)} &= p^{(n)} - \tau \left(r^{(n)} + r^{(n+1)} \right) /2 \end{aligned} \quad \Leftrightarrow \quad \begin{aligned} r^{(n+1)} - \tfrac{\tau}{2} p^{(n+1)} &= r^{(n)} + \tfrac{\tau}{2} p^{(n)} \\ \tfrac{\tau}{2} r^{(n+1)} + p^{(n+1)} &= p^{(n)} - \tfrac{\tau}{2} r^{(n)} \end{aligned}$$

  (Solve 2×2 systems of linear equations in every time step).

- Mid-point rule

$$\begin{aligned} r^{(n+1)} &= r^{(n-1)} + \tau p^{(n)} \\ p^{(n+1)} &= p^{(n-1)} - \tau r^{(n)} \end{aligned}$$

- Störmer-Verlet:

$$\begin{aligned} p^{(n+1/2)} &= p^{(n)} - \frac{\tau}{2} r^{(n)} \\ r^{(n+1)} &= r^{(n)} + \tau p^{(n+1/2)} \\ p^{(n+1)} &= p^{(n)} - \frac{\tau}{2} r^{(n+1)} \end{aligned}$$

- Leapfrog-Version von Störmer-Verlet:

$$\begin{aligned} p^{(n+1/2)} &= p^{(n-1/2)} - \tau r^{(n)} \\ r^{(n+1)} &= r^{(n)} + \tau p^{(n+1/2)} \end{aligned}$$

c) For the single step methods, formulate one timestep as matrix-vector product. What can you conclude for the longterm behaviour of the methods? Calculate the eigen vectors or their product respectively for each method.

Hint: The product of the eigenvalues can also be calculated from the determinant.

Answer:

We consider the vectors $\mathbf{x}^{(n+1)} := \left(r^{(n+1)}, p^{(n+1)}\right)^T$ and $\mathbf{x}^{(n)} := \left(r^{(n)}, p^{(n)}\right)^T$ and represent the time steps as matrix-vector products and vector operations. Then we get the following expression for each time step:

$$\mathbf{x}^{(n+1)} = A\mathbf{x}^{(n)} \Rightarrow \mathbf{x}^{(n)} = A^n\mathbf{x}^{(0)}.$$

From the eigen vectors of A we can see the behaviour of the solutions. E.g. if all eigenvalues are < 1, then $r^{(n)}$ and $p^{(n)}$ will decrease from time step to time step – or increase, if all eigenvalues are > 1. In the 1D-case the analytical solutions are uniform sine and cosine oscillations. Only of eigenvalues of magnitude 1 we can expect the numerical solution to give the uniform oscillations, too, i.e. that position (amplitude) and impulse will repeat ever and ever.

Hint: The length of a vector $(r, p)^T$ is just $\sqrt{r^2 + p^2}$ – note that r^2 corresponds to the potential energy (in the case of Hooke's Law) and p^2 to the kinetic energy ("velocity squared"). If the length of the vectors is conserved (i.e. in the case when all eigen vectors are of magitude 1), this expresses the conservation of energy!

- Explicit Euler method

$$\begin{pmatrix} r^{(n+1)} \\ p^{(n+1)} \end{pmatrix} = \begin{pmatrix} 1 & \tau \\ -\tau & 1 \end{pmatrix} \begin{pmatrix} r^{(n)} \\ p^{(n)} \end{pmatrix}$$

  We get the eigenvalues of the time step matrix as the zero points of the characteristic polynomial $(1 - \lambda)^2 + \tau^2$:

$$(1 - \lambda)^2 + \tau^2 = 0 \Leftrightarrow (1 - \lambda)^2 = -\tau^2 \Leftrightarrow 1 - \lambda = \pm i\tau \Leftrightarrow \lambda = 1 \mp i\tau$$

  Thus, the magnitude of the eigenvalues is > 1 and the product of the eigenvalues is > 1.

- Implicit Euler method

$$\begin{pmatrix} 1 & -\tau \\ \tau & 1 \end{pmatrix} \begin{pmatrix} r^{(n+1)} \\ p^{(n+1)} \end{pmatrix} = \begin{pmatrix} r^{(n)} \\ p^{(n)} \end{pmatrix} \quad \Leftrightarrow \quad \begin{pmatrix} r^{(n+1)} \\ p^{(n+1)} \end{pmatrix} = \begin{pmatrix} 1 & -\tau \\ \tau & 1 \end{pmatrix}^{-1} \begin{pmatrix} r^{(n)} \\ p^{(n)} \end{pmatrix}$$

  The time step matrix is the transposed and inverted matrix of the explicit Euler method. Transposition doesn't change the eigenvalues, Inversion also inverts the eigenvalues. Thus we get

$$\lambda = (1 \mp i\tau)^{-1}$$

  These are of magnitude < 1, just as the product of both eigenvalues.

– Trapezoidal rule:

$$\begin{pmatrix} 1 & -\frac{\tau}{2} \\ \frac{\tau}{2} & 1 \end{pmatrix} \begin{pmatrix} r^{(n+1)} \\ p^{(n+1)} \end{pmatrix} = \begin{pmatrix} 1 & \frac{\tau}{2} \\ -\frac{\tau}{2} & 1 \end{pmatrix} \begin{pmatrix} r^{(n)} \\ p^{(n)} \end{pmatrix}$$

is equivalent to:

$$\begin{pmatrix} r^{(n+1)} \\ p^{(n+1)} \end{pmatrix} = \begin{pmatrix} 1 & -\frac{\tau}{2} \\ \frac{\tau}{2} & 1 \end{pmatrix}^{-1} \begin{pmatrix} 1 & \frac{\tau}{2} \\ -\frac{\tau}{2} & 1 \end{pmatrix} \begin{pmatrix} r^{(n)} \\ p^{(n)} \end{pmatrix}$$

The calculation of of the eigenvalues is tidious, but we can at least determine the determinant, which gives us the product of the eigenvalues. The determinant for both matrices is given by $1^2 + \left(\frac{\tau}{2}\right)^2$ and $\left(1^2 + \left(\frac{\tau}{2}\right)^2\right)^{-1}$. The determinant of the time step matrix is equal to the product of both determinants, i.e. 1.

Hint: With help of Matlab both eigenvalues can be calculated resulting in the complex values $\frac{1}{4+\tau^2}\left(2 \pm i\tau\right)^2$. Both are of magnitude 1. Thus, in every time step the length of the vector $(r, p)^T$ is conserved and consequently the total energy of the system is kept constant.

– Störmer-Verlet: This case is comparably complicated – therefor we restrict ourselves to the (essentially equivalent) Leapfrog variant of the scheme.

– Leapfrog variant of Störmer-Verlet: We set $q^{(n+1)} := p^{(n+1/2)}$, so we get the following method:

$$\begin{aligned} q^{(n+1)} &= q^{(n)} - \tau r^{(n)} \\ r^{(n+1)} &= r^{(n)} + \tau q^{(n+1)} = r^{(n)} + \tau q^{(n)} - \tau^2 r^{(n)} \end{aligned}$$

In matrix-vector notation this is equivalent to

$$\begin{pmatrix} r^{(n+1)} \\ q^{(n+1)} \end{pmatrix} = \begin{pmatrix} 1-\tau^2 & \tau \\ -\tau & 1 \end{pmatrix} \begin{pmatrix} r^{(n)} \\ q^{(n)} \end{pmatrix}$$

The determinant, i.e. the product of both eigenvalues, reads in this case $(1-\tau^2)\cdot 1 - (-\tau)\tau = 1-\tau^2+\tau^2 = 1$. With Matlab or with the help of characteristic polynomials both eigenvalues can be computed – these are equal to $1 - \frac{\tau^2}{2} \pm \frac{\tau}{2}\sqrt{-4+\tau^2} \neq 1$. Thus, this method does not conserve energy exactly. In the (r, p)-diagramme we don't obtain a circle, but a slightly skewed ellipsoid.

Since the result is nevertheless a periodic movement, the fluctuations in the energy remain limited and the method is also suitable for long-running simulations. In contrast to the trapezoidal rule this is an explicit method and therefore also suitable with respect to computing time.