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Computational Physics: Problem Set 3

Discussion: 01/03/2023

1 Analysis of time integrators – Kepler problem

This is a continuation of problem 2 from week 3.

a) The Kepler problem is nonlinear. Its analytic solutions (planetary orbits) are ellipses, but in general the function $\mathbf{r}(t)$ is a bit complicated, so we only use the circular orbit as a test case. Find the momentum and thereby the initial condition that corresponds to a circular orbit of the form $\mathbf{r}_{\text{ref}}(t) = [\cos(\Omega t); \sin(\Omega t)]^T$. Also find the analytical value for Ω.

b) Run the program with this initial condition up to various end times and with various time step sizes that seem plausible. Plot the error $E(t) = ||\mathbf{r}(t) - \tilde{\mathbf{r}}(t)||$ on a semilog plot versus t and on a doublelog plot versus h. Is the numerical solution stable? If so, what is the convergence order?

c) Repeat the same with the error $E'(t) = |\mathcal{E}(t) - \tilde{\mathcal{E}}(t)|$ of the total energy $\mathcal{E}(t) = \frac{1}{2}|\mathbf{p}|^2 - |\mathbf{r}|^{-1}$.

d) Replace Euler's method with the leapfrog integrator and check for stability and convergence order.

e) The function *ode45* in matlab implements a 4th order Runge-Kutta. Test convergence and consistency with this time-evolution (if you use octave instead of matlab, you can use the implementation *rk4* that is uploaded on itslearning; comments and example inside the file *rk4.m*).

2 A simple matrix exponential integrator

a) In the lecture, the matrix exponential was represented as a Taylor series:

$$\exp(M) = \mathbb{I} + \sum_{n=1}^{\infty} \frac{M^n}{n!}.$$

Show that this series really is the same as our original definition

$$\exp(M) = R^{-1} \begin{pmatrix} \exp(\lambda_1) & 0 & \cdots & 0 \\ 0 & \exp(\lambda_2) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \exp(\lambda_n) \end{pmatrix} R,$$

where $M = R^{-1}\Lambda R$ and Λ is diagonal with the eigenvalues $\Lambda_{ii} = \lambda_i$ as entries.

b) Show that

$$\exp(M) = [\exp(M/2^n)]^{2^n}. \tag{1}$$

Using the Cauchy-Schwarz inequality $||AB|| \leq ||A|| \cdot ||B||$, and the triangle inequality $||A + B|| \leq ||A|| + ||B||$, give an estimate for the error of $\exp(M)$ in terms of the norm $||M||$ of M, assuming the Taylor expansion is truncated after N terms (at this point it does not matter how exactly the norm of a matrix is defined, only that it can be defined and that it is correlated to how large the matrix components are). Using this, motivate how Equation (1) is useful for time integration with a truncated Taylor series.

c) Implement the truncated exponential time-evolution

$$\tilde{\mathcal{U}}(\tau) = \mathbb{I} + A\tau\left(\mathbb{I} + \frac{1}{2}A\tau\left(\mathbb{I} + \frac{1}{3}A\tau\left(\mathbb{I} + \frac{1}{4}A\tau\right)\right)\right). \tag{2}$$

Approximate the total time evolution operator

$$\mathcal{U}(t) = \exp(At) \approx [\tilde{\mathcal{U}}(\tau)]^{2^n}, \tag{3}$$

where $\tau = t/2^n$. Using the maximum norm $||A|| = \max_{i,j} |A_{ij}|$ (i.e. the absolute value of the largest matrix element) and the identity $||A\tau|| = |\tau| \cdot ||A||$, implement a rule that finds n (and thereby τ) such that the error of $\tilde{\mathcal{U}}(\tau)$ is on the order of 10^{-4}.

Note 1: Equation (2) is written in Horner's form, which is a favorable way to evaluate polynomials.

Note 2: Equation (3) turns the method into a multi-step method, so it's not unconditionally stable like a single-step matrix exponential method.

Note 3: The right hand side of Equation (3) is best evaluated by repeatedly squaring matrices.

d) Apply this time-evolution to the harmonic oscillator problem, check the stability in the four regimes and study the convergence with respect to τ (controlled by manually changing n).

e) How can you recover Euler's method by modifying Equation (2)?

f) Extra-problem: Try to find the stability contour of the time-evolution with a Taylor series truncated after the fourth power. Can you recognize it from the lecture slides of week 4?

Students are encouraged to solve these problems in groups. They should be able to informally present their solution in the problem class on 01/03/2023 at the white board (no PowerPoint slides to be prepared).