Concepts and Algorithms of Scientific and Visual Computing

–Stiff Differential Equations–

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Stiff Cauchy Problems

According to the Picard-Lindelöf theorem, the Cauchy problem

$$\mathrm{d}_x(y(x)) = f(x, y(x))$$

with initial value $y_0(x_0) = y_0$ and Lipschitz continuity of f, i.e.

$$|f(x, y_1) - f(x, y_2)| \leq N\,|y_1 - y_2|$$

for all (x, y_1) and (x, y_2) in a neighborhood G of (x_0, y_0) has a unique local solution.

If the constant N takes high values, although the solution y runs smoothly, explicit integration methods have to take very small step sizes in order to approximate y appropriately.

Such a scenario is called a stiff Cauchy problem.

Stiff Cauchy Problems

According to the classical definition of [Curtiss 1952] the term “stiff” means:
“...where certain implicit methods perform better than explicit ones”.

Stiffness as such is not a characteristic of the differential equations nor is it a property of the numerical methods applied in order to solve them. It is just an issue of efficiency because we want a numerical integration method to sample the important time scales as quickly as possible.

Dahlquist Equation

According to [Dahlquist 1963] we consider the differential equation

$$\mathrm{d}_t(y(x)) = f(y(x)), \quad y(0) = y_0$$

with $f(y(x)) = -\lambda y(x)$ and $\lambda \in \mathbb{R}^{>0}$, and its analytical solution

$$y(x) = \exp(-x\lambda)y_0.$$

We apply the explicit and the implicit Euler method so that we obtain the scheme

$$y(x + \Delta x) = (1 - \Delta x\lambda)y(x)$$

for the explicit case and

$$y(x + \Delta x) = \frac{1}{1 + \Delta x\lambda}y(t)$$

for the implicit case.

Dahlquist Equation

The absolute value of the exact solution is decreasing monotonically. Hence

$$|1 - \Delta x \lambda| \leq 1$$

is a necessary criterion for the convergence of the explicit Euler method. The analogous criterion for the implicit method is given by

$$\left|\frac{1}{1 + \Delta x \lambda}\right| \leq 1.$$

The first condition is only fulfilled for small step sizes Δx, whereas the second one is fulfilled for all $\Delta x > 0$.

Semi-analytical Exponential Integrator

We consider the symplectic construction of a so-called semi-analytical exponential integrator for second-order differential equations of motion.

$$\ddot{x} + Ax = g(x)$$

$$\downarrow$$

$$\begin{aligned}
x_{n+1} \leftarrow \quad & 2\cos\left(\Delta t\sqrt{A}\right)x_n - x_{n-1} + \int\int_{n\Delta t}^{(n+1)\Delta t} g\left(x(t)\right)\mathrm{d}t^2 \\
\approx \quad & 2\cos\left(\Delta t\sqrt{A}\right)x_n - x_{n-1} + \Delta t^2\,\psi\left(\Delta t\sqrt{A}\right)g\left(\phi\left(\Delta t\sqrt{A}\right)x_n\right)
\end{aligned}$$

$$\downarrow$$

$$(x_{n-1}, x_n) \mapsto (x_n, x_{n+1}) \quad \cong \quad \Phi_{\Delta t} : (x_n, v_n) \mapsto (x_{n+1}, v_{n+1})$$

$$\downarrow$$

$$\Phi_{\Delta t} \text{ symplectic, iff } \psi(\cdot) = \mathrm{sinc}(\cdot)\phi(\cdot)$$

$$(\psi, \phi) = (\mathrm{sinc}^2, \mathrm{sinc}) \ \checkmark$$

Semi-analytical Exponential Integrator

Finally we obtain the so-called exponential integrator of Gautschi type, see [Gautschi 1961].

$$\ddot{\mathbf{x}} + \mathbf{A}\mathbf{x} = \mathbf{g}(\mathbf{x})$$

$$\downarrow$$

$$\mathbf{x}_{n+1} = 2\cos\left(\Delta t\sqrt{\mathbf{A}}\right)\mathbf{x}_n - \mathbf{x}_{n-1} + \Delta t^2 \operatorname{sinc}^2\left(\Delta t\sqrt{\mathbf{A}}\right)\mathbf{g}\left(\operatorname{sinc}\left(\Delta t\sqrt{\mathbf{A}}\right)\mathbf{x}_n\right)$$

This is a composition of a partial analytical solution and a low-pass filtered nonlinearity leading to an explicit, symplectic, and time-reversible scheme of second order.

Splitting / Variational Implicit-explicit Integrator

Splitting of the potential into a fast (i.e. highly oscillatory) and a slow component is often possible. Based on this observation the midpoint quadrature rule is applied to a fast quadratic potential and the trapezoidal quadrature rule to the remaining slow potential term resulting in Λ.

The application of the discrete Euler-Lagrange formalism leads to the so-called variational implicit-explicit integrator which takes the form

$$\mathbf{x}_{n+1} = 2\mathbf{x}_n - \mathbf{x}_{n-1} - \Delta t^2 \left(\mathbf{1} + \Delta t^2/4\,\mathbf{K}\right)^{-1} \left(\mathbf{K}\,\mathbf{x}_n + \mathbf{\Lambda}\left(\mathbf{x}_n\right)\right).$$

Since it is based on a discrete variational principle, it is naturally symplectic. Moreover, its symmetry can be followed easily by calculation.