Remark on Dissipative ODEs

A dissipative system of ODEs has the form

$$\frac{du}{dt} = f - au$$

with $a > 0$. More generally $u \in \mathbb{C}^n$ and

$$\frac{du}{dt} = f - Au$$

→ The dissipative term au (or Au) may render the ODE stiff and preclude the use of explicit Runge-Kutta.

<u>example</u> : The Navier-Stokes equation:

$$\frac{\partial u_a}{\partial t} + u_b \partial_b u_a = -\partial_a p + \nu \nabla^2 u_a + f_a$$

$$\partial_a u_a = 0 \leftarrow \text{incompressibility condition.}$$

In Fourier space, the dissipative term $\nu \nabla^2 u_a$ gives $-\nu k^2 \hat{u}_a(k)$ with k^2 ranging over 6 or more orders of magnitude! $\leftrightarrow$ leads to stiffness.

→ The <u>integrating factor method</u> : substitute $v = u \exp(at)$.

Note that

$$\frac{dv}{dt} = \frac{d}{dt}\left(ue^{at}\right) = \frac{du}{dt}e^{at} + uae^{at} =$$
$$= (f-au)e^{at} + aue^{at} = fe^{at}.$$

Do an explicit Runge-Kutta step on the v equation:

$$v_{n+1} = v_n + \Delta t \, R[f_n e^{at_n}]$$

and note that $R[\,]$ is <u>linear</u>

$$R[\lambda f] = \lambda R[f] \quad , \forall \lambda \in \mathbb{C}$$

and
$$v_n = u_n \exp(at_n)$$
$$t_n = n\Delta t.$$

It follows that

$$\begin{aligned} u_{n+1} &= v_{n+1} e^{-at_{n+1}} \\ &= \exp(-at_{n+1}) \left[v_n + \Delta t \, R[f_n e^{at_n}] \right] \\ &= \exp(-at_{n+1}) \left[u_n \exp(at_n) + \exp(at_n) \Delta t \, R[f_n] \right] \\ &= \exp(-a\Delta t) \left[u_n + \Delta t \, R[f_n] \right]. \end{aligned}$$

Consequently we have the scheme:

$$\boxed{\begin{aligned} u^* &= u_n + \Delta t \, R[f_n] \\ u_{n+1} &= \exp(-a\Delta t)\, u^* \end{aligned}}$$

For a system of ODEs, the scheme generalizes to

$$\boxed{\begin{aligned} u^* &= u_n + \Delta t \, R[f_n] \\ u_{n+1} &= \exp(-\Delta t A)\, u^* \end{aligned}}$$

using the "matrix exponential"

Solution of nonlinear equations for Implicit Runge-Kutta

Implicit Runge-Kutta methods require solving the equation

$$K_a = \Delta t f\left(t + c_a \Delta t,\, y + \sum_{b=1}^{s} A_{ab} k_b\right),$$

$$\forall a \in \{1, 2, \dots, s\}.$$

In more general form:

$$\boxed{x = \varphi(x)} \quad \text{with} \quad x \in \mathbb{R}^n$$

1 Fixed-point iteration

- Start from a guess x_0 and iterate

$$\boxed{x_{n+1} = \varphi(x_n).}$$

- A solution exists if there is a region $I \subseteq \mathbb{R}^n$ such that
  a) φ continuous at I
  b) $\forall x \in I : \varphi(x) \in I$

- The fixed-point iteration converges iff

$$\exists\, \ell \in [0,1) : \forall x_1, x_2 \in I : \|\varphi(x_1) - \varphi(x_2)\|_\infty \leqslant \ell \|x_1 - x_2\|_\infty$$

- <u>Application to Implicit RK</u>

Consider the ODE

$$\frac{dy}{dt} = f(t,y)$$

and assume that

$$\exists\, L \in [0,+\infty) : \forall y_1, y_2 \in \mathbb{R}^n : \forall t \in [0,T] : \|f(t,y_1) - f(t,y_2)\|_\infty \leqslant L \|y_1 - y_2\|_\infty$$

- Solving the implicit RK method with fixed-point iteration requires

$$\boxed{|\Delta t| \leqslant \frac{1}{L\|A\|_\infty}} \leftarrow \text{Impractical.}$$

<u>Proof</u>

Let $\varphi_a(k) = \Delta t\, f\left(t + c_a \Delta t,\, y + \sum_{b=1}^{s} A_{ab} k_b\right)$

and assume that t, y are fixed.

For any $K, \bar{K} \in I \subseteq \mathbb{R}^s$ define

$$Y_a = y + \sum_{b=1}^{s} A_{ab} k_b$$

$$\bar{Y}_a = y + \sum_{b=1}^{s} A_{ab} \bar{k}_b$$

Then

$$\|\varphi(k) - \varphi(\bar{k})\|_\infty = \max_{a=1}^{s} \| [f(t + c_a \Delta t, Y_a) - f(t + c_a \Delta t, \bar{Y}_a)] \Delta t \|_\infty$$

$$\leqslant \max_{a=1}^{s} \| \Delta t \, L \, (Y_a - \bar{Y}_a) \|_\infty =$$

$$= \max_{a=1}^{s} \| \Delta t \, L \sum_{b=1}^{s} A_{ab} (k_b - \bar{k}_b) \|$$

$$\leqslant |\Delta t| \, L \sum_{b=1}^{s} \max_{a=1}^{s} |A_{ab}| \, \|k_b - \bar{k}_b\|$$

$$\leqslant |\Delta t| \, L \, \|A\|_\infty \max_{a=1}^{s} \|k_b - \bar{k}_b\|$$

$$\leqslant |\Delta t| \, L \, \|A\|_\infty \, \|k - \bar{k}\|_\infty$$

Thus the ~~contract~~ fixed-point iteration will solve $k = \varphi(k)$ when

$$|\Delta t| \, L \, \|A_\infty\| < 1 \quad !! \qquad \square$$

② Newton Iteration

- Less efficient but circumvents the need for small Δt required by fixedpoint iteration.

- One nonlinear equation $\longleftrightarrow$ $f(x)=0$

Given an initial guess $x_0 \in [a,b]$, the iteration

$$\boxed{x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}}$$

converges to the solution of $f(x)=0$ if the following conditions are satisfied:

a) $f(a)f(b) < 0$

b) $f \in C^2[a,b]$

c) $\forall x \in [a,b] : f'(x) \neq 0$

d) $[\forall x \in [a,b] : f''(x) \geq 0] \vee [\forall x \in [a,b] : f''(x) \leq 0]$

e) For $c \in \{a,b\}$ such that $|f'(c)| \leq |f'(a)|$ and $|f'(c)| \leq |f'(a)|$ we have

$$\left| \frac{f(c)}{f'(c)} \right| \leq b-a.$$

▶ Nonlinear system of equations ⟷ $f_a(\vec{x}) = 0$

Calculate the Jacobian matrix:

$$f'(x) = [\partial f_a(x) / \partial x_b]$$

and do the iteration

$$\boxed{f'(x_n)[x_{n+1} - x_n] = -f(x_n)}$$

Requires an LU or QR decomposition per iteration. The simplified Newton iteration is

$$\boxed{f'(x_0)[x_{n+1} - x_n] = -f(x_n)}$$

Requires only one decomposition, but may require more iterations to converge.

▶ Application to the equation ⟷ $x_a = \varphi_a(x)$

For $f_a(x) = x_a - \varphi_a(x) \Rightarrow f'_{ab}(x) = \delta_{ab} - \varphi'_{ab}(x)$

thus the Newton iteration is

$$[I - \varphi'(x_n)][x_{n+1} - x_n] = -[x_n - \varphi(x_n)]$$

The simplified Newton iteration is

$$[I - \varphi'(x_0)][x_{n+1} - x_n] = -[x_n - \varphi(x_n)]$$

- **Application to implicit Runge-Kutta**

Specialize from previous case by substituting

$$\varphi_a(k) = \Delta t\, f\Big(t + c_a \Delta t,\ y + \sum_{b=1}^{s} A_{ab} k_b\Big)$$

$$\varphi'_{ab}(k) = \frac{\partial \varphi_a(k)}{\partial k_b}$$

$$\cancel{= \Delta t}$$

$$= \Delta t \sum_{\gamma=1}^{N} \frac{\partial f}{\partial y_\gamma}$$