Numerical Methods for Fractional Differential Equations

Review of:
I. Podlubny "Matrix approach to discrete fractional calculus"
I. Podlubny et al. "Matrix approach to discrete fractional calculus II: Partial fractional differential equations"

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NNF Summer Reading Group
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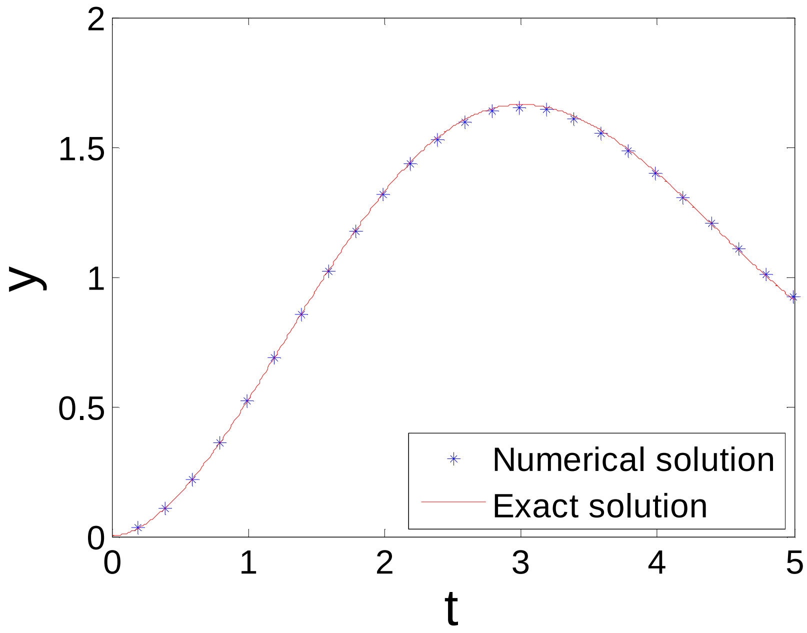
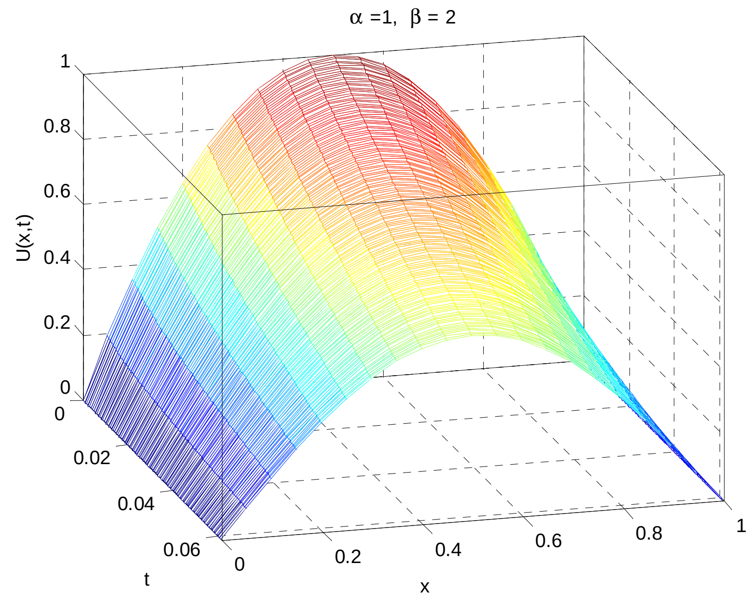
Overview

- I. Podlubny, Matrix approach to discrete fractional calculus, *Fractional Calculus and Applied Analysis* **3** 359–386 (2000)
  - Properties and manipulations with triangular strip matrices
  - Integer order differentiation/integration with matrices
  - Fractional order differentiation
  - Fractional order integration
  - Numerical examples



- I. Podlubny et al., Matrix approach to discrete fractional calculus II: Partial fractional differential equations” *Journal of Computational Physics* **228** 3137–3153 (2009)
  - Numerical methods for PDEs
  - Riesz derivatives
  - Numerical examples of fractional diffusion



Quick reference to fractional operators

- Caputo derivative

$$ {}_a^C D_x^{\mu} \phi(x) = \frac{1}{\Gamma(m-\mu)} \int_a^x \frac{\phi^{(m)}(\xi) d\xi}{(x-\xi)^{\mu-m+1}} \quad (m-1 < \mu \leqslant m) $$

- Riemann-Liouville derivative

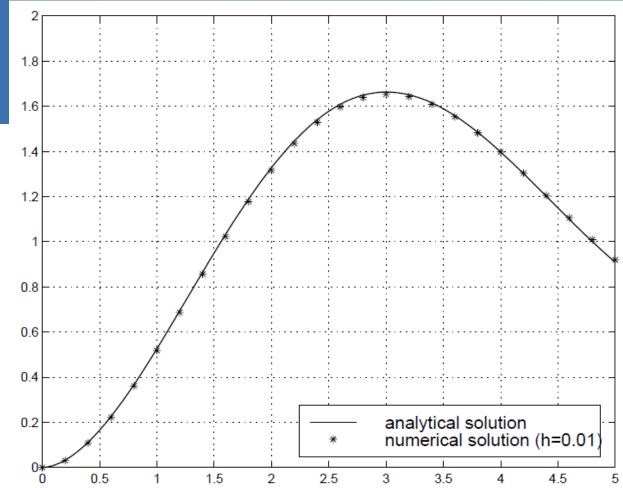
$$ {}_a D_x^{\mu} \phi(x) = \frac{1}{\Gamma(m-\mu)} \left(\frac{d}{dx}\right)^m \int_a^x \frac{\phi(\xi) d\xi}{(x-\xi)^{\mu-m+1}} \quad (m-1 < \mu \leqslant m), $$

$$ {}_x D_b^{\mu} \phi(x) = \frac{1}{\Gamma(m-\mu)} \left(-\frac{d}{dx}\right)^m \int_x^b \frac{\phi(\xi) d\xi}{(\xi-x)^{\mu-m+1}} \quad (m-1 < \mu \leqslant m). $$

- Riesz derivative

$$ \frac{d^{\beta} \phi(x)}{d|x|^{\beta}} = D_R^{\beta} \phi(x) = \frac{1}{2} \left({}_a D_x^{\beta} \phi(x) + {}_x D_b^{\beta} \phi(x) \right) $$

Numerical example for ODE

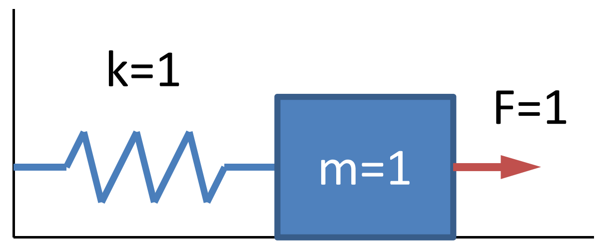


- Example 2 from Part I:

$$y^{(1.8)}(t)+y(t)=1$$
$$y(0)=0$$
$$y^{(1)}(0)=0$$

- Similar ODE:

$$y^{(2)}(t)+y(t)=1$$
$$y(0)=0$$
$$y^{(1)}(0)=0$$

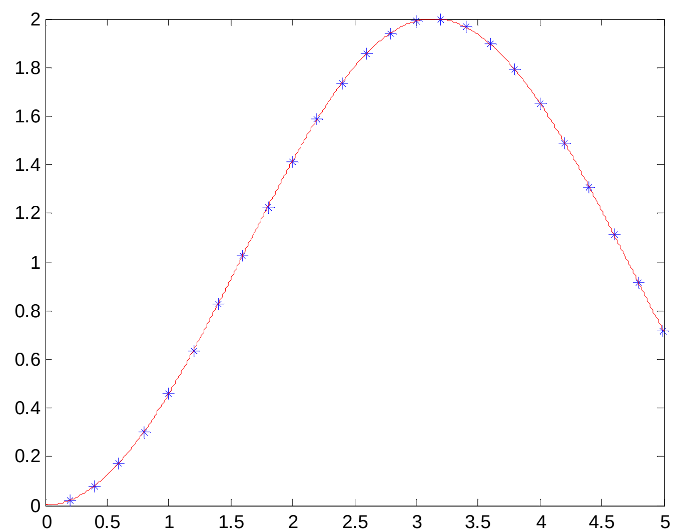


- Backward difference approximation of differential operator

$$y^{(2)}(t_k)\approx\frac{\nabla^2 y}{h^2}=\frac{y_k-2y_{k-1}+y_{k-2}}{h^2}$$

- Recursive relation:

$$y_k=\left(1-\frac{1}{h^2}\right)^{-1}\left[1+\frac{2}{h^2}y_{k-1}-\frac{1}{h^2}y_{k-2}\right]$$
$$y_0=y(0)$$
$$y_1=y(0)+y^{(1)}(0)h$$

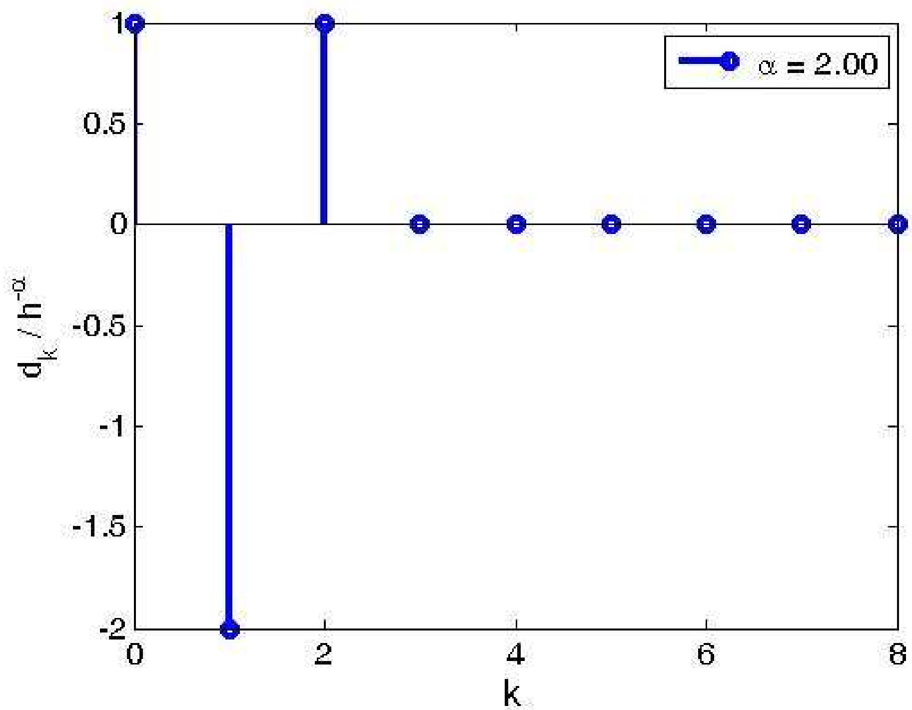


Generalize this method for FDE

- Left-sided fractional operator:

$$D^{\alpha} y(t_k) \approx \frac{\nabla^{\alpha} y}{h^{\alpha}} = \sum_{j=0}^{k} \underbrace{h^{-\alpha} (-1)^{j} \binom{\alpha}{j}}_{d_j} y_{k-j}$$

$$D^{\alpha} y(t_k) \approx d * y$$



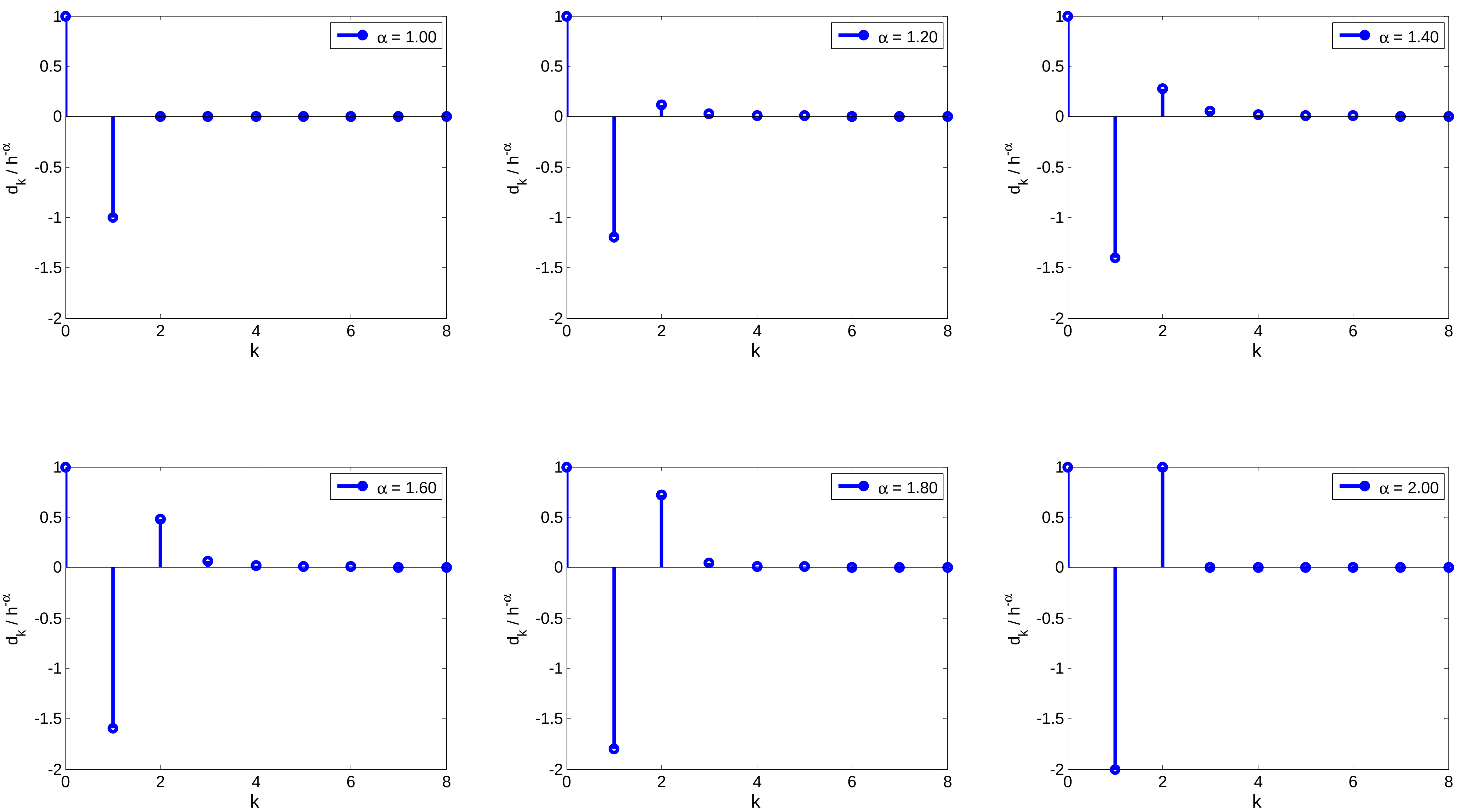
- Time series for calculating fractional derivative is infinite-duration!
- Generalized form for differential equation:

$$\sum_{i=1}^{m} p_i(t) D^{\alpha_i} y(t) = f(t)$$

- Recursion equation:

$$y_k = \left[\sum_{i=1}^{m} \frac{p_i(t)}{h^{\alpha_i}} \right]^{-1} \left[f_k - \sum_{i=1}^{m} p_i(t) \sum_{j=1}^{k} \frac{(-1)^{j}}{h^{\alpha}} \binom{\alpha}{j} y_{k-j} \right]$$

Impulse response of fractional derivative operators



Demo #1

"…unwieldy recurrence relationships…"

Numerical manipulations and initial conditions

- Calculation of binomial coefficients

$$\binom{\alpha}{k} = \frac{\Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(\alpha-k+1)} \qquad \binom{\alpha}{k} = \frac{\alpha-k+1}{k}\binom{\alpha}{k-1}$$

Numerically efficient

  - In MATLAB use : bincoef = cumprod([1, ((alpha+1)./(1:k)-1)])
- Initial conditions
  - Substitute functions to make initial conditions zero
  - Integer-order ICs (for Caputo derivatives)

$$y^{(\alpha)}(t) + y(t) = 1, \quad y(0) = c_0, \quad y'(0) = c_1 \quad \xrightarrow{y(t) = c_0 + c_1 t + z(t)} \quad z^{(\alpha)}(t) + z(t) = 1 - c_0 - c_1 t, \quad z(0) = 0, \quad z'(0) = 0.$$

  - Fractional order ICs

$$y^{(\alpha)}(t) + y(t) = 1, \quad y^{(\alpha-1)}(0) = c_0, \quad y^{(\alpha-2)}(0) = c_1 \quad \xrightarrow{y(t) = c_0 t^{\alpha-1} + c_1 t^{\alpha-2} + z(t)} \quad z^{(\alpha)}(t) + z(t) = 1 - c_0 t^{\alpha-1} - c_1 t^{\alpha-2}, \quad z(0) = 0, \quad z'(0) = 0.$$

Rheological example – fractional springpot (Nutting model)

Material model:

- Shear relaxation modulus (Friedrich et al. 1999):

$$G(t) = \frac{E}{\Gamma(1-\beta)}\left(\frac{t}{\lambda}\right)^{-\beta}$$

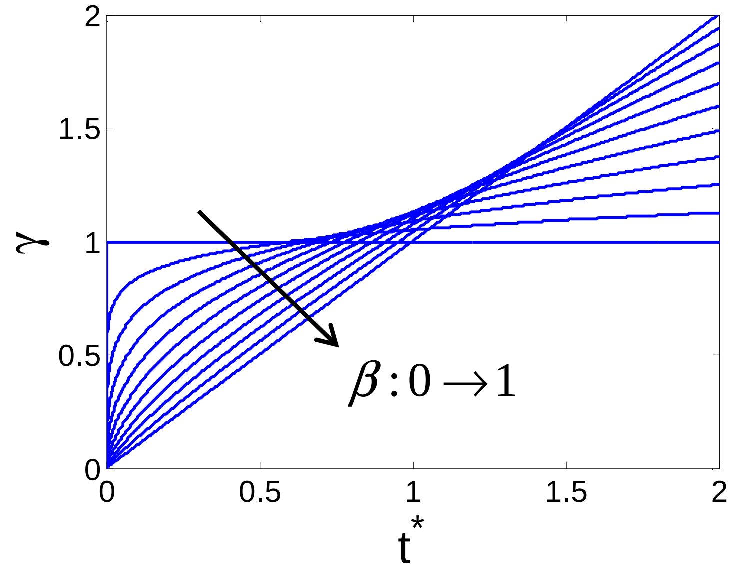
- Non-dimensional constitutive relation:

$$\tau^* = \tau / E, t^* = t / \lambda$$

$$\tau^* = \frac{d^\beta \gamma}{d\left(t^*\right)^\beta}$$

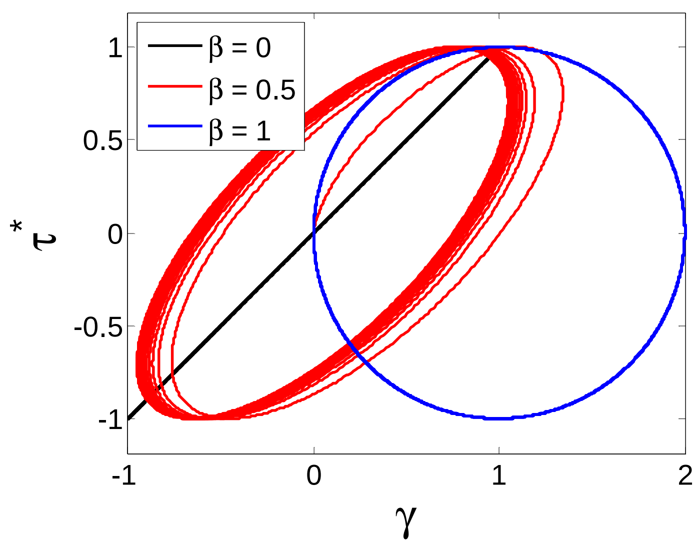
Creep:

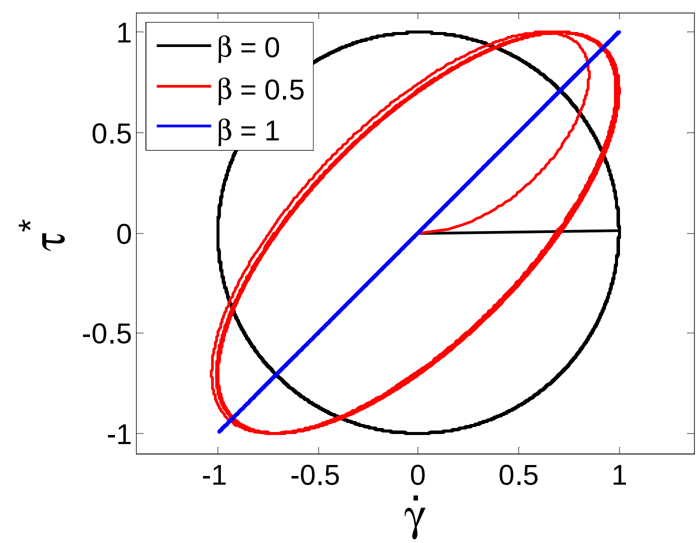
$$\tau^* = \begin{cases} 0 & t^* \le 0 \\ 1 & t^* > 0 \end{cases}$$



Oscillatory shear flow:

$$\tau^* = \begin{cases} 0 & t^* \le 0 \\ \sin\left(t^*\right) & t^* > 0 \end{cases}$$





- Note that the Newtonian fluid $(\beta = 1)$ the Lissajous curve is shifted in strain due to the initial condition

Matrix approach

- The generalized form of FDE:

$$\sum_{k=1}^{m} p_k(t) D^{\alpha_k} y(t) = f(t) \qquad 0 \le \alpha_1 < \alpha_2 < \ldots < \alpha_m, \qquad n-1 < \alpha_m < n$$

- Converted into matrix form:

$$\sum_{k=1}^{m} P_N^{(k)} B_N^{\alpha_k} Y_N = F_N$$

$$Y_N = \big(y(t_0), y(t_1), \ldots, y(t_N)\big)^T, \qquad F_N = \big(f(t_0), f(t_1), \ldots, f(t_N)\big)^T$$

$$P_N^{(k)} = \operatorname{diag}\big(p_k(t_0), p_k(t_1), \ldots, p_k(t_N)\big)$$

$$B_N^{\alpha} = \frac{1}{h^{\alpha}} \begin{bmatrix} \omega_0^{(\alpha)} & 0 & 0 & 0 & \cdots & 0 \\ \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & 0 & 0 & \cdots & 0 \\ \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \cdots & \cdots \\ \omega_{N-1}^{(\alpha)} & \ddots & \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & 0 \\ \omega_N^{(\alpha)} & \omega_{N-1}^{(\alpha)} & \ddots & \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} \end{bmatrix} \qquad \omega_j^{(\alpha)} = (-1)^j \binom{\alpha}{j}$$

Same equations with the recursive method!

Other derivatives

- Right-sided fractional derivative

$$F_N^{\alpha} = \frac{1}{h^{\alpha}} \begin{bmatrix} \omega_0^{(\alpha)} & \omega_1^{(\alpha)} & \ddots & \ddots & \omega_{N-1}^{(\alpha)} & \omega_N^{(\alpha)} \\ 0 & \omega_0^{(\alpha)} & \omega_1^{(\alpha)} & \ddots & \ddots & \omega_{N-1}^{(\alpha)} \\ 0 & 0 & \omega_0^{(\alpha)} & \omega_1^{(\alpha)} & \ddots & \ddots \\ \cdots & \cdots & \cdots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & 0 & \omega_0^{(\alpha)} & \omega_1^{(\alpha)} \\ 0 & 0 & \cdots & 0 & 0 & \omega_0^{(\alpha)} \end{bmatrix}$$

$$\left(B_N^{\alpha}\right)^T = F_N^{\alpha}, \qquad \left(F_N^{\alpha}\right)^T = B_N^{\alpha}$$

- Sequential fractional derivatives

$${}_a\mathcal{D}_t^{\vec{\alpha}} f(t) = {}_aD_t^{\alpha_1}\, {}_aD_t^{\alpha_2} \,\ldots\, {}_aD_t^{\alpha_n} f(t),$$

$$\vec{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_n),$$

$$\mathcal{B}_N^{\vec{\alpha}} = B_N^{\alpha_1} B_N^{\alpha_2} \ldots B_N^{\alpha_n} = \prod_{k=1}^{n} B_N^{\alpha_k}$$

Fractional integration

- Left-sided fractional integral

$$ {}_aD_t^{-\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-\tau)^{\alpha-1} f(\tau) d\tau $$

$$ I_N^\alpha = \left(B_N^\alpha\right)^{-1} $$

$$ \omega_j^{(\alpha)} = (-1)^j \binom{\alpha}{j} $$

$$ I_N^\alpha = h^\alpha \begin{bmatrix} \omega_0^{(-\alpha)} & 0 & 0 & 0 & \cdots & 0 \\ \omega_1^{(-\alpha)} & \omega_0^{(-\alpha)} & 0 & 0 & \cdots & 0 \\ \omega_2^{(-\alpha)} & \omega_1^{(-\alpha)} & \omega_0^{(-\alpha)} & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \cdots & \cdots \\ \omega_{N-1}^{(-\alpha)} & \ddots & \omega_2^{(-\alpha)} & \omega_1^{(-\alpha)} & \omega_0^{(-\alpha)} & 0 \\ \omega_N^{(-\alpha)} & \omega_{N-1}^{(-\alpha)} & \ddots & \omega_2^{(-\alpha)} & \omega_1^{(-\alpha)} & \omega_0^{(-\alpha)} \end{bmatrix} $$

- Right-sided fractional integral

$$ J_N^\alpha = h^\alpha \begin{bmatrix} \omega_0^{(-\alpha)} & \omega_1^{(-\alpha)} & \ddots & \ddots & \omega_{N-1}^{(-\alpha)} & \omega_N^{(-\alpha)} \\ 0 & \omega_0^{(-\alpha)} & \omega_1^{(-\alpha)} & \ddots & \ddots & \omega_{N-1}^{(-\alpha)} \\ 0 & 0 & \omega_0^{(-\alpha)} & \omega_1^{(-\alpha)} & \ddots & \ddots \\ \cdots & \cdots & \cdots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & 0 & \omega_0^{(-\alpha)} & \omega_1^{(-\alpha)} \\ 0 & 0 & \cdots & 0 & 0 & \omega_0^{(-\alpha)} \end{bmatrix} $$

PDEs – Spatial derivatives

- The left-sided fractional derivative is a natural choice for time derivative due to causality. This does not apply for spatial derivative
- Riesz derivative:

$$\frac{d^\beta \phi(x)}{d|x|^\beta} = D_R^\beta \phi(x) = \frac{1}{2}\left({}_aD_x^\beta \phi(x) + {}_xD_b^\beta \phi(x)\right)$$

$${}_aD_x^\mu \phi(x) = \frac{1}{\Gamma(m-\mu)}\left(\frac{d}{dx}\right)^m \int_a^x \frac{\phi(\xi)d\xi}{(x-\xi)^{\mu-m+1}} \quad (m-1<\mu\leqslant m),$$

$${}_xD_b^\mu \phi(x) = \frac{1}{\Gamma(m-\mu)}\left(-\frac{d}{dx}\right)^m \int_x^b \frac{\phi(\xi)d\xi}{(\xi-x)^{\mu-m+1}} \quad (m-1<\mu\leqslant m).$$

- Matrix approximation: (Ortigueira*, Int J Math and Math Sci*, 2006)

$$R_m^{(\beta)} = h^{-\beta}\begin{bmatrix} \omega_0^{(\beta)} & \omega_1^{(\beta)} & \omega_2^{(\beta)} & \omega_3^{(\beta)} & \cdots & \omega_m^{(\beta)} \\ \omega_1^{(\beta)} & \omega_0^{(\beta)} & \omega_1^{(\beta)} & \omega_2^{(\beta)} & \cdots & \omega_{m-1}^{(\beta)} \\ \omega_2^{(\beta)} & \omega_1^{(\beta)} & \omega_0^{(\beta)} & \omega_1^{(\beta)} & \cdots & \omega_{m-2}^{(\beta)} \\ \ddots & \ddots & \ddots & \ddots & \cdots & \cdots \\ \omega_{m-1}^{(\beta)} & \ddots & \omega_2^{(\beta)} & \omega_1^{(\beta)} & \omega_0^{(\beta)} & \omega_1^{(\beta)} \\ \omega_m^{(\beta)} & \omega_{m-1}^{(\beta)} & \ddots & \omega_2^{(\beta)} & \omega_1^{(\beta)} & \omega_0^{(\beta)} \end{bmatrix},$$

$$\omega_k^{(\beta)} = \frac{(-1)^k \Gamma(\beta+1)\cos(\beta\pi/2)}{\Gamma(\beta/2-k+1)\Gamma(\beta/2+k+1)}, \quad k=0,1,\ldots,m.$$

Demo #2

FPDEs with online Matlab routines

I. Podlubny, A. Chechkin, T. Skovranek, Y. Chen, B. Vinagre Jara,
Matrix approach to discretization of ODEs and PDEs of arbitrary real order (2008)
http://www.mathworks.com/matlabcentral/fileexchange/22071

Conclusions

- Straightforward to implement the fractional operators in numerical schemes
- Long duration impulse response of operator requires care in implementation
- Codes available online to simulate 1-D and 2-D problems