

An introduction to fractional calculus

Fundamental ideas and numerics

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May, 2022



Where are we?

We know a general way to obtain FLMM methods of the form

$$y^{(n)} = T_{m-1}(t_n) + \tau^\beta \sum_{j=0}^s w_{n,j} f(t_j, y^{(j)}) + \tau^\alpha \sum_{j=0}^n \omega_{n-j} f(t_j, y^{(j)}),$$

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- 📋 we need to discuss how we compute the starting values for a multi-step method,
- 📋 we still need to discuss how we can efficiently treat the memory term.

Computing the starting values

To **initialize the computation** we need the values $y^{(0)}, \dots, y^{(s)}, s+1$, $s = |\mathcal{A}| = \mathcal{A}_{p-1} \cup \{p-1\}$ with p the order of convergence of the FLMM, and $\mathcal{A}_{p-1} = \{\nu \in \mathbb{R} \mid \nu = i + j\alpha, \quad i, j \in \mathbb{N}, \nu < p-1\}$.

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- To avoid mixing methods we evaluate all the approximations at the same time by solving

$$\begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(s)} \end{bmatrix} = \begin{bmatrix} T_{m-1}(t_1) \\ T_{m-1}(t_2) \\ \vdots \\ T_{m-1}(t_s) \end{bmatrix} + \tau^\alpha \begin{bmatrix} (\omega_1 + w_{1,0})f_0 \\ (\omega_2 + w_{2,0})f_0 \\ \vdots \\ (\omega_s + w_{s,0})f_0 \end{bmatrix} + \tau^\alpha (\Omega \otimes I + W \otimes I) \begin{bmatrix} f(t_1, y^{(1)}) \\ f(t_2, y^{(2)}) \\ \vdots \\ f(t_s, y^{(s)}) \end{bmatrix}$$

where

$$\Omega = \begin{bmatrix} \omega_0 & & & \\ \omega_1 & \omega_0 & & \\ \vdots & \vdots & \ddots & \\ \omega_{s-1} & \omega_{s-2} & \cdots & \omega_0 \end{bmatrix}, \quad W = \begin{bmatrix} w_{1,1} & w_{1,2} & \cdots & w_{1,s} \\ w_{2,1} & w_{2,2} & \cdots & w_{2,s} \\ \vdots & \vdots & \ddots & \vdots \\ w_{s,1} & w_{s,2} & \cdots & w_{s,s} \end{bmatrix}$$

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- This will be in general an $s \times \dim(y^{(j)})$ nonlinear system that we need to solve before starting the iteration.
- If the value of α is not very small, viz s is moderate, and the system of ODEs is moderate this is manageable.

Treating the memory term

If we compute the sum on the coefficients ω_j naively for

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we end up having a $O(N^2)$ cost! If we do not perform this task efficiently the numerical solution degenerates in an unworkable task as we either refine our grid or enlarge our computational domain.

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- We can consider using a stretched grid towards t_0 to reduce N ,
- We can try an approach with nested meshes to reduce the load,
- We can exploit the fact that this is a convolution and adopt some FFT tricks.

The FFT trick (Hairer, Lubich, and Schlichte 1985)

The treatment remains the same indifferently for both PI and FLMM method, let us focus here on the generic formulation

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- Let r be a moderate number of step, e.g., $r = 2^k$ for a small k , we compute the first steps directly

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💡 We can use FFT!

If we call $S_r(n, 0, r-1) = \sum_{j=0}^{r-1} c_{n-j} f_j$, $n \in \{r, r+1, \dots, 2r-1\}$, the set of partial sums each of length r we can evaluate them with FFT in $O(2r \log_2(2r))$.

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- We can apply the same process recursively if we double every time-interval under consideration

$$y^{(n)} = \phi_n + \sum_{j=0}^{2r-1} c_{n-j} f_j + \sum_{j=2r}^n c_{n-j} f_j, \quad n \in \{2r, 2r+1, \dots, 3r-1\},$$

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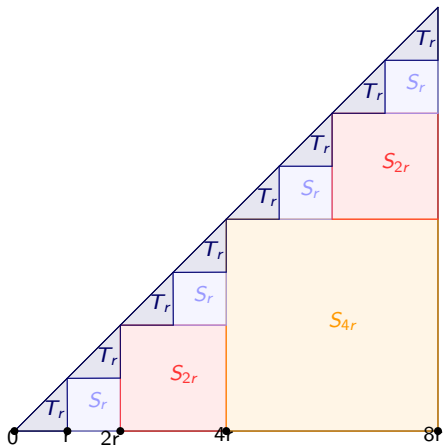
If we call $S_{2r}(n, 0, 2r-1) = \sum_{j=0}^{2r-1} c_{n-j} f_j$, and $S_r(n, 2r, 3r-1) = \sum_{j=2r}^{3r-1} c_{n-j} f_j$ the set of partial sums of lengths $2r$ and r we can evaluate them with FFT in $O(4r \log_2(4r))$ and $O(2r \log_2(2r))$ respectively.

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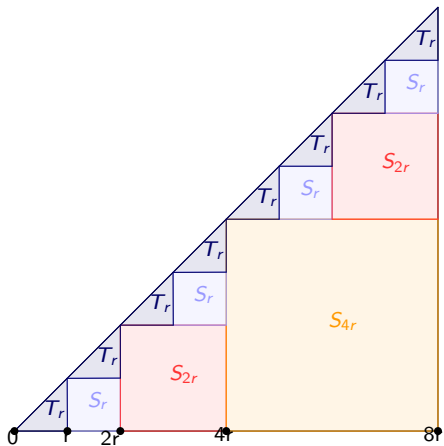
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- We can iterate the process for the $4r$ approximations in the interval $n \in \{4r, \dots, 8r - 1\}$, together with the partial sums $S_{4r}(n, 0, 4r - 1)$, $S_{2r}(n, 4r, 6r - 1)$, $S_r(n, 6r, 7r - 1)$ that can be evaluated in $O(8r \log_2(8r))$, $O(4r \log_2(4r))$ and $O(2r \log_2(2r))$ respectively,

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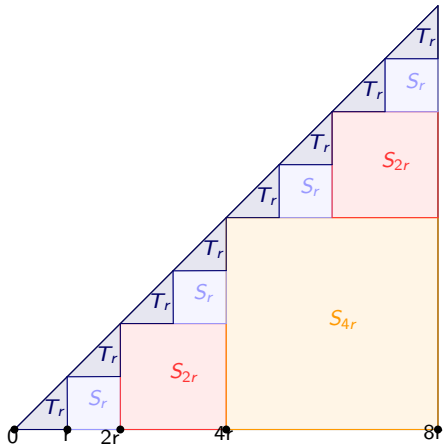
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- At each level we have to complete the recursion by computing

$$T_r(p, n) = \sum_{j=p}^n c_{n-j} f_j, \quad p = \ell r,$$

$$n \in \{\ell r, \ell r + 1, \dots, (\ell + 1)r - 1\},$$

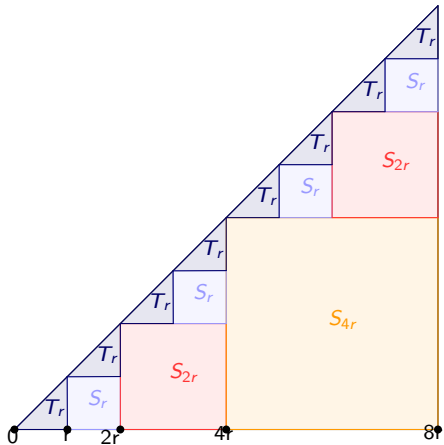
$$\ell = 0, 1, 2, \dots$$

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To determine the whole cost we just have to sum the various components

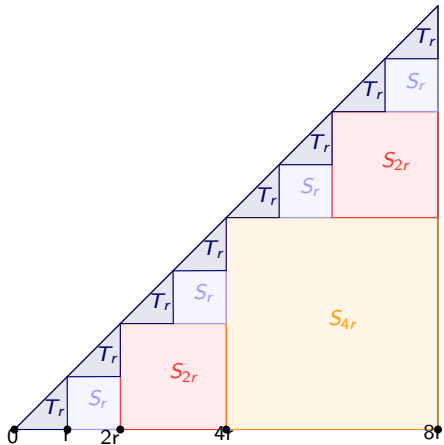
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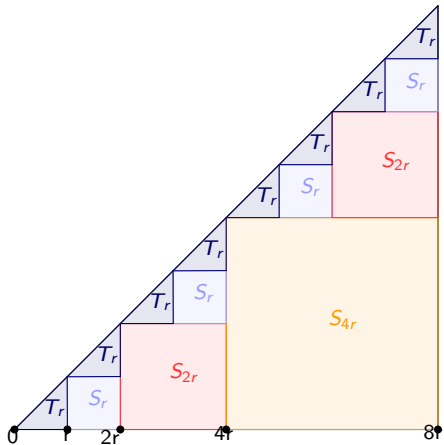
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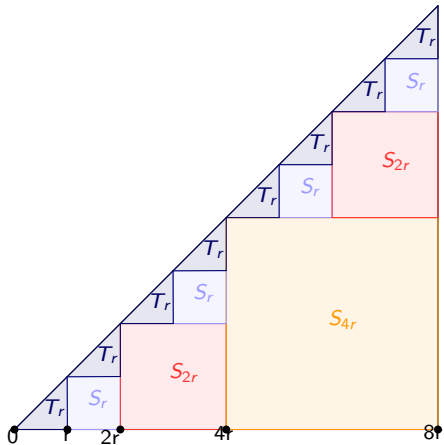
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- Assume that $N = 2^{n_t}$
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- + $O(N/2 \log_2 N/2)$ for 2 S_{2r}

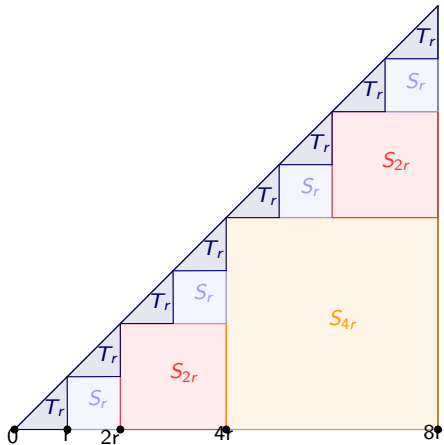
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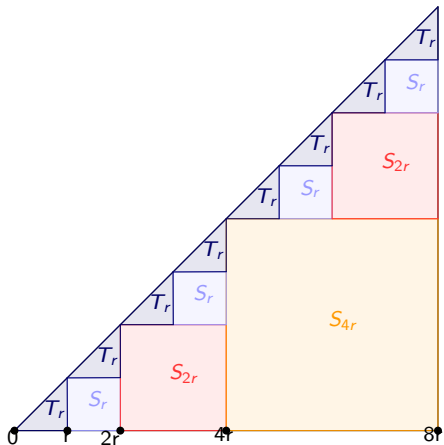
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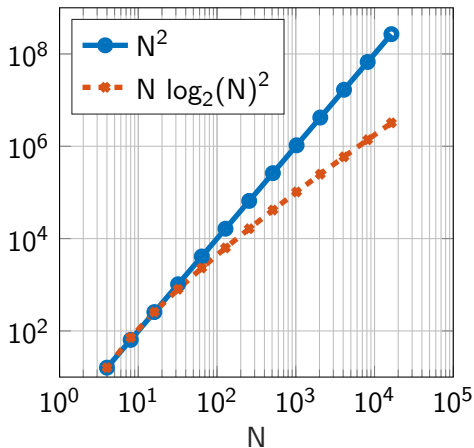
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- + $r(r+1)/2$ for the N/r convolutions T_r
- In general:

$$N \log_2 N + 2 \frac{N}{2} \log_2 \frac{N}{2} + 4 \frac{N}{4} \log_2 \frac{N}{4} + \dots$$

$$+ p \frac{N}{p} \log_2 \frac{N}{p} + \frac{N}{r} \frac{r(r+1)}{2}, \quad p = \frac{N}{2r}$$

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- + $r(r+1)/2$ for the N/r convolutions T_r
- In general:

$$\sum_{j=0}^{\log_2 p} N \log_2 \frac{N}{2^j} + N \frac{r+1}{2} = O(N(\log_2 N)^2).$$

Short-memory principle (Ford and Simpson 2001)

We can try to use a “fixed memory length” to reduce the computational (and memory) load.

$$\begin{aligned} y(t_{n+1}) = & y(t_n) + \frac{1}{\Gamma(\alpha)} \int_{t_n}^{t_{n+1}} (t_{n+1} - \tau)^{\alpha-1} f(\tau, x(\tau)) d\tau \\ & + \frac{1}{\Gamma(\alpha)} \int_0^{t_n} ((t_{n+1} - \tau)^{\alpha-1} - (t_n - \tau)^{\alpha-1}) f(\tau, y(\tau)) d\tau, \quad \alpha \in (0, 1). \end{aligned}$$

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Let us introduce now a fixed window T_M of memory, then

$$\begin{aligned} E &= \left| \frac{1}{\Gamma(\alpha)} \int_0^{t_n - T_M} ((t_{n+1} - \tau)^{\alpha-1} - (t_n - \tau)^{\alpha-1}) f(\tau, y(\tau)) d\tau \right| \\ &\leq \frac{M}{\Gamma(\alpha)} \left| \int_0^{t_n - T_M} ((t_{n+1} - \tau)^{\alpha-1} - (t_n - \tau)^{\alpha-1}) d\tau \right| \end{aligned}$$

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Let us introduce now a fixed window T_M of memory, then If we have a global error bound E_{global} with step-length τ we just need to choose

$$T_M > \left(\frac{M}{\Gamma(\alpha) E_{\text{global}}} \right)^{1/1-\alpha}, \quad \alpha \in (0, 1),$$

while if we have a local error bound E_{local}

$$T_M > \left(\frac{M\tau}{\Gamma(\alpha) E_{\text{local}}} \right)^{1/1-\alpha}, \quad \alpha \in (0, 1).$$

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But now to preserve the order of accuracy, we must choose

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The idea can be refined by using *nested meshes*.

Nested meshes

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Given $p \in \mathbb{N}$ we then have

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$$\Omega_\tau^\alpha f(n\tau) \approx I_{[0,t]}^\alpha f(n\tau), \text{ step length } \tau$$

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- In summary for any $p \in \mathbb{N}$ we get

$$\Omega_\tau^\alpha f(n\tau) = \sum_{j=0}^n \omega_{n-j} f(j\tau) \Leftrightarrow \Omega_{w^p \tau}^\alpha f(nw^p \tau) = w^{p\alpha} \sum_{j=0}^n \omega_{n-j} f(jw^p \tau).$$

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Given $\tau \in \mathbb{R}^+$, the mesh $M_\tau = \{\tau n, n \in \mathbb{N}\}$. Selected $w, r, p \in \mathbb{N}$, $w > 0$, $r > p$, we have $M_{w^p \tau} \supset M_{w^r \tau}$ and we decompose the interval as

$$[0, t] = [0, t - w^m T] \cup [t - w^m T, t - w^{m-1} T] \cup \dots \cup [t - wT, t - T] \cup [t - T, t]$$

for $m \in \mathbb{N}$ the smallest integer such that $t < w^{m+1} T$.

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Proof. For integration over a fixed interval $[0, t]$ the choice of T fixes (independent of h) the number of subranges over which the integral is evaluated, on each of them we have an error $O(h^p)$.

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- 🚩 This approach cost $O(w^m)$ with respect to $O(w^{2m})$ of the full method,
- ⚙️ We could use linear extrapolation techniques to improve the results.
- ⚙️ Selecting the various parameter may need a bit of tuning.

</> Available codes

With respect to the ordinary case for which there exists many reliable and high-performance codes, the choices for computing the solution of fractional differential equation is much more *sparse*.

- From (Garrappa 2018)
 - </> FDE_PI1_Ex.m - [Explicit Product-Integration of rectangular type](#)
 - </> FDE_PI1_Im.m - [Implicit Product-Integration of rectangular type](#)
 - </> FDE_PI2_Im.m - [Implicit Product-Integration of trapezoidal type](#)
 - </> FDE_PI12_PC.m - [Product-Integration with predictor-corrector](#)
- From (Garrappa 2015)
 - </> FLMM2 Matlab code - [Three implicit second order Fractional Linear Multistep Methods](#).

A remark

All these methods use direct-solver for the Newton method inside them, there is space to make improvement on the solution strategies. Furthermore, a challenge that yet remains: can we find a strategy that combines the convolution features and savings on the memory?

What do we have now

We know a general way to obtain FLMM methods of the form

$$y^{(n)} = T_{m-1}(t_n) + \tau^\beta \sum_{j=0}^s w_{n,j} f(t_j, y^{(j)}) + \tau^\alpha \sum_{j=0}^n \omega_{n-j} f(t_j, y^{(j)}),$$

- ✓ starting from the polynomials (ρ, σ) of an implicit order p method,
- ✓ we have seen how to compute the convolution coefficients ω_n ,
- ✓ we have seen how to compute the starting nodes $w_{n,j}$,
- ✓ we know how we can compute the starting values for a multi-step method by solving a nonlinear system with Newton,
- ✓ we have some hints on how we can efficiently treat the memory term.

A worked out example

Let us write everything for a case, let us start from the 2nd order BDF formula for ODEs

$$y^{(n+2)} - \frac{4}{3}y^{(n+1)} + \frac{1}{3}y^{(n)} = \frac{2}{3}\tau f_{n+2},$$

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$$\rho(\zeta) = \zeta^2 - \frac{4}{3}\zeta + \frac{1}{3}, \quad \sigma(\zeta) = \frac{2}{3}\zeta^2.$$

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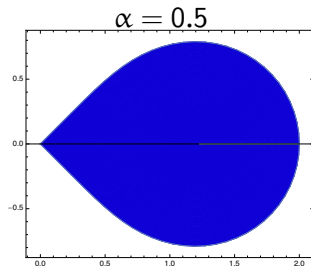
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$$\rho(\zeta) = \zeta^2 - \frac{4}{3}\zeta + \frac{1}{3}, \quad \sigma(\zeta) = \frac{2}{3}\zeta^2.$$

- Then we compute the generating function $\omega(\zeta)$

$$\omega(\zeta) = \frac{\rho(1/\zeta)}{\sigma(1/\zeta)} = \frac{2}{3(1 - 4\zeta/3 + \zeta^2/3)}.$$



$$\{1/\omega(\zeta)^\alpha : |\zeta| \leq 1\}$$

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Now we need to expand the convolution coefficients of

$$\omega^\alpha(\zeta) = (\omega(\zeta))^\alpha = \frac{2^\alpha}{3^\alpha} (1 - 4\zeta/3 + \zeta^2/3)^{-\alpha}.$$

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Theorem (Henrici 1974, Theorem 1.6c, p. 42)

Let $\phi(\zeta) = 1 + \sum_{n=1}^{+\infty} a_n \zeta^n$ be a formal power series. Then for any $\alpha \in \mathbb{C}$, we have

$$(\phi(\zeta))^\alpha = \sum_{n=0}^{+\infty} v_n^{(\alpha)} \zeta^n,$$

where coefficients $v_n^{(\alpha)}$ can be evaluated recursively as

$$v_0^{(\alpha)} = 1, \quad v_n^{(\alpha)} = \sum_{j=1}^n \left(\frac{(\alpha+1)j}{n} - 1 \right) a_j v_{n-j}^{(\alpha)}$$

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- $a_1 = -4/3$, $a_2 = 1/3$, $a_j = 0$ if $j \geq 3$, thus using

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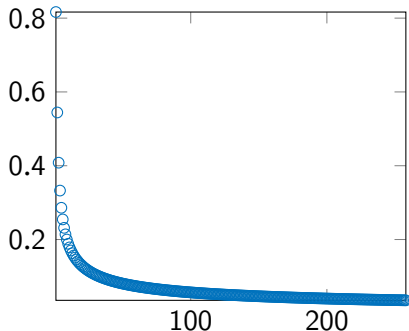
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- we get $\tilde{\omega}_0 = 1$, $\tilde{\omega}_1 = 4/3\alpha\tilde{\omega}_0 = 4\alpha/3$,

$$\tilde{\omega}_n = \frac{4}{3} \left(1 + \frac{\alpha-1}{n} \right) \tilde{\omega}_{n-1} + \frac{4}{3} \left(\frac{2(1-\alpha)}{n} - 1 \right) \tilde{\omega}_{n-2}.$$

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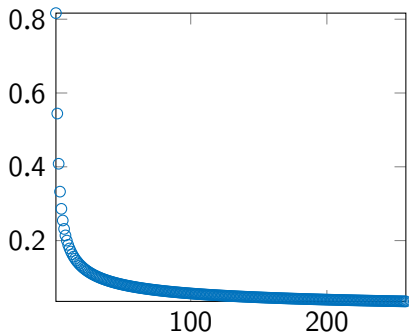


$\alpha = 0.5$.

- Since the a_j are a finite small number, we can compute the coefficients in an $O(N)$ operations,

```
omega = zeros(1,N+1) ;  
onethird = 1/3 ; fourthird = 4/3;  
twothird_oneminusalpha = 2/3*(1-alpha);  
fourthird_oneminusalpha = 4/3*(1-alpha);  
omega(1) = 1 ; omega(2) = fourthird*alpha*omega(1);  
for n = 2 : N  
    omega(n+1) = (fourthird -  
        ↪ fourthird_oneminusalpha/n)*omega(n) + ...  
        (twothird_oneminusalpha/n - onethird)*omega(n-1);  
end  
omega = omega*((2/3)^(alpha));
```

A worked out example

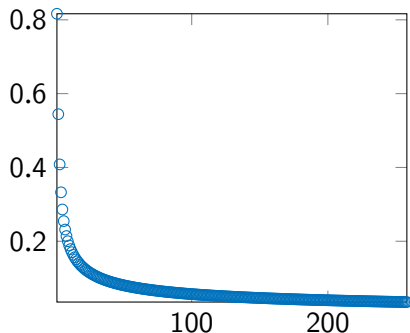


$\alpha = 0.5.$

- Since the a_j are a finite small number, we can compute the coefficients in an $O(N)$ operations,
- We can solve ${}_C D_{[0,2]}^{0.5} y(t) = -2y(t)$, $y(0) = 1$

τ	$ y^{(n)} - y(2) $	order
2^{-6}	1.44e-04	1.61
2^{-7}	4.42e-05	1.71
2^{-8}	1.28e-05	1.79
2^{-9}	3.57e-06	1.84
2^{-10}	9.68e-07	1.88
2^{-11}	2.85e-07	1.76
2^{-12}	8.17e-08	1.80
2^{-13}	2.29e-08	1.84
2^{-14}	6.27e-09	1.87

A worked out example



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- Since the a_j are a finite small number, we can compute the coefficients in an $O(N)$ operations,
- We can solve ${}_C D_{[0,2]}^{0.5} y(t) = -2y(t)$, $y(0) = 1$
- For the starting weights we have to solve a 3×3 Vandermonde system:

$$\begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & \sqrt{2} \\ 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} w_{n,0} \\ w_{n,1} \\ w_{n,2} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

number of time-step times.

Reuse

Since we have a fixed time-grid we can reuse the same factorization for the Vandermonde system and compute all the weights in a single sweep.

Fractional Brusselator

The Brusselator is a model of the **autocatalytic chemical reaction**, it is described by

$$\begin{cases} \dot{x}_1 = a - (\mu + 1)x_1 + x_1^2 x_2, \\ \dot{x}_2 = \mu x_1 - x_1^2 x_2, \end{cases} \quad a, \mu > 0.$$

- If $\mu > a^2 + 1$ then a single Brusselator has a *unique limit cycle*,

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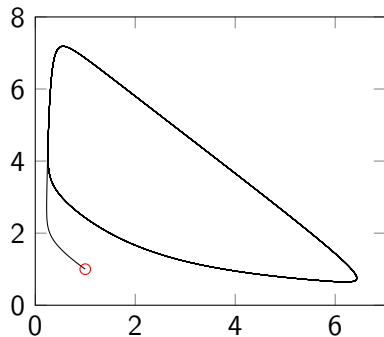
- If $\mu > a^2 + 1$ then a single Brusselator has a *unique limit cycle*,
- If $(a - 1)^2 < \mu \leq a^2 + 1$ all the orbits tend to the steady state.

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```
a = 1 ; mu = 4 ;  
param = [ a , mu ] ;  
f_fun = @(t,y,param) [ ...  
par(1) - (par(2)+1)*y(1) + y(1)^2*y(2) ; ...  
par(2)*y(1) - y(1)^2*y(2) ] ;  
t0 = 0 ; T = 100 ;  
y0 = [ 1 ; 1 ] ;  
[T,Y] = ode45(@(t,y)  
    ↪ f_fun(t,y,param), [t0,T], y0);  
figure(1)  
plot(Y(:,1),Y(:,2), 'k-', y(1,1), y(2,1), 'ro')
```



Fractional Brusselator

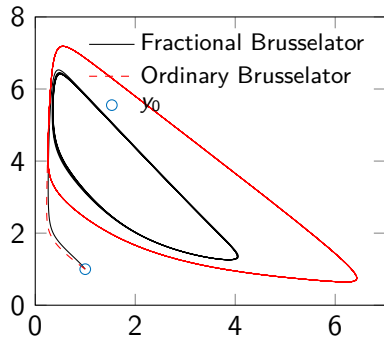
The Brusselator is a model of the **autocatalytic chemical reaction**, it is described by

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```
alpha = [0.8,0.7] ;  
h = 1e-2;  
[t, y] =  
↳ fde_pi1_ex(alpha,f_fun,t0,T,y0,h,param) ;
```

The cycle of the single fractional Brusselator is contained in the region

$$\left\{ (x_1, x_2) : \frac{a}{\mu + 1} < x_1 < \frac{2a}{\mu}, 0 < x_2 < \frac{\mu(1 + \mu)}{a} \right\}$$



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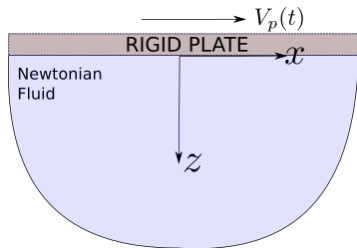
? Of interest (Wang and Li 2007)

Finding the smallest values α_1, α_2 for which a limit cycle exist is of interest.

Bagley-Torvik Model (Bagley and Torvik 1986)

Stoke's Second Problem

Can we determine the behavior of a half-space of Newtonian, viscous fluid undergoing the motion induced by the prescribed uniform sinusoidal motion of a plate on the surface?



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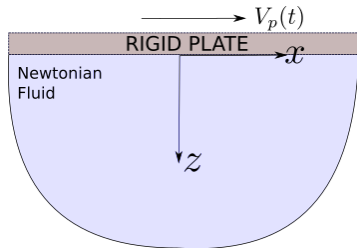
If we write down the **equation of motion** we find

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$$\rho \frac{\partial v}{\partial t} = \mu \frac{\partial^2 v}{\partial z^2}$$

- ρ is the *fluid density*, μ is the viscosity, v is the profile of the *transverse fluid velocity*.

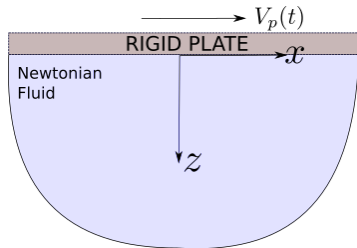


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$$\rho[s\tilde{v}(s, z) - v(0, x)] = \mu \frac{d^2 \tilde{v}(s, z)}{dz^2},$$

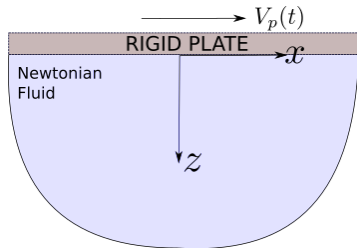
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$$\tilde{v}(s, z) = \tilde{v}_p(s) \exp\left(\sqrt{\frac{\rho s}{\mu}} z\right)$$

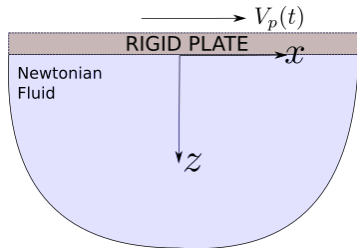
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$$\tilde{\sigma}(s, z) = \sqrt{\mu\rho}\sqrt{s}\tilde{v}(s, z) = \sqrt{\mu\rho}\frac{1}{\sqrt{s}}s\tilde{v}(s, z)$$

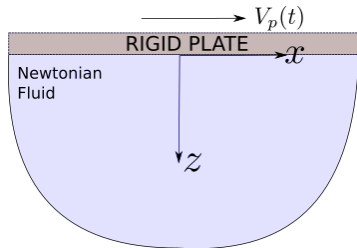
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$$\tilde{\sigma}(s, z) = \sqrt{\mu\rho} \mathcal{L} \left\{ \frac{1}{\Gamma(1/2) t^{1/2}} \right\} * \mathcal{L} \{ v_t \}$$

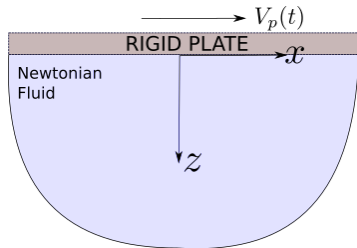
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$$\sigma(t, z) = \sqrt{\mu\rho} \frac{1}{\Gamma(1/2)} \int_0^t (t - \tau)^{1/2} v_\tau(\tau, z) d\tau.$$

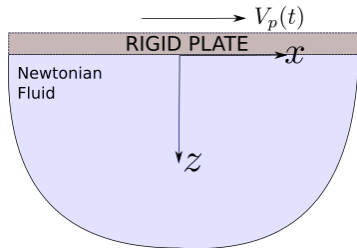
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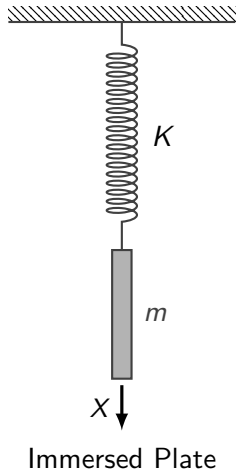
$$\sigma(t, z) = \sqrt{\mu \rho} C A D_{[0, t]}^{1/2} v(t, z).$$

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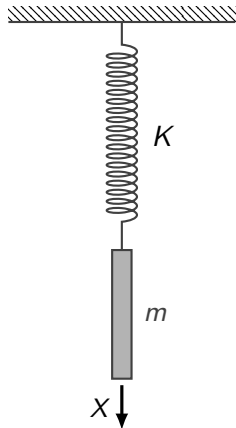
Bagley-Torvik Model (Bagley and Torvik 1986)

Assumptions:

- The spring is massless and its oscillations do not disturb the fluid,
- The area A of the plate is sufficiently large as to produce in the fluid adjacent to the plate the velocity field and stresses we just derived,



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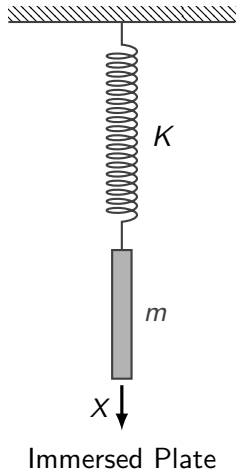
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Deriving the equation:

$$m\ddot{X} = F_X = -KX - 2A\sigma(t, 0)$$

Immersed Plate

Bagley-Torvik Model (Bagley and Torvik 1986)



Assumptions:

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Deriving the equation:

$$m\ddot{X} = F_X = -KX - 2A\sigma(t, 0)$$

Using the expression for the *strain* and $V_p(t, 0) = \dot{X}(t)$ we find

$$m\ddot{X} + 2A\sqrt{\mu\rho}CA D_{[0,t]}^{3/2}X + KX = 0.$$

Linear Multi-Term FDEs

The Bagley-Torvik model is an example of a **Linear Multi-Term FDE**, that is, something of the form

$$\lambda_{QCA} D^{\alpha_Q} y(t) + \lambda_{Q-1CA} D^{\alpha_{Q-1}} y(t) + \cdots + \lambda_{2CA} D^{\alpha_2} y(t) + \lambda_{1CA} D^{\alpha_1} y(t) = f(t, y(t)),$$

with

- $\lambda_i \in \mathbb{R} \ \forall i = 1, \dots, Q$,
- $0 < \alpha_1 < \alpha_2 < \dots < \alpha_{Q-1} < \alpha_Q$ and $\alpha_Q \neq 0$.

For this problem we have $m_Q = \max m_i$, $m_i = \lceil \alpha_i \rceil$, $i = 1, \dots, Q$ **initial conditions:**

$$y(t_0) = y_0, y'(t_0) = y_0^{(1)}, \dots, y^{(m_Q-1)}(t_0) = y_0^{(m_Q-1)}.$$

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❓ How can we solve them?

Linear Multi-Term FDEs

We need to **recall one of the properties** we have seen of the Caputo derivatives

$$(P_1) \quad I_{[t_0, T]}^{\alpha} {}^{CA}D_{[t_0, T]}^{\alpha} y(t) = y(t) - T_{m-1}[y, t_0](t),$$

$$(P_2) \quad I_{[t_0, T]}^{\beta} {}^{CA}D_{[t_0, T]}^{\alpha} y(t) = I_{[t_0, T]}^{\beta} {}^{RL}D_{[t_0, T]}^{\alpha} [y(t) - T_{m-1}[y; t_0](t)] = \\ I_{[t_0, T]}^{\beta-\alpha} [y(t) - T_{m-1}[y; t_0](t)], \quad \beta > \alpha.$$

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We start from the multi-term equation

$$\lambda_Q {}_{CA}D^{\alpha_Q} y(t) + \lambda_{Q-1} {}_{CA}D^{\alpha_{Q-1}} y(t) + \cdots + \lambda_2 {}_{CA}D^{\alpha_2} y(t) + \lambda_1 {}_{CA}D^{\alpha_1} y(t) = f(t, y(t)),$$

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We start from the multi-term equation

$$\lambda_Q I_{[t_0, T]}^{\alpha_Q} [{}_{CA}D^{\alpha_Q} y(t)] = -I_{[t_0, T]}^{\alpha_Q} \left[\sum_{i=1}^{Q-1} \lambda_i {}_{CA}D^{\alpha_i} y(t) + f(t, y(t)) \right],$$

- we multiply both sides by $I_{[t_0, T]}^{\alpha_Q}$,

Linear Multi-Term FDEs

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We start from the multi-term equation

$$y(t) - T_{m_Q-1}[y, t_0](t) = - \sum_{i=1}^{Q-1} \frac{\lambda_i}{\lambda_Q} I_{[t_0, t]}^{\alpha_Q - \alpha_i} [y(t) - T_{m_i-1}[y; t_0](t)] + \frac{1}{\lambda_Q} I_{[t_0, T]}^{\alpha_Q} f(t, y(t))$$

- we multiply both sides by $I_{[t_0, T]}^{\alpha_Q}$,
- we use P_1 on the left-hand side, P_2 on the right-hand side,

Linear Multi-Term FDEs

We need to **recall one of the properties** we have seen of the Caputo derivatives

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We start from the multi-term equation

$$y(t) = T_{m_{Q-1}}[y, t_0](t) - \sum_{i=1}^{Q-1} \frac{\lambda_i}{\lambda_Q} I_{[t_0, t]}^{\alpha_Q - \alpha_i} [y(t) - T_{m_i-1}[y; t_0](t)] + \frac{1}{\lambda_Q} I_{[t_0, T]}^{\alpha_Q} f(t, y(t))$$

- we multiply both sides by $I_{[t_0, T]}^{\alpha_Q}$,
- we use P_1 on the left-hand side, P_2 on the right-hand side,
- and re-arrange to get an expression for the solution.

Linear Multi-Term FDEs: generalizing PI rules

First we do a bit of rewriting of

$$y(t) = T_{m_{Q-1}}[y, t_0](t) - \sum_{i=1}^{Q-1} \frac{\lambda_i}{\lambda_Q} I_{[t_0, t]}^{\alpha_Q - \alpha_i} [y(t) - T_{m_{i-1}}[y; t_0](t)] + \frac{1}{\lambda_Q} I_{[t_0, T]}^{\alpha_Q} f(t, y(t))$$

- we employ the usual fractional integral for polynomials:

$$I_{[t_0, t]}^{\alpha} T_{m-1}[y; t_0](t) = \sum_{k=0}^{m-1} \frac{(t - t_0)^{k+\alpha}}{\Gamma(k + \alpha)} y^{(k)}(t_0), \quad \begin{array}{l} \alpha \in \{\alpha_1, \dots, \alpha_{Q-1}\}, \\ m \in \{m_1, \dots, m_{Q-1}\}. \end{array}$$

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$$y(t) = T_{m_{Q-1}}[y, t_0](t) - \sum_{i=1}^{Q-1} \frac{\lambda_i}{\lambda_Q} I_{[t_0, t]}^{\alpha_Q - \alpha_i} [y(t) - T_{m_{i-1}}[y; t_0](t)] + \frac{1}{\lambda_Q} I_{[t_0, T]}^{\alpha_Q} f(t, y(t))$$

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- We use it to **simplify the expression**

$$\tilde{T}(t) = T_{m_{Q-1}}[y; t_0](t) + \sum_{i=1}^{Q-1} \frac{\lambda_i}{\lambda_Q} \sum_{k=0}^{m_i-1} \frac{(t - t_0)^{k + \alpha_Q - \alpha_i}}{\Gamma(k + \alpha_Q - \alpha_i + 1)} y^{(k)}(t_0).$$

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$$y(t) = \tilde{T}(t) - \sum_{i=1}^{Q-1} \frac{\lambda_i}{\lambda_Q} I_{[t_0, t]}^{\alpha_Q - \alpha_i} y(t) + \frac{1}{\lambda_Q} I_{[t_0, T]}^{\alpha_Q} f(t, y(t)).$$

- we employ the usual fractional integral for polynomials:

$$I_{[t_0, t]}^{\alpha} T_{m-1}[y; t_0](t) = \sum_{k=0}^{m-1} \frac{(t - t_0)^{k+\alpha}}{\Gamma(k + \alpha)} y^{(k)}(t_0), \quad \begin{array}{l} \alpha \in \{\alpha_1, \dots, \alpha_{Q-1}\}, \\ m \in \{m_1, \dots, m_{Q-1}\}. \end{array}$$

- We use it to simplify the expression

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Linear Multi-Term FDEs: generalizing PI rules

Now we have an expression that we can treat by adapting one of the Product Integral rules

$$y(t) = \tilde{T}(t) - \sum_{i=1}^{Q-1} \frac{\lambda_i}{\lambda_Q} I_{[t_0, t]}^{\alpha_Q - \alpha_i} y(t) + \frac{1}{\lambda_Q} I_{[t_0, T]}^{\alpha_Q} f(t, y(t)).$$

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We can start from the **explicit rectangular product integral rule** on a uniform grid

$$y^{(n)} = \tilde{T}(t_n) - \sum_{i=1}^{Q-1} \frac{\lambda_i}{\lambda_Q} \tau^{\alpha_Q - \alpha_i} \sum_{j=0}^{n-1} b_{n-j-1}^{(\alpha_Q - \alpha_i)} y^{(j)} + \frac{1}{\lambda_Q} \sum_{j=0}^{n-1} b_{n-j-1}^{(\alpha_Q)} f(t_j, y^{(j)}).$$

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$$b_n^{(\alpha)} = [(n+1)^\alpha - n^\alpha]/\alpha, \quad n = 1, \dots, N.$$

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We can do it similarly for the **Implicit Trapezoidal Rule** and then for the **Predictor-Corrector method** (Diethelm [2003](#)).

Linear Multi-Term FDEs: generalizing PI rules

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Available codes (Garrappa 2018):

⌕ MT_FDE_PI1_Ex.m - Explicit Product-Integration of rectangular type

⌕ MT_FDE_PI1_Im.m - Implicit Product-Integration of rectangular type

⌕ MT_FDE_PI2_Im.m - Implicit Product-Integration of trapezoidal type

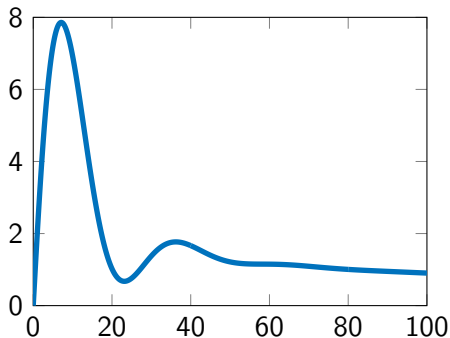
⌕ MT_FDE_PI12_PC.m - Product-Integration with predictor-corrector

Linear Multi-Term FDEs: back to Bagley-Torvik

We reached the equation

$$m\ddot{X} + 2A\sqrt{\mu\rho_{CA}}D_{[0,t]}^{3/2}X + KX = 0.$$

```
m = 10; A = 6; K = 3;
mu = 2; rho = 2;
alpha = [2 3/2] ;
lambda = [m 2*A*sqrt(mu*rho)] ;
f_fun = @(t,X) -K*X;
J_fun = @(t,X) -K;
t0 = 0 ; T = 100 ;
X0 = [0 , 2 ] ;
h = 1e-2;
[t, X] = mt_fde_pi1_ex(alpha, lambda, f_fun,
    ↪ t0, T, X0, h);
```

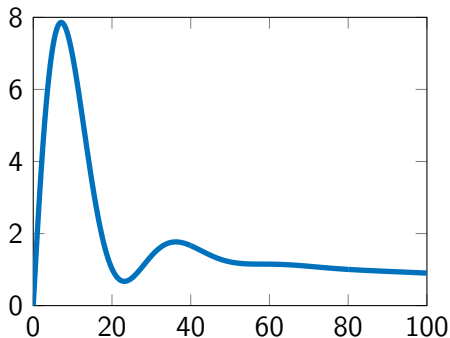


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But does it fit the reality?

Linear Multi-Term FDEs: back to Bagley-Torvik

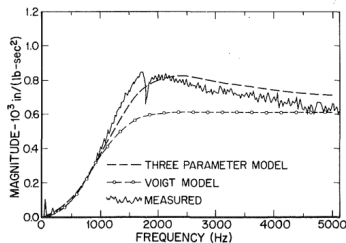


Fig. 5 The magnitude of the transfer function for Case 1

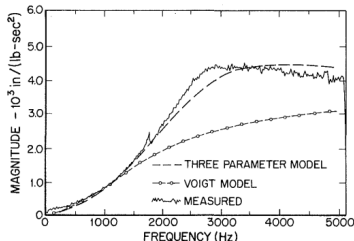


Fig. 7 The magnitude of the transfer function for Case 5

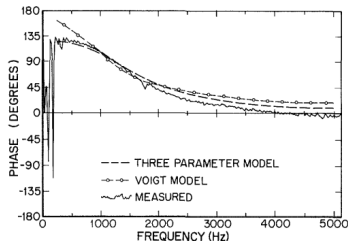


Fig. 6 The phase of the transfer function for Case 1

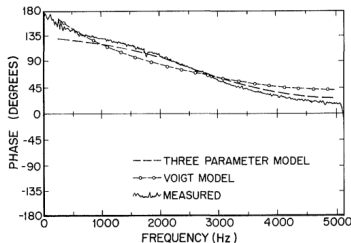


Fig. 8 The phase of the transfer function for Case 5

The model we have derived is a model of the form

$$\begin{aligned}\sigma(t) &= G_0 \epsilon(t) + G_1 \dot{\epsilon}(t), \\ \epsilon(t) &= \frac{x(t)}{\delta} \\ f(t) &= m\ddot{x}(t) + f_p(t), \\ f_p(t) &= \frac{2A}{\delta} (G_0 + G_1 {}_C A D^\alpha x(t)).\end{aligned}$$

One can do *parameter tuning* to find the fractional order from experimental data and compare the results with the integer-order model. The results on the left by Bagley and Torvik 1986 show that the fractional model obtain a better fit with the measured data.

Equivalent formulations of the Multi-Term FDEs

In the integer-order case we know how to rewrite the equation

$$y^{(n)}(t) = f(t, y^{(n-1)}(t), \dots, y^{(1)}(t), y(t)), \quad y^{(j)}(0) = y_0^{(j)}, \quad j = 0, 1, \dots, n-1,$$


as a **system of first-order equations**.

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 Can we do something similar in the fractional case?

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(A1) Let us assume that our multi-term equation is of the form

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for $\alpha_k > \alpha_{k-1} > \dots > \alpha_1 > 0$, $\alpha_j - \alpha_{j-1} \leq 1 \quad \forall j = 1, 2, \dots, k$, $0 < \alpha_1 \leq 1$.

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(A2) Assume also that $\alpha_j \in \mathbb{Q} \quad \forall j = 1, 2, \dots, k$, and that M is the least common multiple of $\alpha_1, \alpha_2, \dots, \alpha_k$.

Equivalent formulations of the Multi-Term FDEs

Theorem (Diethelm 2010, Theorem 8.1)

Under the assumptions (A1) and (A2), set $\gamma = 1/M$, and $N = M\alpha_k$, then the IVP is equivalent to

$$\begin{cases} {}_{CA}D^\gamma y_0(t) = y_1(t), \\ {}_{CA}D^\gamma y_1(t) = y_2(t), \\ \vdots \\ {}_{CA}D^\gamma y_{N-2}(t) = y_{N-1}(t), \\ {}_{CA}D^\gamma y_{N-1}(t) = f(t, y_0(t), y_{\alpha_{k-1}/M}(t), \dots, y_{\alpha_1/M}(t), y(t)) \end{cases} \quad y_i(0) = \begin{cases} y_0^{(j/m)}, & \text{if } \frac{j}{M} \in \mathbb{N}_0, \\ 0, & \text{otherwise.} \end{cases}$$

\Rightarrow whenever $y = (y_0, \dots, y_{N-1})^T$ with $y_0 \in \mathcal{C}^{[\alpha_k]}[0, b]$, for some $b > 0$, is a solution of the N -dimensional system, then $y \equiv y_0$ is a solution of the multi-term FDE.

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\Leftarrow whenever $y \in \mathcal{C}^{[\alpha_k]}([0, b])$ is a solution of the multi-term FDE, then the vector function $\mathbf{y} = (y, {}_{CA}D^\gamma y, {}_{CA}D^{2\gamma} y, \dots, {}_{CA}D^{(N-1)\gamma} y)^T$ solves the N -dimensional system.

Equivalent formulations of the Multi-Term FDEs

We can relax (A2) from the *rationality requirement* to a requirement on being commensurable².

(A2)' Let $1 \geq \alpha_k > \alpha_{k-1} > \dots > \alpha_1 > 0$ and assume the equation to be *commensurate*, then we define $\tilde{\alpha}_j = \alpha_j/\alpha_1$ for $j = 1, \dots, k$, let \tilde{M} be the least common multiple of the denominators of the values $\tilde{\alpha}_1, \dots, \tilde{\alpha}_k$.

Theorem (Diethelm 2010, Theorem 8.2)

Under the assumption (A1) and (A2)', set $\gamma = \alpha_1/\tilde{M}$ and $N = \tilde{M}\alpha_k/\alpha_1$, then the equivalence relation of the N -dimensional system and of the multi-term FDE holds as in the previous result.

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- ⚙ See (Ford and Connolly 2009) for other reformulations and comparisons.

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The Method of Lines

Consider a partial differential equations of the form

$$\text{Find } u(\mathbf{x}, t) \text{ s.t. } u_t = \mathcal{L}u, \quad \mathbf{x} \in \Omega \subseteq \mathbb{R}^d, t \in I \subseteq \mathbb{R}_+,$$

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A *classical* way of approaching this task is using a **Method Of Lines** (MOL) approach, that is

1. we discretize w.r.t. the *space variables* with some method (e.g., Finite Elements/Differences/Volumes, meshfree/meshless methods, spectral methods...)

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2. now we have a (possibly nonlinear, non-autonomous) system of ODEs to which we can apply an integrator.

PDEs with fractional derivatives with respect to time

We can think of using the methods we have seen until now for solving PDEs in which the **derivative with respect to time** has been substituted by the **fractional derivative in the Caputo sense**

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Examples:

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$${}_{CA}D_t^\alpha u = \operatorname{div}(p(x) \operatorname{grad} u) - q(x)u + F(x, t), \quad 0 < \alpha \leq 1.$$

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- Time-fractional Schrödinger equation

$$(iT_\rho)^\alpha {}_{CA}D_t^\alpha \psi = -\frac{L_\rho^2}{2N_m} \nabla^2 \psi + N_v \psi, \quad 0 < \alpha \leq 1.$$

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 Time-fractional (incompressible) Navier–Stokes equation

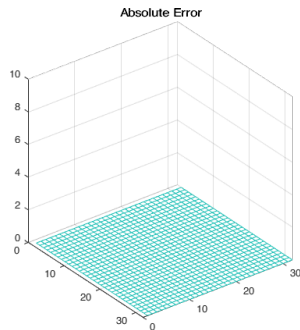
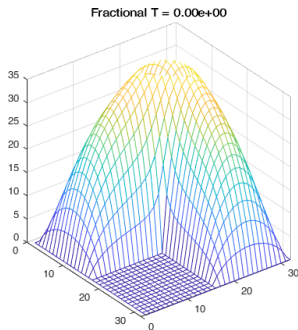
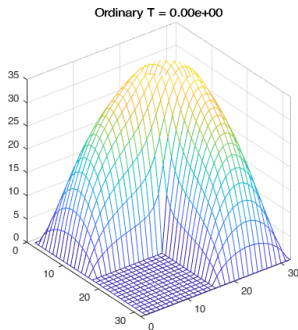
$$\begin{cases} {}_{CA}D_t^\alpha (u \cdot \nabla) u = \nu \nabla^2 u - \frac{1}{\rho} \nabla p + f, \\ \nabla \cdot u = 0. \end{cases} \quad 0 < \alpha \leq 1.$$

An example with diffusion

Let us consider the case of

$${}_C D_t^\alpha u = 0.05 \nabla^2 u, \quad \alpha = 0.3, 1.$$

and integrate it with the FBDF2 with $\tau = 10^{-2}$.

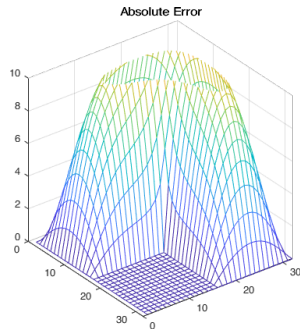
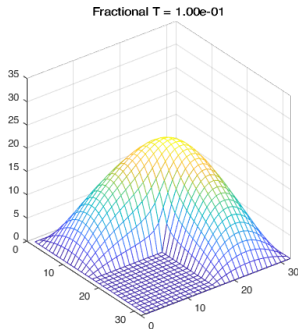
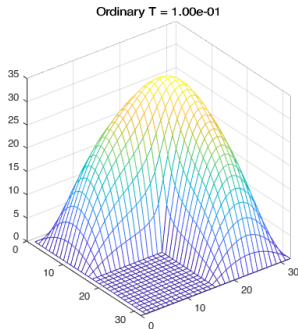


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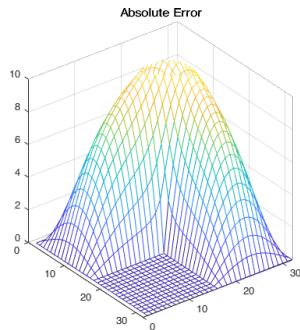
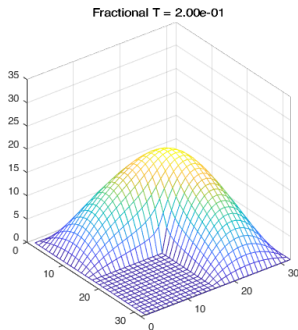
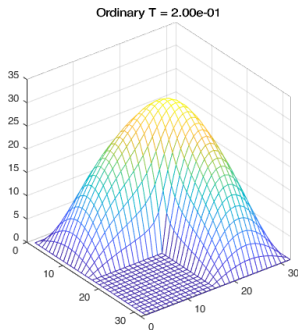


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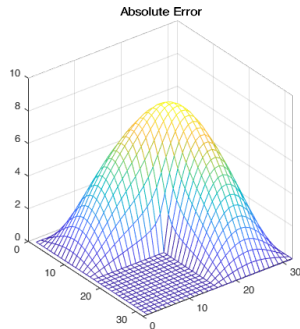
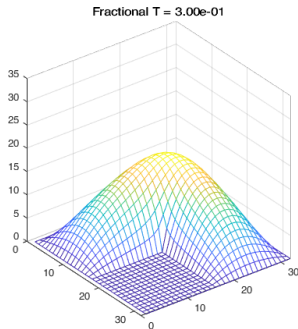
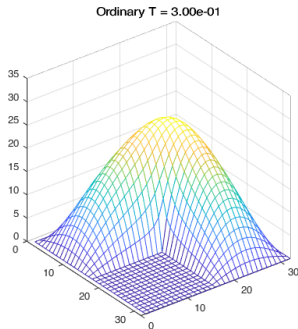


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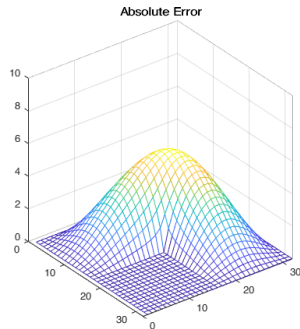
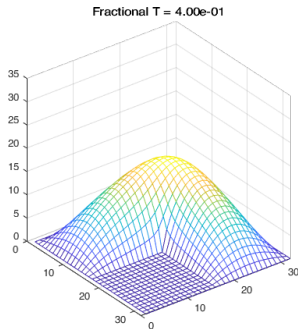
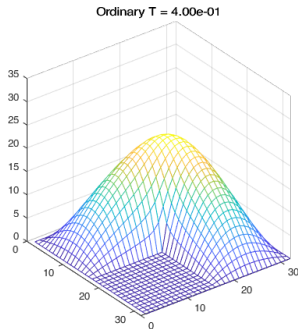


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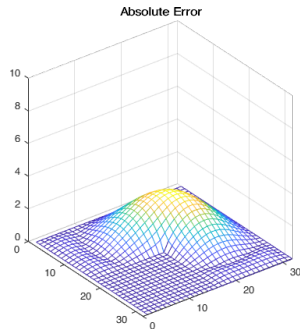
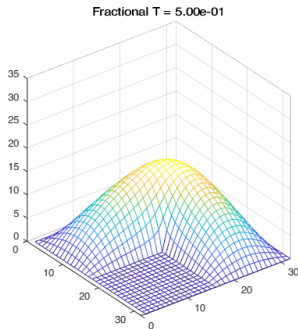
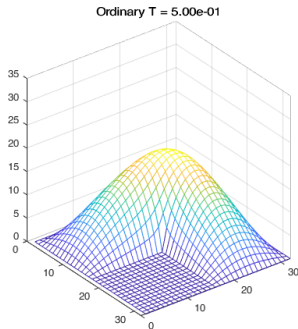


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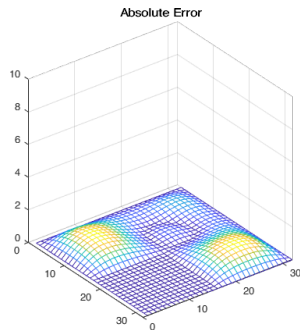
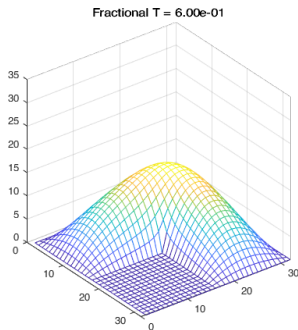
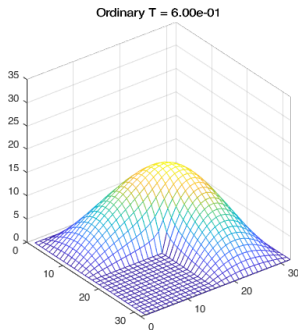


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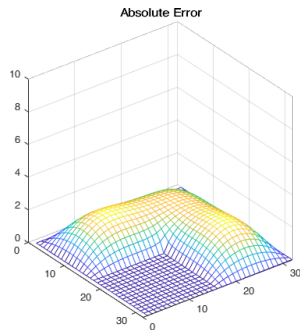
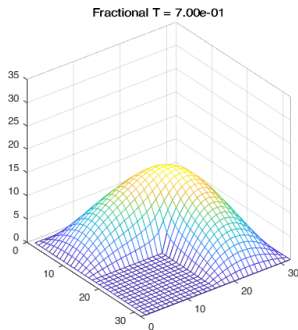
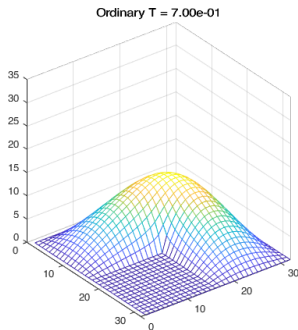


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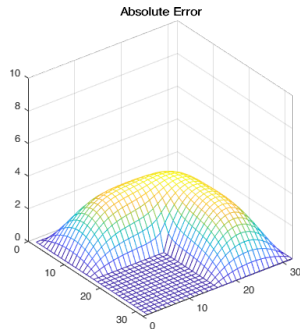
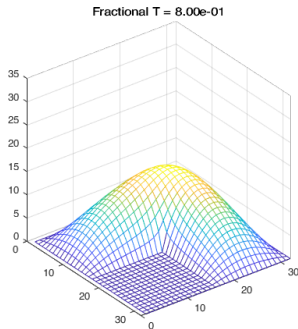
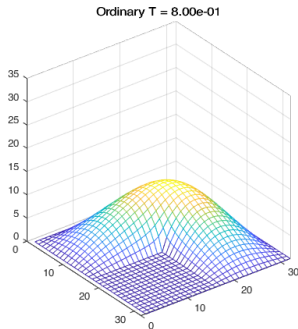


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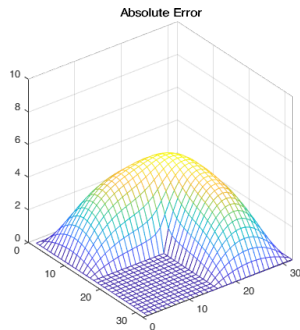
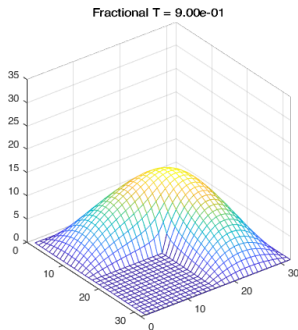
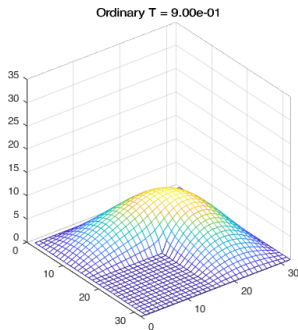


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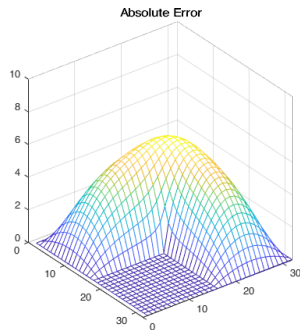
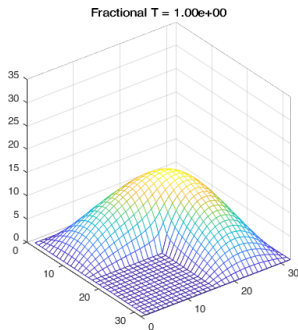
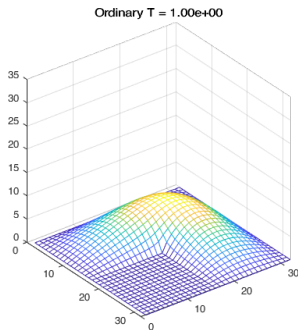


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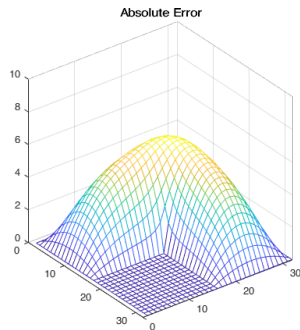
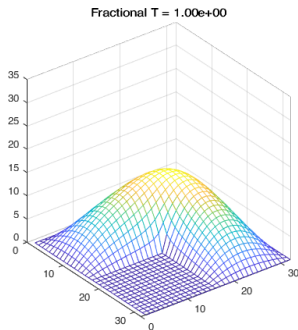
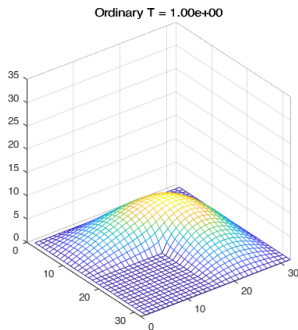


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