Numerical methods for non-standard fractional operators in the simulation of dielectric materials

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Outline

Numerical methods for non-standard fractional operators in the simulation of dielectric materials

1. The problem
2. The operator
3. The numerical method

Financial support:

- EU Cost Action 15225 - Fractional Systems
- Istituto Nazionale di Alta Matematica (INdAM-GNCS)

Maxwell's equations:

Standard Maxwell's equations:

$$\begin{cases} \nabla \times \mathbf{H} = \epsilon_0 \dfrac{\partial}{\partial t}\mathbf{E} & \text{Ampere's law} \\ \nabla \times \mathbf{E} = -\mu_0 \dfrac{\partial \mathbf{H}}{\partial t} & \text{Faraday's law} \end{cases}$$

E: electric field   **H**: magnetic field

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E: electric field **H**: magnetic field

Real world applications

- design of data and energy storage devices
- design of antennas
- medical diagnostic (MRI), cancer therapy, ...

Maxwell's equations:

Standard Maxwell's equations with polarization:

$$\begin{cases} \nabla \times \mathbf{H} = \epsilon_0 \dfrac{\partial}{\partial t}\mathbf{E} + \dfrac{\partial}{\partial t}\mathbf{P} & \text{Ampere's law} \\ \nabla \times \mathbf{E} = -\mu_0 \dfrac{\partial \mathbf{H}}{\partial t} & \text{Faraday's law} \end{cases}$$

E: electric field **H**: magnetic field **P**: polarization

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E: electric field **H**: magnetic field **P**: polarization

The complex susceptibility

The polarization **P** depends on the electric field **E** (constitutive law)

$$\hat{\mathbf{P}} = \varepsilon_0 \, \hat{\chi}(\omega) \, \hat{\mathbf{E}}$$

- $\hat{\chi}(\omega)$ is a specific feature of the matter (or system)

Simplified notation (just for easy of presentation)

Determining the complex susceptibility $\hat{\chi}(\omega)$

How to derive $\hat{\chi}(\omega) = \hat{\chi}'(\omega) - \mathrm{i}\hat{\chi}''(\omega)$?

Determining the complex susceptibility $\hat{\chi}(\omega)$

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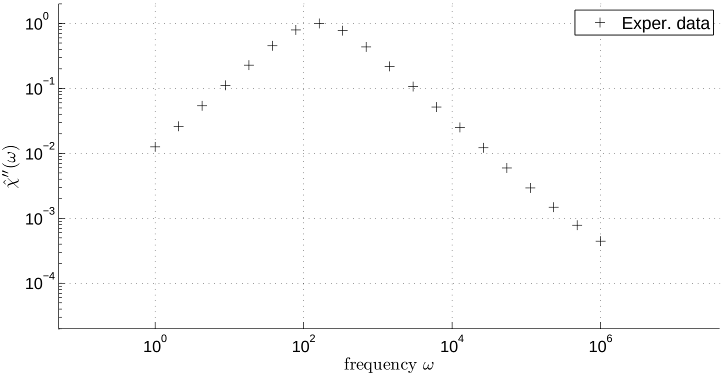
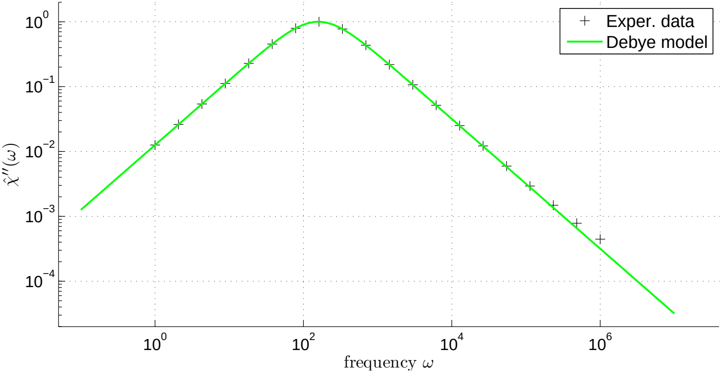
Experimental data (in the frequency domain): $\hat{P} = \hat{\chi}(\omega)\hat{E}$



Match experimental data into a mathematical model

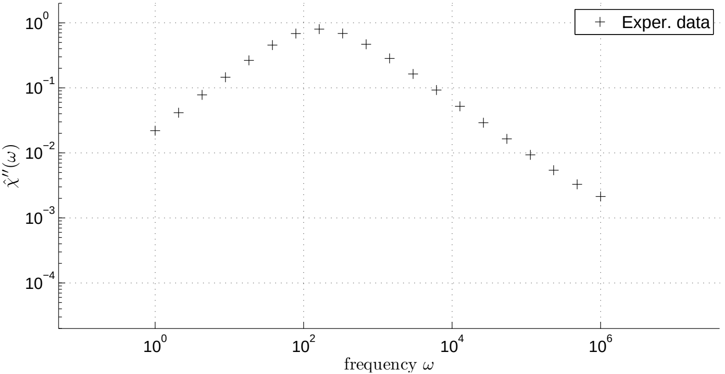
Determining the complex susceptibility $\hat{\chi}(\omega)$



The Debye model: $\hat{\chi}(\omega) = \dfrac{1}{1 + \mathrm{i}\omega\tau}$ (standard materials)

Ordinary differential equation: $\tau \dfrac{d}{dt} P(t) + P(t) = E(t)$

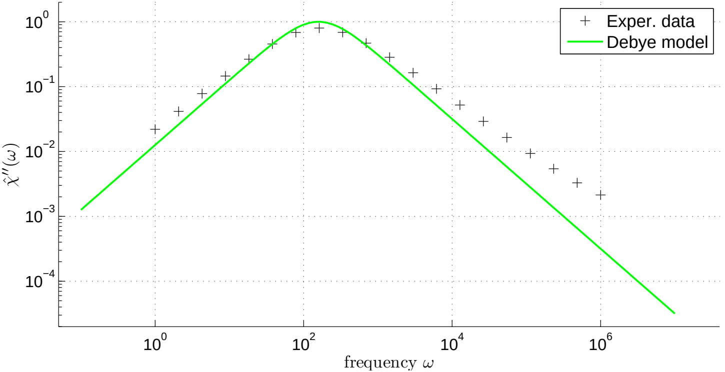
Determining the complex susceptibility $\hat{\chi}(\omega)$



Materials with anomalous dielectric properties:

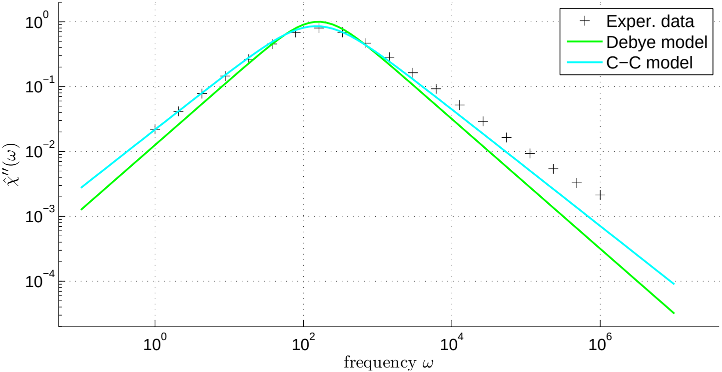
- amorphous polymers
- complex systems (biological tissues)

Determining the complex susceptibility $\hat{\chi}(\omega)$



Debye model not satisfactory

Determining the complex susceptibility $\hat{\chi}(\omega)$

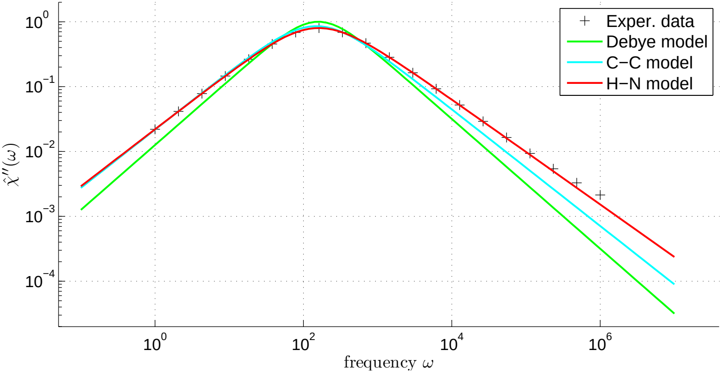


The Cole-Cole model: $\hat{\chi}(\omega) = \dfrac{1}{1 + (\mathrm{i}\omega\tau)^{\alpha}}$ $\quad 0 < \alpha < 1$

Fractional differential equation: $\tau^{\alpha} \dfrac{d^{\alpha}}{dt^{\alpha}} P(t) + P(t) = E(t)$

Only partially satisfactory

Determining the complex susceptibility $\hat{\chi}(\omega)$

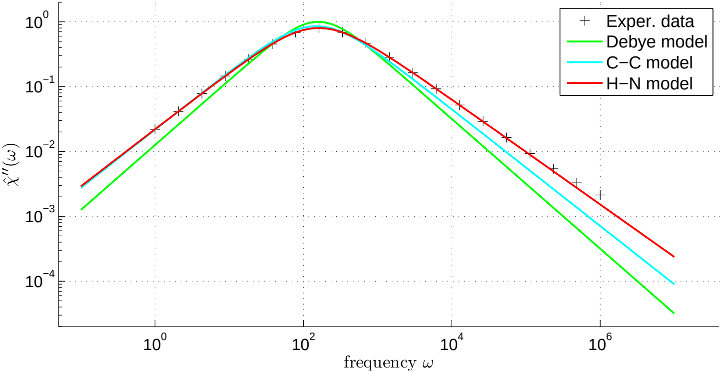


The Havriliak-Negami model: $$\hat{\chi}(\omega) = \frac{1}{\big(1 + (\mathrm{i}\omega\tau)^{\alpha}\big)^{\gamma}} \qquad 0 < \alpha, \alpha\gamma \leq 1$$

Better matching thanks to three parameters α, γ and τ

S. Havriliak and S. Negami "A complex plane representation of dielectric and mechanical relaxation processes in some polymers". In: *Polymer* (1967)

Determining the complex susceptibility $\hat{\chi}(\omega)$



The Havriliak-Negami model: $\hat{\chi}(\omega) = \dfrac{1}{\left(1+(\mathrm{i}\omega\tau)^{\alpha}\right)^{\gamma}}$ $\quad 0 < \alpha, \alpha\gamma < 1$

Fractional pseudo-differential equation: $\left(1 + \tau^{\alpha}\dfrac{d^{\alpha}}{dt^{\alpha}}\right)^{\gamma} P(t) = E(t)$?

Other models for complex susceptibility $\hat{\chi}(\omega)$

- Modified Havriliak-Negami or JWS (Jurlewicz, Weron and Stanislavsky)

$$\hat{\chi}_{\text{JWS}}(\mathrm{i}\omega) = 1 - \frac{1}{\Big(1 + \big(\mathrm{i}\tau_\star\omega\big)^{-\alpha}\Big)^{\gamma}} = 1 - (\mathrm{i}\tau_\star\omega)^{\alpha\gamma}\chi_{\text{HN}}(\mathrm{i}\omega)$$

- EW: Excess wing (Hilfer, Nigmatullin and others)

$$\hat{\chi}_{\text{EW}}(\mathrm{i}\omega) = \frac{1 + (\tau_2\mathrm{i}\omega)^{\alpha}}{1 + (\tau_2\mathrm{i}\omega)^{\alpha} + \tau_1\mathrm{i}\omega}.$$

- Multichannel excess wing (Hilfer)

$$\hat{\xi}(s) = \frac{1}{1 + \left[\displaystyle\sum_{k=1}^{n}(\mathrm{i}\omega\tau_k)^{-\alpha_k}\right]^{-1}}$$

This talk focuses on the Havriliak-Negami model

Garrappa R., Mainardi F. and Maione G., "Models of dielectric relaxation based on completely monotone functions". In: *Frac. Calc. Appl. Anal.* 19(5) (2016)

Dealing with the Havriliak-Negami model

$$\hat{\mathbf{P}}(\omega) = \frac{1}{((\mathrm{i}\omega\tau)^{\alpha} + 1)^{\gamma}} \hat{\mathbf{E}}(\omega)$$

Few contributions on simulation of this constitutive law:

- C.S.Antonopoulos, N.V.Kantartzis, I.T.Rekanos "FDTD Method for Wave Propagation in Havriliak-Negami Media Based on Fractional Derivative Approximation". In: *IEEE Trans Magn.* 53(6) (2017)
- P.Bia et al. "A novel FDTD formulation based on fractional derivatives for dispersive Havriliak–Negami media". In: *Signal Processing*, 107 (2015) 312–318
- M.F.Causley, P.G.Petropoulos, "On the Time-Domain Response of Havriliak-Negami Dielectrics". In: *IEEE Trans. Antennas Propag.*, 61(6) (2013) 3182–3189
- M.F.Causley, P.G.Petropoulos, and S. Jiang "Incorporating the Havriliak-Negami dielectric model in the FD-TD method". In: *J. Comput. Phys.*, 230 (2011), 3884–3899.

Main problems:

- Define time-domain operator for HN
- Discretize the operator for simulations

Operators in the time domain

$$\hat{\mathbf{P}}(\omega) = \frac{1}{((\mathrm{i}\omega\tau)^{\alpha}+1)^{\gamma}}\hat{\mathbf{E}}(\omega) \qquad \Longleftrightarrow \qquad \left(\tau^{\alpha}\,{}_0D_t^{\alpha}+1\right)^{\gamma}\mathbf{P}(t) = \mathbf{E}(t) \quad ???$$

How to define the fractional pseudo-differential operator $\left(\tau^{\alpha}\,{}_0D_t^{\alpha}+1\right)^{\gamma}$?

Operators in the time domain

$$\hat{\mathbf{P}}(\omega) = \frac{1}{((\mathrm{i}\omega\tau)^{\alpha}+1)^{\gamma}}\hat{\mathbf{E}}(\omega) \qquad \Longleftrightarrow \qquad \left(\tau^{\alpha}{}_0D_t^{\alpha}+1\right)^{\gamma}\mathbf{P}(t) = \mathbf{E}(t) \quad ???$$

How to define the fractional pseudo-differential operator $\left(\tau^{\alpha}{}_0D_t^{\alpha}+1\right)^{\gamma}$?

Combination of fractional operators

$$\left(\tau^{\alpha}{}_0D_t^{\alpha}+1\right)^{\gamma} = \exp\left(-\frac{t}{\alpha\tau^{\alpha}}{}_0D_t^{1-\alpha}\right)\cdot\tau^{\alpha\gamma}{}_0D_t^{\alpha\gamma}\cdot\exp\left(\frac{t}{\alpha\tau^{\alpha}}{}_0D_t^{1-\alpha}\right)$$

Useful for theoretical investigations

R.R.Nigmatullin and Y.E.Ryabov "Cole–Davidson dielectric relaxation as a self–similar relaxation process". In: *Physics of the Solid State* 39.1 (1997)

Operators in the time domain

$$\hat{\mathbf{P}}(\omega) = \frac{1}{((\mathrm{i}\omega\tau)^{\alpha} + 1)^{\gamma}} \hat{\mathbf{E}}(\omega) \qquad \Longleftrightarrow \qquad \left(\tau^{\alpha}{}_0D_t^{\alpha} + 1\right)^{\gamma} \mathbf{P}(t) = \mathbf{E}(t) \quad ???$$

How to define the fractional pseudo-differential operator $\left(\tau^{\alpha}{}_0D_t^{\alpha} + 1\right)^{\gamma}$?

Expansion in infinite series

$$\left(\tau^{\alpha}{}_0D_t^{\alpha} + 1\right)^{\gamma} = \sum_{k=0}^{\infty} \binom{\gamma}{k} \tau^{\alpha(\gamma-k)}{}_0D_t^{\alpha(\gamma-k)}$$

No satisfactory for error control

V.Novikov et al. "Anomalous relaxation in dielectrics. Equations with fractional derivatives". In: *Mater. Sci. Poland* 23.4 (2005)

P.Bia et al. "A novel FDTD formulation based on fractional derivatives for dispersive Havriliak–Negami media". In: *Signal Processing*, 107 (2015) 312–318

Operators in the time domain

$$\hat{\mathbf{P}}(\omega) = \frac{1}{((\mathrm{i}\omega\tau)^{\alpha}+1)^{\gamma}}\hat{\mathbf{E}}(\omega) \qquad \Longleftrightarrow \qquad \left(\tau^{\alpha}{}_0D_t^{\alpha}+1\right)^{\gamma}\mathbf{P}(t) = \mathbf{E}(t) \quad ???$$

How to define the fractional pseudo-differential operator $\left(\tau^{\alpha}{}_0D_t^{\alpha}+1\right)^{\gamma}$?

Prabhakar derivative

$$\left(\tau^{\alpha}{}_0D_t^{\alpha}+1\right)^{\gamma}\mathbf{P}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \left(\frac{u}{\tau}\right)^{-\alpha\gamma} E_{\alpha,1-\alpha\gamma}^{-\gamma}\left(-\left(\frac{u}{\tau}\right)^{\alpha}\right)\mathbf{P}(t-u)\,\mathrm{d}u$$

Prabhakar function: $E_{\alpha,\beta}^{\gamma}(z) = \dfrac{1}{\Gamma(\gamma)}\displaystyle\sum_{k=0}^{\infty}\frac{\Gamma(\gamma+k)z^k}{k!\Gamma(\alpha k+\beta)}$

R.Garra, R.Gorenflo, F.Polito and Z.Tomovski "Hilfer-Prabhakar derivatives and some applications". In: *Appl. Math. Comput.* 242 (2014)

Operators in the time domain

$$\hat{\mathbf{P}}(\omega) = \frac{1}{((\mathrm{i}\omega\tau)^{\alpha} + 1)^{\gamma}} \hat{\mathbf{E}}(\omega) \qquad \Longleftrightarrow \qquad \left(\tau^{\alpha} {}_0D_t^{\alpha} + 1\right)^{\gamma} \mathbf{P}(t) = \mathbf{E}(t) \quad ???$$

How to define the fractional pseudo-differential operator $\left(\tau^{\alpha} {}_0D_t^{\alpha} + 1\right)^{\gamma}$?

Prabhakar derivative of Caputo type

$$\left(\tau^{\alpha} {}_0D_t^{\alpha} + 1\right)^{\gamma} \mathbf{P}(t) = \frac{\mathrm{d}}{\mathrm{d}t} \int_0^t \left(\frac{u}{\tau}\right)^{-\alpha\gamma} E_{\alpha,1-\alpha\gamma}^{-\gamma}\left(-\left(\frac{u}{\tau}\right)^{\alpha}\right) \mathbf{P}(t-u)\,\mathrm{d}u \quad \text{RL}$$

$${}^{C}\left(\tau^{\alpha} {}_0D_t^{\alpha} + 1\right)^{\gamma} \mathbf{P}(t) = \int_0^t \left(\frac{u}{\tau}\right)^{-\alpha\gamma} E_{\alpha,1-\alpha\gamma}^{-\gamma}\left(-\left(\frac{u}{\tau}\right)^{\alpha}\right) \mathbf{P}'(t-u)\,\mathrm{d}u \quad \text{Caputo}$$

$${}^{C}\left(\tau^{\alpha} {}_0D_t^{\alpha} + 1\right)^{\gamma} \mathbf{P}(t) = \left(\tau^{\alpha} {}_0D_t^{\alpha} + 1\right)^{\gamma} \left(\mathbf{P}(t) - \mathbf{P}(0^+)\right)$$

Operators in the time domain

$$\hat{\mathbf{P}}(\omega) = \frac{1}{\left((\mathrm{i}\omega\tau)^{\alpha}+1\right)^{\gamma}}\hat{\mathbf{E}}(\omega) \qquad \Longleftrightarrow \qquad \left(\tau^{\alpha}{}_0D_t^{\alpha}+1\right)^{\gamma}\mathbf{P}(t)=\mathbf{E}(t) \quad ???$$

How to define the fractional pseudo-differential operator $\left(\tau^{\alpha}{}_0D_t^{\alpha}+1\right)^{\gamma}$?

Fractional differences of Grünwald–Letnikov

$$\left(\tau^{\alpha}{}_0D_t^{\alpha}+1\right)^{\gamma}\mathbf{P}(t)=\lim_{h\to 0}\frac{1}{h^{\alpha\gamma}}\sum_{k=0}^{\infty}\Omega_k\mathbf{P}(t-kh)$$

$$\bar{\Omega}_0=1, \quad \bar{\Omega}_k=\frac{\tau^{\alpha}}{\tau^{\alpha}+h^{\alpha}}\sum_{j=1}^{k}\left(\frac{(1+\gamma)j}{k}-1\right)\omega_j^{(\alpha)}\bar{\Omega}_{k-j}, \quad \Omega_k=\left(\tau^{\alpha}+h^{\alpha}\right)^{\gamma}\bar{\Omega}_k$$

R.Garrappa "On Grünwald–Letnikov operators for fractional relaxation in Havriliak-Negami models". In: *Commun. Nonlinear. Sci. Numer. Simul.* 38 (2016)

Operators in the time domain

$$\hat{\mathbf{P}}(\omega) = \frac{1}{((\mathrm{i}\omega\tau)^{\alpha} + 1)^{\gamma}} \hat{\mathbf{E}}(\omega) \qquad \Longleftrightarrow \qquad \left(\tau^{\alpha}{}_0D_t^{\alpha} + 1\right)^{\gamma} \mathbf{P}(t) = \mathbf{E}(t) \quad ???$$

How to define the fractional pseudo-differential operator $\left(\tau^{\alpha}{}_0D_t^{\alpha} + 1\right)^{\gamma}$?

Fractional differences of Grünwald–Letnikov

$$\left(\tau^{\alpha}{}_0D_t^{\alpha} + 1\right)^{\gamma} \mathbf{P}(t_n) \approx \frac{1}{h^{\alpha\gamma}} \sum_{k=0}^{n} \Omega_k \mathbf{P}(t_{n-k}) + \mathcal{O}(h)$$

$${}^{\mathrm{C}}\left(\tau^{\alpha}{}_0D_t^{\alpha} + 1\right)^{\gamma} \mathbf{P}(t_n) \approx \frac{1}{h^{\alpha\gamma}} \sum_{k=0}^{n} \Omega_k \left(\mathbf{P}(t_{n-k}) - \mathbf{P}(t_0)\right) + \mathcal{O}(h)$$

Approximation of first order only !

Integral operator

$$\hat{\mathbf{P}}(\omega) = \frac{1}{\left((\mathrm{i}\omega\tau)^{\alpha} + 1\right)^{\gamma}} \hat{\mathbf{E}}(\omega) \qquad \Longleftrightarrow \qquad \mathbf{P}(t) = \left(\tau^{\alpha} {}_0J_t^{\alpha} + 1\right)^{\gamma} \mathbf{E}(t)$$

Prabhakar integral $\left(\tau^{\alpha} {}_0J_t^{\alpha} + 1\right)^{\gamma}$

$$\mathbf{P}(t) = \frac{1}{\tau^{\alpha\gamma}} \int_0^t (t-u)^{\alpha\gamma-1} E_{\alpha,\alpha\gamma}^{\gamma} \left(-\left(\frac{t-u}{\tau}\right)^{\alpha} \right) \mathbf{E}(u) \, \mathrm{d}u,$$

Integral operator

$$\hat{\mathbf{P}}(\omega) = \frac{1}{\big((\mathrm{i}\omega\tau)^{\alpha}+1\big)^{\gamma}}\hat{\mathbf{E}}(\omega) \qquad \Longleftrightarrow \qquad \mathbf{P}(t) = \big(\tau^{\alpha}\,{}_0J_t^{\alpha}+1\big)^{\gamma}\mathbf{E}(t)$$

Prabhakar integral $\big(\tau^{\alpha}\,{}_0J_t^{\alpha}+1\big)^{\gamma}$

$$\mathbf{P}(t) = \frac{1}{\tau^{\alpha\gamma}}\int_0^t (t-u)^{\alpha\gamma-1}E_{\alpha,\alpha\gamma}^{\gamma}\left(-\left(\frac{t-u}{\tau}\right)^{\alpha}\right)\mathbf{E}(u)\,\mathrm{d}u,$$

Non-local operator

Weakly singular integral

Series of RL integrals [1] $\big(\tau^{\alpha}\,{}_0J_t^{\alpha}+1\big)^{\gamma} = \displaystyle\sum_{k=0}^{\infty}(-1)^k\binom{\gamma}{k}\frac{1}{\tau^{\alpha(k+\gamma)}}J_0^{\alpha(k+\gamma)}$

[1] Giusti A., "A comment on some new definitions of fractional derivative". *Nonlinear Dyn.* (2018)

Integral operator

$$\hat{\mathbf{P}}(\omega) = \frac{1}{((\mathrm{i}\omega\tau)^{\alpha}+1)^{\gamma}}\hat{\mathbf{E}}(\omega) \qquad \Longleftrightarrow \qquad \mathbf{P}(t) = \left(\tau^{\alpha}{}_{0}J_t^{\alpha}+1\right)^{\gamma}\mathbf{E}(t)$$

Prabhakar integral $\left(\tau^{\alpha}{}_{0}J_t^{\alpha}+1\right)^{\gamma}$

$$\mathbf{P}(t) = \frac{1}{\tau^{\alpha\gamma}}\int_0^t (t-u)^{\alpha\gamma-1}E_{\alpha,\alpha\gamma}^{\gamma}\left(-\left(\frac{t-u}{\tau}\right)^{\alpha}\right)\mathbf{E}(u)\,\mathrm{d}u,$$

Preferable in numerical simulation

- Numerical integration is easier than numerical differentiation
- Approximation by quadrature rules
- What kind of quadrature rule ?

Discretization of Maxwell's equations

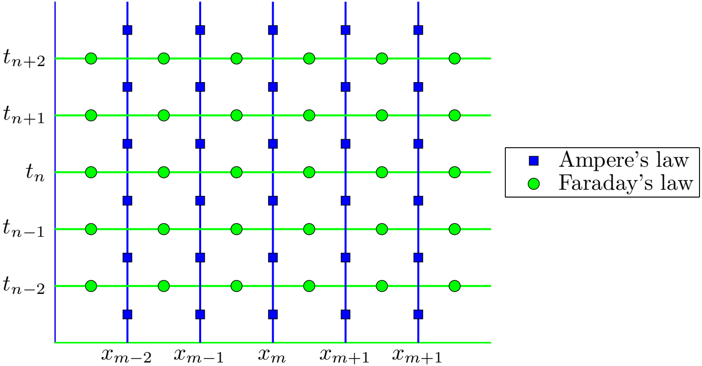
$$
\begin{cases}
\nabla \times \mathbf{H} = \epsilon_0 \dfrac{\partial}{\partial t} \mathbf{E} + \dfrac{\partial}{\partial t} \mathbf{P} & \text{Ampere's law} \\
\nabla \times \mathbf{E} = -\mu_0 \dfrac{\partial \mathbf{H}}{\partial t} & \text{Faraday's law}
\end{cases}
$$

$$
\nabla \times \mathbf{F} = \left(\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z} \right) \mathbf{i} + \left(\frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x} \right) \mathbf{j} + \left(\frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} \right) \mathbf{k}
$$

The Finite Differences Time Domain (FDTD) method:

1. Introduced by K. Yee in 1966
2. Approximation based on centred finite difference operators
3. Use of staggered grids in space and time

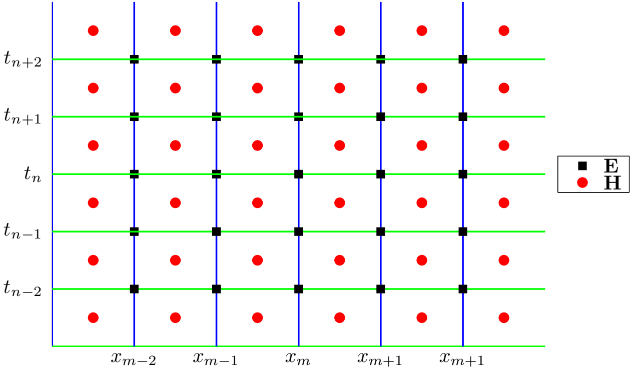
Discretization of Maxwell's equations - FDTD



$$\nabla \times \mathbf{H}_{n+\frac{1}{2},m} = \frac{\mathbf{H}_{m+\frac{1}{2},n+\frac{1}{2}} - \mathbf{H}_{m-\frac{1}{2},n+\frac{1}{2}}}{\Delta_x} + \mathcal{O}\left(\Delta_x^2\right)$$

$$\nabla \times \mathbf{E}_{m+\frac{1}{2},n} = \frac{\mathbf{E}_{m+1,n} - \mathbf{H}_{m-1,n}}{\Delta_x} + \mathcal{O}\left(\Delta_x^2\right)$$

Discretization of Maxwell's equations - FDTD



$$\nabla \times \mathbf{H}_{n+\frac{1}{2},m} = \frac{\mathbf{H}_{m+\frac{1}{2},n+\frac{1}{2}} - \mathbf{H}_{m-\frac{1}{2},n+\frac{1}{2}}}{\Delta_x} + \mathcal{O}\left(\Delta_x^2\right)$$

$$\nabla \times \mathbf{E}_{m+\frac{1}{2},n} = \frac{\mathbf{E}_{m+1,n} - \mathbf{H}_{m-1,n}}{\Delta_x} + \mathcal{O}\left(\Delta_x^2\right)$$

Discretization of the constitutive law

$$\begin{cases} \nabla \times \mathbf{H} = \epsilon_0 \dfrac{\partial}{\partial t}\mathbf{E} + \dfrac{\partial}{\partial t}\mathbf{P} & \text{Ampere's law} \\ \nabla \times \mathbf{E} = -\mu_0 \dfrac{\partial \mathbf{H}}{\partial t} & \text{Faraday's law} \\ \mathbf{P} = \left(\tau^{\alpha}\, {}_0J_t^{\alpha} + 1\right)^{\gamma}\mathbf{E} & \text{Constitutive law} \end{cases}$$

- It is necessary a second-order approximation
- Use of the values of **E** just on grid points (t_n, x_m)

Discretization of the constitutive law

$$\begin{cases} \nabla \times \mathbf{H} = \epsilon_0 \dfrac{\partial}{\partial t}\mathbf{E} + \dfrac{\partial}{\partial t}\mathbf{P} & \text{Ampere's law} \\ \nabla \times \mathbf{E} = -\mu_0 \dfrac{\partial \mathbf{H}}{\partial t} & \text{Faraday's law} \\ \mathbf{P} = \left(\tau^{\alpha}{}_0 J_t^{\alpha} + 1\right)^{\gamma}\mathbf{E} & \text{Constitutive law} \end{cases}$$

- It is necessary a second-order approximation
- Use of the values of **E** just on grid points (t_n, x_m)

Convolution quadratures by Lubich [Lubich, 1988]

- Based on the LT $\hat{\chi}(s) = \dfrac{1}{\left(\tau^{\alpha} s^{\alpha} + 1\right)^{\gamma}}$ (i.e. the complex susceptibility)
- Extension of classical linear multistep methods (LMM) for ODEs
- Preservation of convergence and stability of the LMM

Convolution quadrature rules

$$I(t) = \int_0^t f(t-u)g(u)\mathrm{d}u$$

- Generalizes LMM for ODEs

$$\sum_{j=0}^{k} \rho_j y_{n-j} = h \sum_{j=0}^{k} \sigma_j f(t_{n-j}, y_{n-j}), \quad n \geq k.$$

- Based on the generating function of the LMM

$$\rho(\xi) = \sum_{j=0}^{k} \rho_j \xi^{k-j} \qquad \sigma(\xi) = \sum_{j=0}^{k} \sigma_j \xi^{k-j} \qquad \delta(\xi) = \frac{\rho(1/\xi)}{\sigma(1/\xi)}$$

$$I(t_n) = \underbrace{h^{\mu} \sum_{j=0}^{\nu} w_{n,j} g(t_j)}_{\text{starting term}} + \underbrace{h^{\mu} \sum_{j=0}^{n} \omega_{n-j} g(t_j)}_{\text{convolution term}}$$

Lubich C. "Convolution quadrature and discretized operational calculus (I and II)", In: *Numer. Math.* 52, 129–145 and 413–425 (1988).

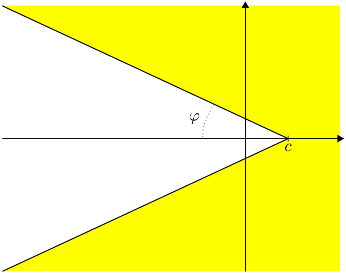
Convolution quadrature rules

$$I(t) = \int_0^t f(t-u)g(u)\mathrm{d}u \quad \Longrightarrow \quad I(t_n) = \underbrace{h^\mu \sum_{j=0}^{\nu} w_{n,j} g(t_j)}_{\text{starting term}} + \underbrace{h^\mu \sum_{j=0}^{n} \omega_{n-j} g(t_j)}_{\text{convolution term}}$$

- Use of LT $F(s)$ of $f(t)$
- $F(s)$ analytic in a sector

  $$\Sigma_{\varphi,c} = \{ s \in \mathbb{C} \,:\, |\arg(s-c)| < \pi - \varphi \}$$

- $F(s) \le M|s|^{-\mu} \quad \mu > 0 \quad M < \infty$
- Weights $F\left(\frac{\delta(\xi)}{h}\right) = \sum_{n=0}^{\infty} \omega_n \xi^n$



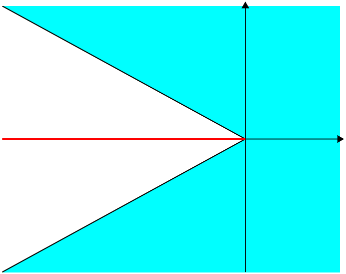
Lubich C. "Convolution quadrature and discretized operational calculus (I and II)", In: *Numer. Math.* 52, 129–145 and 413–425 (1988).

Convolution quadrature for Havriliak-Negami

$$I(t) = \int_0^t f(t-u)g(u)\mathrm{d}u \quad \Longrightarrow \quad I(t_n) = \underbrace{h^{\mu}\sum_{j=0}^{\nu} w_{n,j} g(t_j)}_{\text{starting term}} + \underbrace{h^{\mu}\sum_{j=0}^{n} \omega_{n-j} g(t_j)}_{\text{convolution term}}$$

- $f(t) = t^{\alpha\gamma-1}E^{\gamma}_{\alpha,\alpha\gamma}\left(-t^{\alpha}/\tau^{\alpha}\right)$
- $F(s) = \hat{\chi}(s) = \dfrac{1}{(\tau^{\alpha}s^{\alpha}+1)^{\gamma}}$

  $F(s)$ analytic outside $(-\infty, 0]$
- $F(s) \le M|s|^{-\alpha\gamma} \quad \mu = \alpha\gamma$
- Weights $\hat{\chi}\left(\dfrac{\delta(\xi)}{h}\right) = \displaystyle\sum_{n=0}^{\infty} \omega_n \xi^n$



Convolution quadrature for Havriliak-Negami

$$\mathbf{P} = \left(\tau^{\alpha}{}_{0}J_{t}^{\alpha} + 1\right)^{\gamma}\mathbf{E}$$

$$P(x,t_n) = \underbrace{h^{\alpha\gamma}\sum_{j=0}^{\nu} w_{n,j}E(x,t_j)}_{\text{starting term}} + \underbrace{h^{\alpha\gamma}\sum_{j=0}^{n} \omega_n^{\text{HN}} E(x,t_j)}_{\text{convolution term}}$$

Trapezoidal rule $\quad y_{n+1} - y_n = \dfrac{h}{2}\big(f(t_n,y_n) + f(t_{n+1},y_{n+1})\big)$

Generating function $\quad \delta(\xi) = \dfrac{2(1-\xi)}{1+\xi}$

Convolution weights $\quad h^{\alpha\gamma}\displaystyle\sum_{n=0}^{\infty} \omega_n^{\text{HN}}\xi^n = \hat{\chi}\left(\frac{2(1-\xi)}{h(1+\xi)}\right)$

Evaluation of convolution weights

$$h^{\alpha\gamma} \sum_{n=0}^{\infty} \omega_n^{\mathsf{HN}} \xi^n = \frac{h^{\alpha\gamma}}{2^\alpha \tau^\alpha} \left(\bar{h}^\alpha + \frac{(1-\xi)^\alpha}{(1+\xi)^\alpha} \right)^{-\gamma}, \quad \bar{h} = \frac{h}{2\tau}$$

1) Recursion, FFT and power of FPS

2) Numerical integration of Cauchy integral

Evaluation of convolution weights

$$h^{\alpha\gamma} \sum_{n=0}^{\infty} \omega_n^{\mathrm{HN}} \xi^n = \frac{h^{\alpha\gamma}}{2^\alpha \tau^\alpha} \left(\bar{h}^\alpha + \frac{(1-\xi)^\alpha}{(1+\xi)^\alpha} \right)^{-\gamma}, \quad \bar{h} = \frac{h}{2\tau}$$

1) Recursion, FFT and power of FPS

$$(1-\xi)^\alpha = \sum_{n=0}^{\infty} \hat{\omega}_n \xi^n \quad \hat{\omega}_0 = 1 \quad \hat{\omega}_n = \left(1 - \frac{\alpha+1}{n}\right) \hat{\omega}_{n-1}$$

$$(1+\xi)^{-\alpha} = \sum_{n=0}^{\infty} \bar{\omega}_n \xi^n \quad \bar{\omega}_0 = 1 \quad \bar{\omega}_n = \left(\frac{1-\alpha}{n} - 1\right) \bar{\omega}_{n-1}$$

$$\frac{(1-\xi)^\alpha}{(1+\xi)^\alpha} = \sum_{n=0}^{\infty} \tilde{\omega}_n \xi^n \quad \text{FFT of weights of } (1-\xi)^\alpha \text{ and } (1+\xi)^{-\alpha}$$

$$\left(\bar{h}^\alpha + \sum_{n=0}^{\infty} \tilde{\omega}_n \xi^n \right)^{-\gamma} = \frac{1}{(1+\bar{h}^\alpha)^\gamma} \left(1 + \sum_{n=1}^{\infty} \frac{\tilde{\omega}_n}{1+\bar{h}^\alpha} \tilde{\omega}_n \xi^n \right)^{-\gamma} \text{ unitary FPS}$$

Evaluation of convolution weights

$$h^{\alpha\gamma}\sum_{n=0}^{\infty}\omega_n^{\mathrm{HN}}\xi^n = \frac{h^{\alpha\gamma}}{2^\alpha\tau^\alpha}\left(\bar{h}^\alpha + \frac{(1-\xi)^\alpha}{(1+\xi)^\alpha}\right)^{-\gamma}, \quad \bar{h} = \frac{h}{2\tau}$$

1) Recursion, FFT and power of FPS

Miller's Formula: power $\beta \in \mathbb{C}$ of unitary Formal Power Series

$$\left(1 + a_1\xi + a_2\xi^2 + a_3\xi^3 + \dots\right)^\beta = v_0^{(\beta)} + v_1^{(\beta)}\xi + v_2^{(\beta)}\xi^2 + v_3^{(\beta)}\xi^3 + \dots$$

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

Direct evaluation $\omega_0^{\mathrm{HN}} = 1 \quad \omega_n^{\mathrm{HN}} = \sum_{j=1}^{n}\left(\frac{(1-\gamma)j}{n} - 1\right) \underset{\frac{(1-\xi)^\alpha}{(1+\xi)^\alpha}}{\underset{\downarrow}{\tilde{\omega}_j}}\, \omega_{n-j}^{\mathrm{HN}}$

Evaluation of convolution weights

$$h^{\alpha\gamma} \sum_{n=0}^{\infty} \omega_n^{\mathrm{HN}} \xi^n = \frac{h^{\alpha\gamma}}{2^\alpha \tau^\alpha} \left(\bar{h}^\alpha + \frac{(1-\xi)^\alpha}{(1+\xi)^\alpha} \right)^{-\gamma}, \quad \bar{h} = \frac{h}{2\tau}$$

1) Recursion, FFT and power of FPS

- Weights evaluated in an exact way
- Expensive computation $\mathcal{O}(N^2)$
- Instability due to long recurrences

Evaluation of convolution weights

$$h^{\alpha\gamma} \sum_{n=0}^{\infty} \omega_n^{\mathrm{HN}} \xi^n = \frac{h^{\alpha\gamma}}{2^\alpha \tau^\alpha} \left(\bar{h}^\alpha + \frac{(1-\xi)^\alpha}{(1+\xi)^\alpha} \right)^{-\gamma}, \quad \bar{h} = \frac{h}{2\tau}$$

2) Numerical integration of Cauchy integral

$$\omega_n^{\mathrm{HN}} = \frac{1}{n!} \, \frac{\mathrm{d}^n}{\mathrm{d}\xi^n} G(\xi) \Big|_{\xi=0} \qquad G(\xi) = \left(\bar{h}^\alpha + \frac{(1-\xi)^\alpha}{(1+\xi)^\alpha} \right)^{-\gamma}$$

Representation in terms of Cauchy integrals

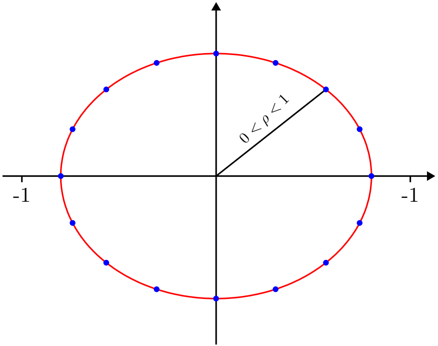
$$\omega_n^{\mathrm{HN}} = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} \xi^{-n-1} G(\xi) \mathrm{d}\xi,$$

Approximation by quadrature rule

Evaluation of convolution weights

$$h^{\alpha\gamma} \sum_{n=0}^{\infty} \omega_n^{\mathsf{HN}} \xi^n = \frac{h^{\alpha\gamma}}{2^\alpha \tau^\alpha} \left(\bar{h}^\alpha + \frac{(1-\xi)^\alpha}{(1+\xi)^\alpha} \right)^{-\gamma}, \quad \bar{h} = \frac{h}{2\tau}$$

2) Numerical integration of Cauchy integral



Contour $|\xi| = \rho \quad 0 < \rho < 1$

Equispaced quadrature nodes

$$\xi_\ell = \rho \mathrm{e}^{2\pi \mathrm{i} \ell / L}, \quad \ell = 0, 1, \ldots, L-1$$

Trapezoidal rule

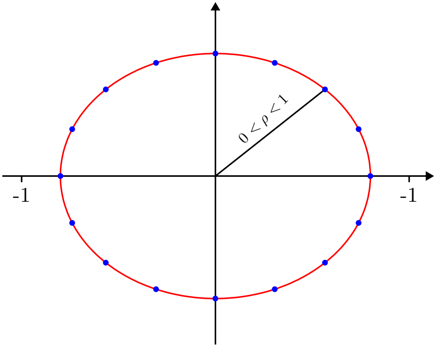
$$\omega_{n,L}^{\mathsf{HN}} = \frac{\rho^{-n}}{L} \sum_{l=0}^{L-1} G(\xi_l) \mathrm{e}^{-2\pi \mathrm{i} n \ell / L}$$

Fast computation by FFT $\mathcal{O}(L \log L)$

Evaluation of convolution weights

$$h^{\alpha\gamma} \sum_{n=0}^{\infty} \omega_n^{\text{HN}} \xi^n = \frac{h^{\alpha\gamma}}{2^\alpha \tau^\alpha} \left(\bar{h}^\alpha + \frac{(1-\xi)^\alpha}{(1+\xi)^\alpha} \right)^{-\gamma}, \quad \bar{h} = \frac{h}{2\tau}$$

2) Numerical integration of Cauchy integral



Choice of ρ and L: error analysis

Discretization error $0 < \rho < r < 1$

$$\left| \omega_n^{\text{HN}} - \omega_{n,L}^{\text{HN}} \right| \leq \rho^{-n} C_r \frac{(r/\rho)^n}{(r/\rho)^L - 1}$$ [a]

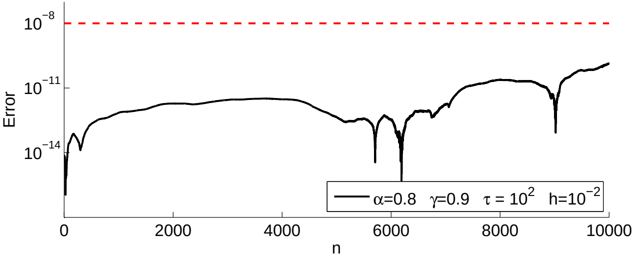
Round-off error

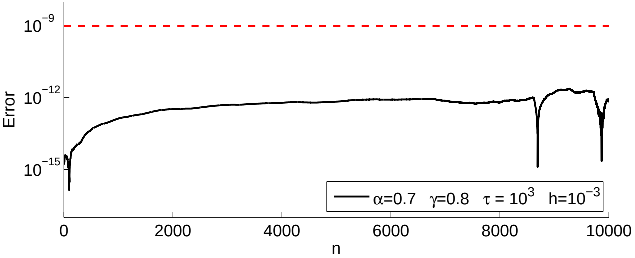
$$\left| \omega_{n,L}^{\text{HN}} - \hat{\omega}_{n,L}^{\text{HN}} \right| \leq \rho^{-n} C_\rho \epsilon$$

Balancing of the two errors: target accuracy $\varepsilon > \epsilon$

[a] Trefethen & Weideman in [SIAM Review 2014]

Numerical integration of Cauchy integral





Evaluation of the starting term

$$P(x,t_n) = \underbrace{h^{\alpha\gamma}\sum_{j=0}^{\nu} w_{n,j} E(x,t_j)}_{\text{starting term}} + \underbrace{h^{\alpha\gamma}\sum_{j=0}^{n} \omega_n^{\mathrm{HN}} E(x,t_j)}_{\text{convolution term}}$$

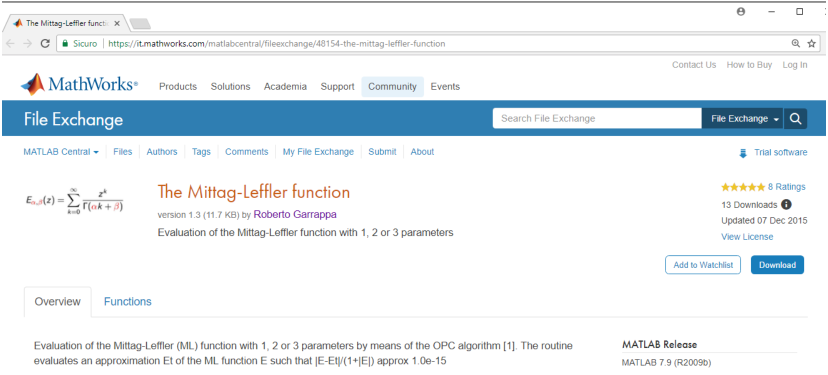
- Handling the singularity at the origin
- $w_{n,j}$ obtained by imposing the rule exact for $\{1, t^{\alpha\gamma}, t\}$ when $\alpha\gamma > \frac{1}{2}$
- Solution of small systems of algebraic equations

$$\begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 2^{\alpha\gamma} \\ 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} w_{n,0} \\ w_{n,1} \\ w_{n,2} \end{pmatrix} = \begin{pmatrix} n^{\alpha\gamma} E^{\gamma}_{\alpha,\alpha\gamma+1}(-(t_n/\tau)^{\alpha}) - \displaystyle\sum_{j=0}^{n} \omega_{n-j}^{\mathrm{HN}} \\ \gamma_\alpha n^{2\alpha\gamma} E^{\gamma}_{\alpha,2\alpha\gamma+1}(-(t_n/\tau)^{\alpha}) - \displaystyle\sum_{j=0}^{n-j} \omega_{n}^{\mathrm{HN}} j^{\alpha\gamma} \\ n^{\alpha\gamma+1} E^{\gamma}_{\alpha,\alpha\gamma+2}(-(t_n/\tau)^{\alpha}) - \displaystyle\sum_{j=0}^{n} \omega_{n-j}^{\mathrm{HN}} j \end{pmatrix}$$

$\gamma_\alpha = \Gamma(\alpha\gamma + 1)$ Simple inversion of the matrix

Evaluation of Prabhakar (three-parameter ML) function

Matlab code available



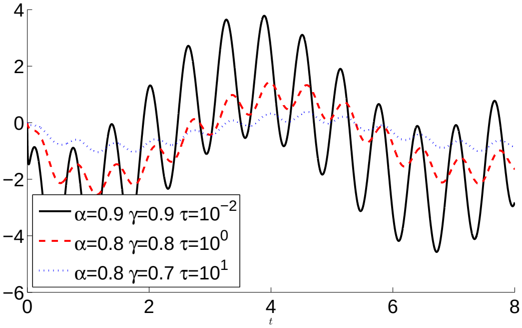
Possible evaluation of $E^{\gamma}_{\alpha,\beta}(z)$ when $|\arg(z)| > \alpha\pi$

Also available code for ML function with matrix arguments

Testing the quadrature rule

$$\mathbf{P}(t) = (\tau^{\alpha}\,{}_0J_t^{\alpha} + 1)^{\gamma}\,\mathbf{E}(t) \qquad \mathbf{E}(t) = \sum_{k=0}^{N} a_k \cos\omega_k t + \sum_{k=0}^{N} b_k \sin\omega_k t$$

	α	γ	τ
Set 1	0.8	0.9	10^{-2}
Set 2	0.8	0.8	10^{0}
Set 3	0.8	0.7	10^{1}



Numerical experiments: errors and EOC

$$\mathbf{P}(t) = \left(\tau^{\alpha}{}_0 J_t^{\alpha} + 1\right)^{\gamma} \mathbf{E}(t) \qquad \mathbf{E}(t) = \sum_{k=0}^{N} a_k \cos \omega_k t + \sum_{k=0}^{N} b_k \sin \omega_k t$$

	$\alpha = 0.9 \quad \gamma = 0.9$, $\tau = 10^{-2}$		$\alpha = 0.8 \quad \gamma = 0.8$, $\tau = 10^{0}$		$\alpha = 0.8 \quad \gamma = 0.7$, $\tau = 10^{1}$	
h	Error	EOC	Error	EOC	Error	EOC
2^{-4}	5.10(−3)		6.21(−3)		2.04(−3)	
2^{-5}	1.18(−3)	2.118	1.52(−3)	2.030	4.83(−4)	2.080
2^{-6}	2.85(−4)	2.043	3.80(−4)	2.000	1.21(−4)	1.999
2^{-7}	7.02(−5)	2.021	9.51(−5)	2.000	3.02(−5)	1.998
2^{-8}	1.73(−5)	2.022	2.35(−5)	2.014	7.50(−6)	2.013
2^{-9}	4.12(−6)	2.071	5.61(−6)	2.069	1.79(−6)	2.068

$$\mathrm{EOC} = \log_2\left(E(h)/E\left(\frac{h}{2}\right)\right)$$

Numerical experiments: errors and EOC

$$\mathbf{P}(t) = (\tau^{\alpha}\,{}_0J_t^{\alpha} + 1)^{\gamma}\,\mathbf{E}(t) \qquad \mathbf{E}(t) = \sum_{k=0}^{N} a_k t^{\alpha k} + \sum_{k=0}^{N} b_k t^{\gamma k} + \sum_{k=0}^{N} c_k t^{k}$$

	$\alpha = 0.9$ $\gamma = 0.9$ $\tau = 10^{-2}$		$\alpha = 0.8$ $\gamma = 0.8$ $\tau = 10^{0}$		$\alpha = 0.8$ $\gamma = 0.7$ $\tau = 10^{1}$	
h	Error	EOC	Error	EOC	Error	EOC
2^{-4}	1.28(−4)		1.26(−3)		1.43(−4)	
2^{-5}	3.11(−5)	2.041	3.15(−4)	1.996	3.68(−5)	1.960
2^{-6}	7.69(−6)	2.015	7.88(−5)	1.999	9.29(−6)	1.987
2^{-7}	1.91(−6)	2.009	1.97(−5)	2.003	2.32(−6)	2.001
2^{-8}	4.72(−7)	2.018	4.86(−6)	2.017	5.73(−7)	2.019
2^{-9}	1.12(−7)	2.071	1.16(−6)	2.070	1.36(−7)	2.075

$$\mathrm{EOC} = \log_2\left(E(h)/E(\tfrac{h}{2})\right)$$

The Excess Wing model

$$\mathbf{P}(t) = \frac{1 + (\tau_2 \mathrm{i}\omega)^\alpha}{1 + (\tau_2 \mathrm{i}\omega)^\alpha + \tau_1 \mathrm{i}\omega} \mathbf{E}(t)$$

1) Linear multiterm fractional differential equation

$$D_t \mathbf{P}(t) + \frac{\tau_2^\alpha}{\tau_1} {}_0D_t^\alpha \mathbf{P}(t) + \frac{1}{\tau_1} \mathbf{P}(t) = \Big(\frac{1}{\tau_1} \mathbf{E}(t) + \frac{\tau_2^\alpha}{\tau_1} {}_0D_t^\alpha \mathbf{E}(t) \Big)$$

1) Convolution quadrature rule

$$h^{1-\alpha} \sum_{n=0}^{\infty} \omega_n^{\mathrm{EW}} \xi^n = h^{1-\alpha} \frac{h^\alpha + 2^\alpha \tau_2^\alpha \dfrac{(1-\xi)^\alpha}{(1+\xi)^\alpha}}{h + 2^\alpha \tau_2^\alpha h^{1-\alpha} \dfrac{(1-\xi)^\alpha}{(1+\xi)^\alpha} + \tau_1 \dfrac{(1-\xi)}{(1+\xi)}}$$

Concluding remarks

- The Havriliak-Negami dielectric model can be described in the time-domain by Prabhakar derivatives and integrals
- Prabhakar derivatives and integrals are non standard fractional-order operators depending on several parameters
- Discretization of Prbhakar operators by means of Lubich's convolution quadratures: direct use of the complex susceptibility
- General approach: extension to other models: Excess Wing, multichannel Excess Wing, and others ...

Further developments

- Improving computational efficiency (memory term)
- Validation with experimental data (Technical University of Bari)
- Releasing robust software for solving Maxwell's systems with anomalous dielectric relaxation

Some references

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