A Survey of Numerical Methods in Fractional Calculus

Fractional Derivatives in Mechanics: State of the Art

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Outline

- The basic problem
- Grünwald-Letnikov methods
- Lubich's fractional linear multistep methods
- Methods based on quadrature theory
- Examples
- Extensions

The Basic Problem

Find a numerical solution for the fractional differential equation

$$D^\alpha y(x) = f(x, y(x))$$

with appropriate initial condition(s), where D^α is

- either the Riemann-Liouville derivative
- or the Caputo derivative.

Fundamental Definitions

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Grünwald-Letnikov Methods

Integer-order derivatives:

$$D^{n} \; y(x) = \lim_{h \to 0} \frac{1}{h^n} \sum_{k=0}^{\infty} \frac{(-1)^k \quad \Gamma(n+1)}{\Gamma(k+1)\Gamma(n-k+1)} y(x-kh) \qquad (n \in \mathbb{N})$$

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Fractional extension (Liouville 1832, Grünwald 1867, Letnikov 1868):

$$D^{\alpha}_{\mathrm{GL}} y(x) = \lim_{h \to 0} \frac{1}{h^{\alpha}} \sum_{k=0}^{\infty} \frac{(-1)^k \quad \Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(\alpha-k+1)} y(x-kh) \qquad (\alpha > 0)$$

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y defined only on $[0, X]$; thus assume $y(x) = 0$ for $x < 0$.

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y defined only on $[0, X]$; thus assume $y(x) = 0$ for $x < 0$.

$\Rightarrow \qquad D^{\alpha}_{\mathrm{GL}} y(x) = D^{\alpha} y(x)$ if y is smooth.

Grünwald-Letnikov Methods

Exact analytical expression:

$$D^{\alpha}_{\mathrm{GL}} y(x) = \lim_{h \to 0} \frac{1}{h^{\alpha}} \sum_{k=0}^{\lfloor x/h \rfloor} \frac{(-1)^k \quad \Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(\alpha-k+1)} y(x - kh)$$

Grünwald-Letnikov Methods

Numerical approximation:

$$ {}_hD^{\alpha}_{\mathrm{GL}}y(x) = \qquad \frac{1}{h^{\alpha}} \sum_{k=0}^{\lfloor x/h \rfloor} \frac{(-1)^k \quad \Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(\alpha-k+1)} y(x-kh) $$

for some $h > 0$.

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Error $= O(h) + O(f(0))$ if f is smooth, i.e.

- slow convergence if $f(0) = 0$,
- completely unfeasible if $f(0) \neq 0$.

Fractional Linear Multistep Methods

Generalization of classical linear multistep methods for first-order ODEs (Lubich 1983–1986)

General form:

$$y_m = \sum_{j=0}^{\lceil \alpha \rceil - 1} y_0^{(j)} \frac{x_m^j}{j!} + h^\alpha \sum_{j=0}^{m} \omega_{m-j} f(x_j, y_j) + h^\alpha \sum_{j=0}^{s} w_{m,j} f(x_j, y_j)$$

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initial condition — convolution weights — starting weights

Computation of convolution weights directly from coefficients of underlying classical linear multistep method

Fractional Linear Multistep Methods

Computation of starting weights: Linear system of equations

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Properties of linear system depend strongly on α:

Fractional Linear Multistep Methods

Computation of starting weights: Linear system of equations

Properties of linear system depend strongly on α:

Assume underlying classical method to be of order p, and let

$$\mathcal{A} = \{\gamma = j + k\alpha : j, k = 0, 1, \ldots, \quad \gamma \leq p - 1\}.$$

Then,

- error of resulting fractional method $= O(h^p)$,
- dimension of linear system $=$ cardinality of $\mathcal{A}$,
- condition of linear system depends on distribution of elements of $\mathcal{A}$.

Fractional Linear Multistep Methods

Further comments on linear system for starting weights:

- needs to be solved at every grid point,
- coefficient matrix always identical,
- coefficient matrix has generalized Vandermonde structure,
- right-hand sides change from one grid point to another,
- accuracy of numerical computation of right-hand side suffers from cancellation of digits.

Fractional Linear Multistep Methods

A well-behaved example:

$p = 4$, $\alpha = 1/3 \quad \Rightarrow \quad \mathcal{A} = \left\{0, \frac{1}{3}, \frac{2}{3}, 1, \frac{4}{3}, \frac{5}{3}, \ldots, 3\right\}.$

- $\mathrm{card}(\mathcal{A}) = 10$,
- highly regular spacing of elements of $\mathcal{A}$ (equispaced)
  $\Rightarrow$ Matrix of coefficients can be transformed to usual Vandermonde form
- mildly ill conditioned system
- special algorithms can be used for sufficiently accurate solution (Björck & Pereyra 1970)

Fractional Linear Multistep Methods

A badly behaved example:

$p = 4$, $\alpha = 0.33$

$$\Rightarrow \quad \mathcal{A} = \{0, 0.33, 0.66, 0.99, 1, 1.32, 1.33, \ldots, 2.97, 2.98, 2.99, 3\}$$

- $\mathrm{card}(\mathcal{A}) = 22$,
- spacing of the elements of $\mathcal{A}$ is highly irregular (in particular, some elements are very close together)
- severely ill conditioned system
- no algorithms for sufficiently accurate solution known

(Diethelm, Ford, Ford & Weilbeer 2006)

Quadrature-Based Methods

Direct approach:

- Use representation $D^\alpha y(x) = \frac{1}{\Gamma(-\alpha)} \int_0^x (x-t)^{-\alpha-1} y(t) \mathrm{d}t$ (finite-part integral) in differential equation
- Discretize integral by classical quadrature techniques
- Example: Replace y in integrand by piecewise linear interpolant with step size h (Diethelm 1997)
  $\Rightarrow$ product trapezoidal method; Error $= O(h^{2-\alpha})$

Similar concept applicable to Caputo derivatives

Quadrature-Based Methods

Indirect approach: (Diethelm, Ford & Freed 1999–2004)

- Rewrite Caputo initial value problem as integral equation

$$y(x) = \sum_{k=0}^{\lceil \alpha \rceil - 1} y_0^{(k)} \frac{x^k}{k!} + J^\alpha [f(\cdot, y(\cdot))](x)$$

- Apply product integration idea to J^α
- Example 1: Product rectangle quadrature

  $\Rightarrow$ fractional Adams-Bashforth method

  - explicit method
  - Error $= O(h)$

Quadrature-Based Methods

Indirect approach (continued):

- Example 2: Product trapezoidal quadrature
  $\Rightarrow$ fractional Adams-Moulton method
  - implicit method
  - Error $= O(h^2)$
- P(EC)^{m}E scheme: Combine Adams-Bashforth predictor and m Adams-Moulton correctors
  $\Rightarrow$ Error = $O(h^p)$, $p = \min\{2, 1 + m\alpha\}$

Similar concept applicable to Riemann-Liouville derivatives

Quadrature-Based Methods

Common properties:

- Coefficients can be computed in accurate and stable way without problems
- Method is applicable for any type of differential equation
- Reasonable rate of convergence can be achieved

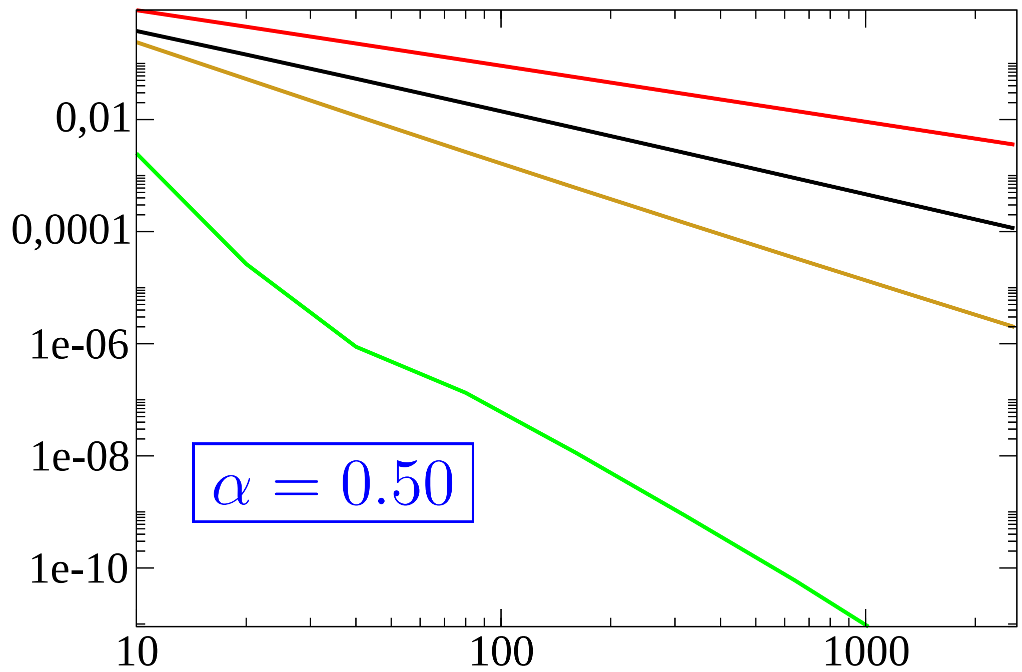
Example 1

$$D_*^\alpha y(x) = x^4 + 1 + \frac{24}{\Gamma(5-\alpha)} x^{4-\alpha} - y(x), \qquad y(0) = 1$$

exact solution on $[0,2]$: $y(x) = x^4 + 1$

$|$Error at $x = 2|$ vs. no. of nodes

- Grünwald-Letnikov
- direct quadrature
- indirect quadrature
- multistep (BDF4)



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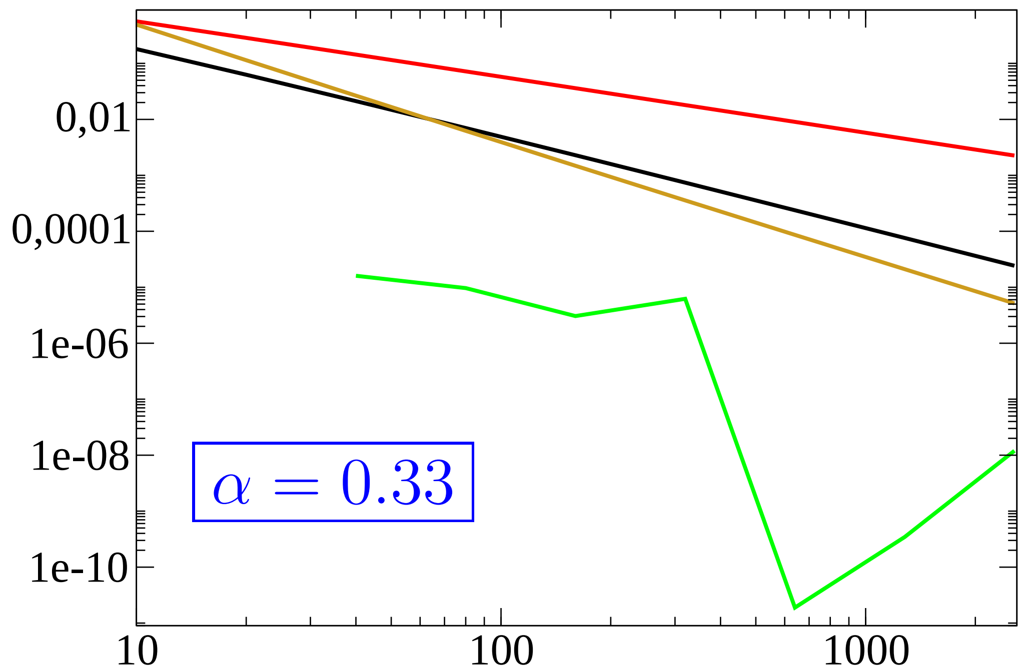

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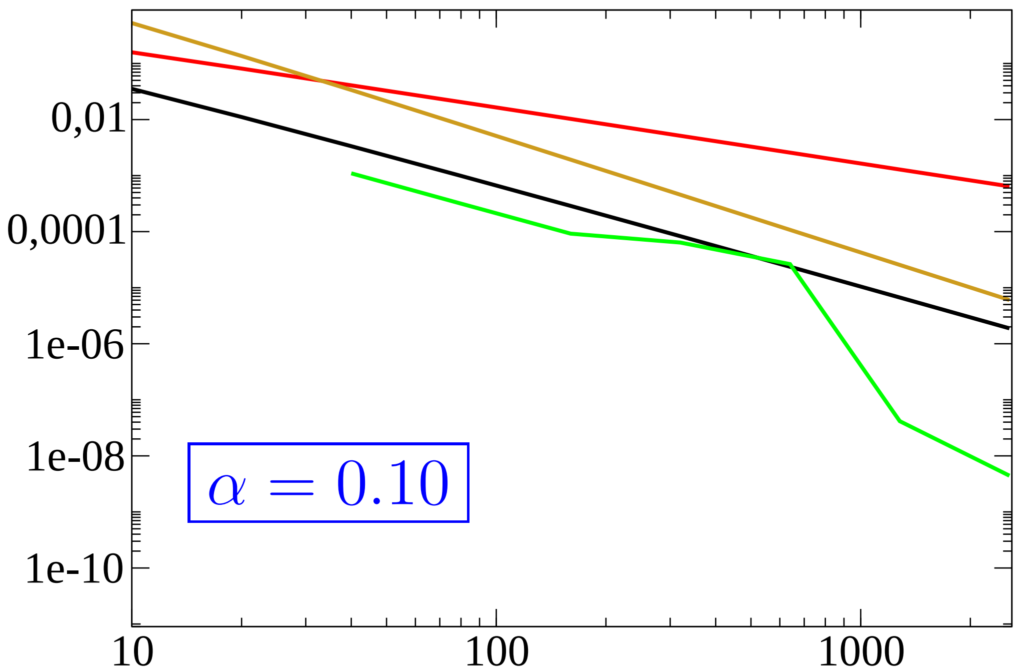

Example 2

$$D_*^\alpha y(x) = \frac{40320}{\Gamma(9-\alpha)} x^{8-\alpha} - 3\frac{\Gamma(5+\alpha/2)}{\Gamma(5-\alpha/2)} x^{4-\alpha/2} + \frac{9}{4}\Gamma(\alpha+1) + \left(1.5x^{\alpha/2} - x^4\right)^3 - y(x)^{3/2}, \qquad y(0) = 0$$

exact solution on $[0,1]$: $y(x) = x^8 - 3x^{4+\alpha/2} + 2.25x^\alpha$

$|$Error at $x=1|$ vs. no. of nodes

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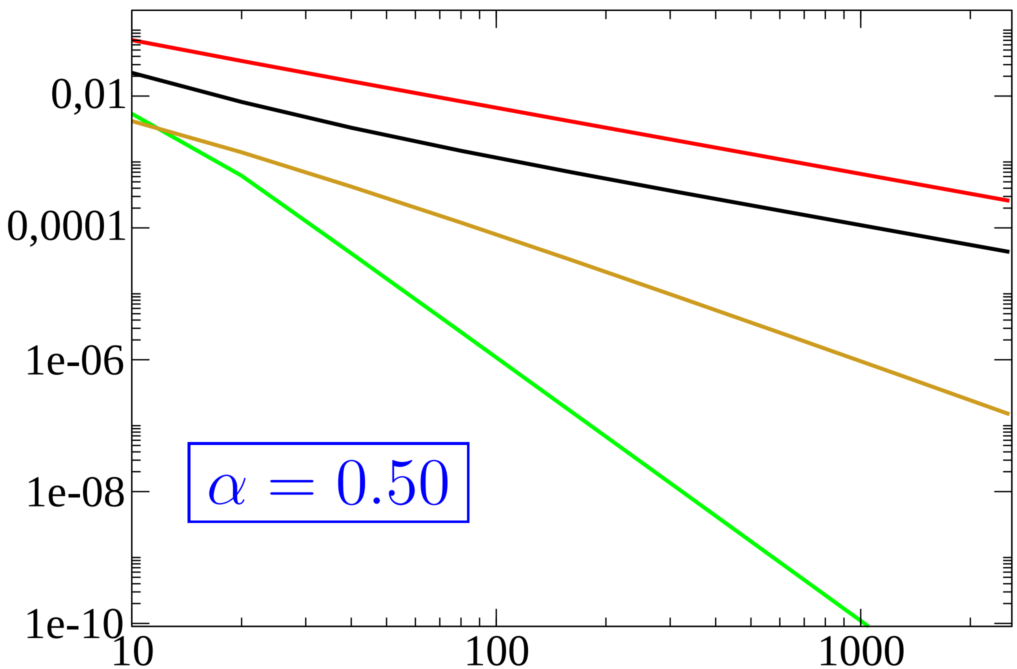

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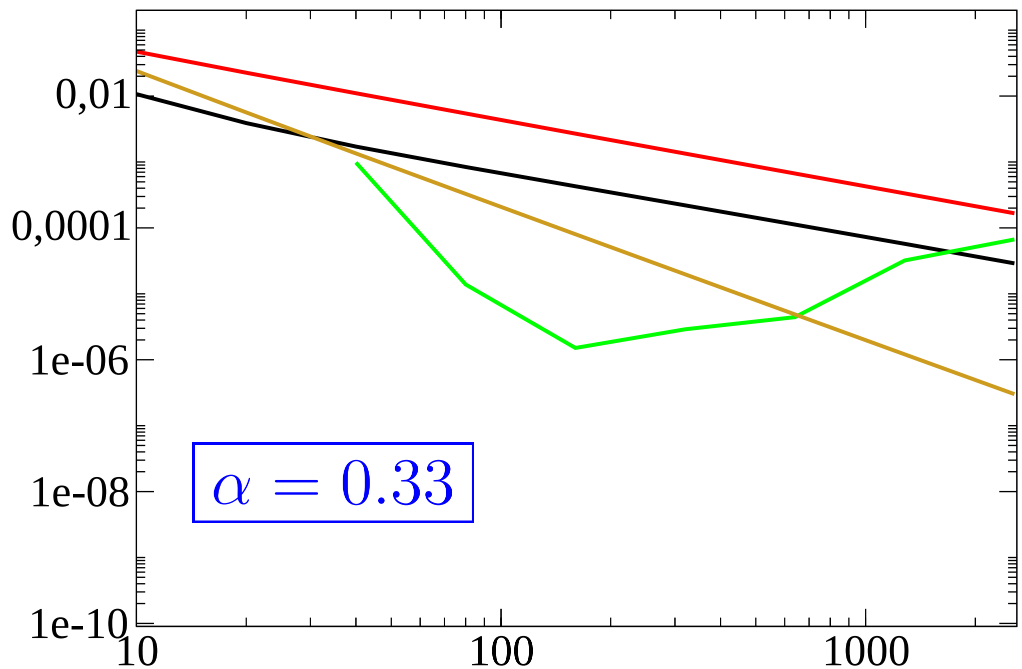

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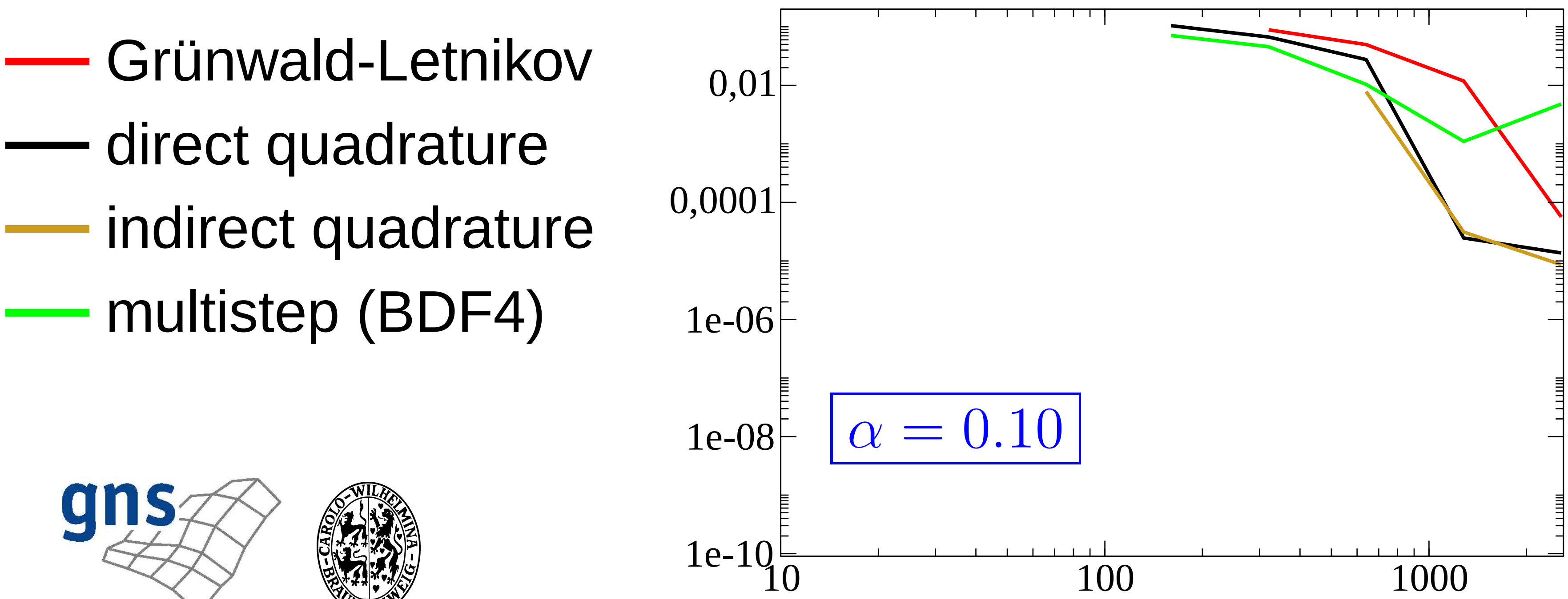
$|$Error at $x = 1|$ vs. no. of nodes



Example 3

$$D_*^\alpha y(x) = -x^{1-\alpha} E_{1,2-\alpha}(-x) + \exp(-2x) - y(x)^2, \qquad y(0) = 1$$

exact solution on $[0,5]$: $y(x) = \exp(-x)$

$|\text{Error at } x=5|$ vs. no. of nodes

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- direct quadrature
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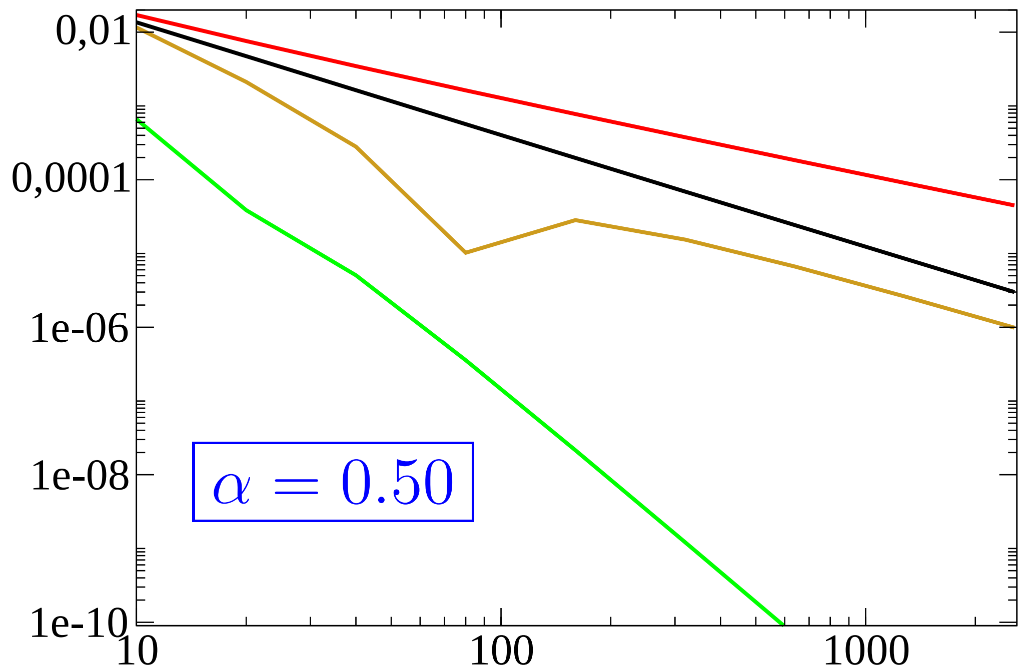

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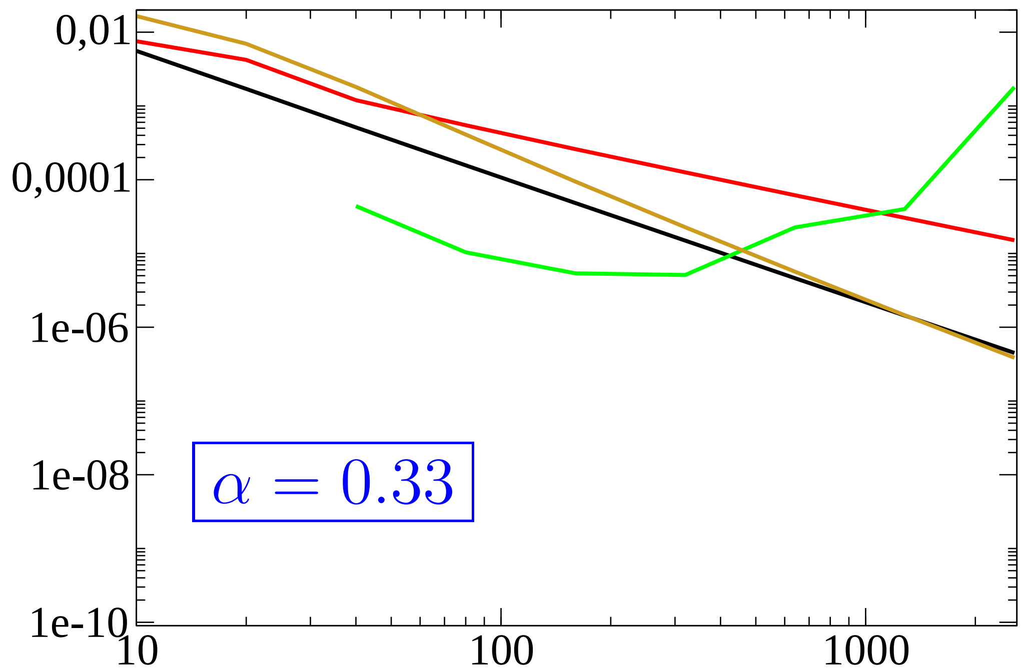

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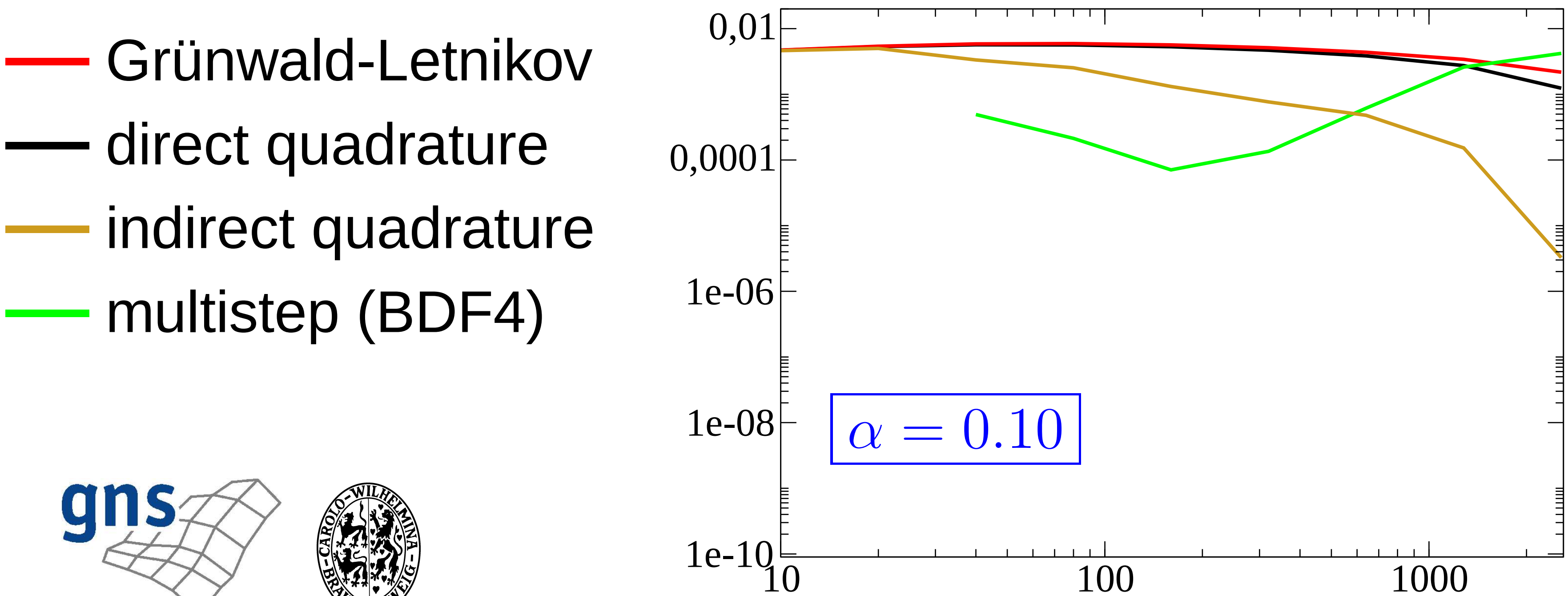

Summary

- Grünwald-Letnikov: reliable but slowly convergent
- Linear multistep methods: very bad for some values of α, very good for others
- Quadrature-based methods: useful compromise, in particular because of simple speed-up possibility
- All types of basic routines available in GNS Numerical Fractional Calculus Library (presently FORTRAN77)

Extensions

- Application of methods to
  - time-/space-fractional partial differential equations,
  - fractional optimal control problems.
- Common problem: High arithmetic complexity due to non-locality of fractional operators.
  Solution for quadrature methods: Nested mesh concept (Ford & Simpson 2001).

Merci pour votre attention!

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