Lecture 9

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Numerical Methods for Time-Dependent PDEs, Spring 2024

Outline

- PART 1:

Fractional calculus and fractional PDEs

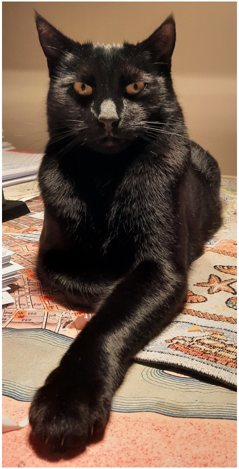
- PART 2:

Boundary-value methods

PART 1

Fractional calculus and fractional PDEs

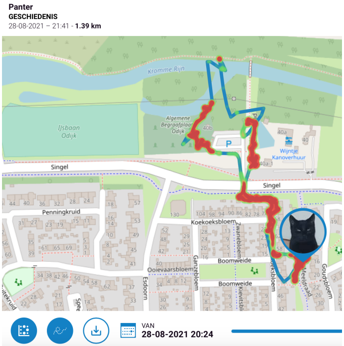
PANTER [1]



PANTER [2]

Panter
GESCHIEDENIS
31-12-2020 – 21:05 - **772.55 m**

VAN
31-12-2020 20:11



Panter
GESCHIEDENIS
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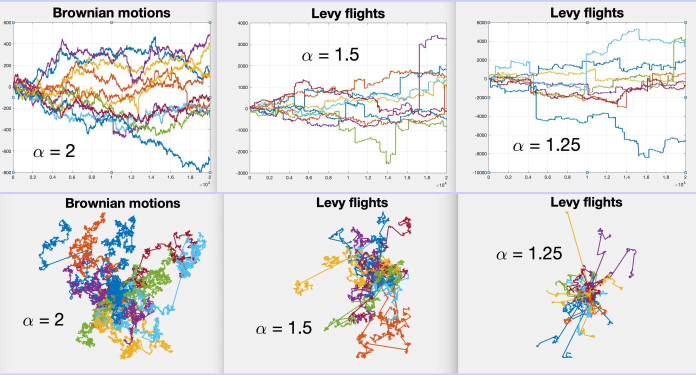
Brownian motions vs Lévy flights: 1d and 2d



$$\boxed{\lim_{N\to\infty} \Rightarrow \frac{\partial^2}{\partial x^2} = \Delta}$$

vs

$$\boxed{\lim_{N\to\infty} \Rightarrow -(-\frac{\partial^2}{\partial x^2})^{\alpha/2} = -(-\Delta)^{\alpha/2}}$$

Brownian motions vs Lévy flights: 3d

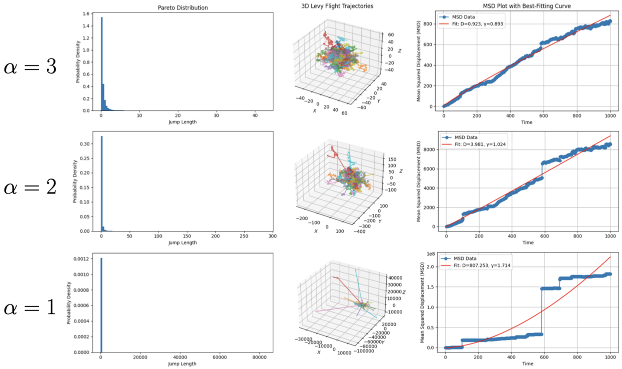


Figure 1.2: Lévy Flights simulations for $\alpha = 3$ (subdiffusion, $\gamma \approx 0.89$), $\alpha = 2$ (normal diffusion, $\gamma \approx 1.02$) and $\alpha = 1$ (superdiffusion, $\gamma \approx 1.71$).

Brownian motions vs Lévy flights: 2d ???

$\alpha \approx 2?$ vs $\alpha \approx 1.5?$

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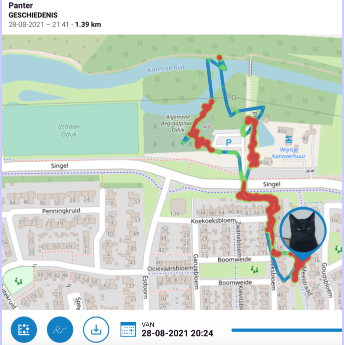

Panter
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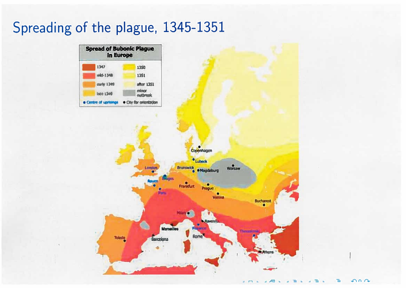
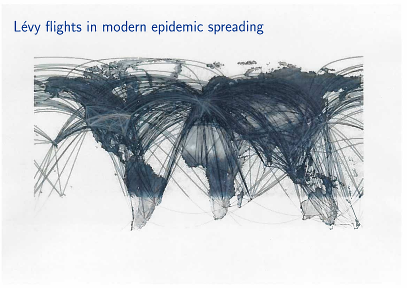
Reaction-diffusion vs *fractional* reaction-diffusion



Spreading of the plague, 1345-1351



Lévy flights in modern epidemic spreading

left: "Fisher PDE" (or "SIR-model") with $\alpha = 2$

vs

right: "fractional Fisher/SIR-model" with $\alpha < 2$

The fractional Laplacian

For $0 \leq \alpha \leq 2$, in one dimension:

$$-(-\Delta)^{\frac{\alpha}{2}} u(x) := \alpha \frac{2^{\alpha-1}\Gamma(\frac{1}{2}+\frac{\alpha}{2})}{\sqrt{\pi}\Gamma(1-\frac{\alpha}{2})} \int_{-\infty}^{\infty} \frac{u(x)-u(x+y)}{|y|^{1+\alpha}}\, dy$$

Theorem ($\alpha \neq 1$):

$$\boxed{-(-\Delta)^{\frac{\alpha}{2}} u(x) = \frac{\partial^{\alpha} u(x)}{\partial |x|^{\alpha}} = -\frac{1}{2\cos(\frac{\pi\alpha}{2})}[\mathcal{D}^{\alpha}_{Left} u(x) + \mathcal{D}^{\alpha}_{Right} u(x)]}$$

$\alpha = 2$: $\quad -(-\Delta)^{\frac{\alpha}{2}} = \frac{\partial^2}{\partial x^2}$

$\alpha = 1$: $\quad -(-\Delta)^{\frac{\alpha}{2}} \neq \pm\frac{\partial}{\partial x}$

$\alpha = 0$: $\quad -(-\Delta)^{\frac{\alpha}{2}} = -\mathcal{I}$

The case $\alpha = 1$

for $\alpha = 1$:

$$\boxed{(-\Delta)^{\frac{\alpha}{2}} = (-\Delta)^{\frac{1}{2}} = \mathcal{H}(\frac{\partial}{\partial x})}$$

where the Hilbert transform[1] $\mathcal{H}$ is defined by

$$\boxed{[\mathcal{H}u](x) = u(x) \star \frac{1}{\pi x} = \frac{1}{\pi}\ p.v.\ \int_{-\infty}^{\infty} \frac{u(y)}{x-y}\ dy}$$

and

$$p.v. \int_{-a}^{a} f(x)\ dx = \lim_{\epsilon \to 0^+} [\int_{-a}^{-\epsilon} f(x)\ dx + \int_{\epsilon}^{a} f(x)\ dx]$$

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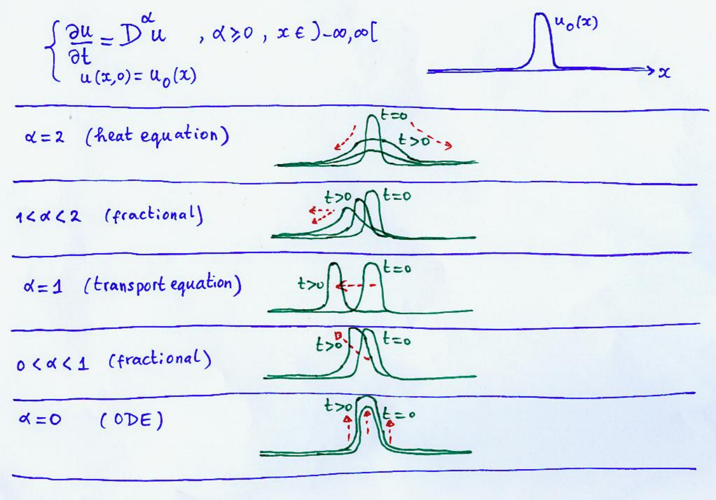
[1] used in signal processing

The *"left"*-fractional heat equation



$$\begin{cases} \frac{\partial u}{\partial t} = D^{\alpha} u & , \alpha \geq 0 , x \in]-\infty,\infty[\\ u(x,0) = u_0(x) \end{cases}$$

$\alpha = 2$ (heat equation)

$1 < \alpha < 2$ (fractional)

$\alpha = 1$ (transport equation)

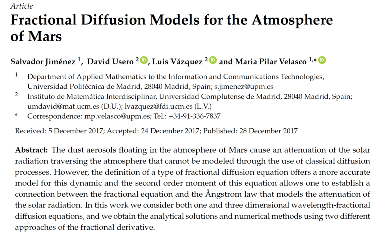
$0 < \alpha < 1$ (fractional)

$\alpha = 0$ (ODE)

Fractional PDEs: application areas [1]

- Hydrology (non-Fickian laws)
- Finance (Lévy-flights, non-Markovian models)
- Non-Brownian motions
- Super- and Sub-diffusion (anomalous transport)
- Visco-elasticity
- Rheology
- Electro-physiology of the heart

Application areas [2]



Article

Fractional Diffusion Models for the Atmosphere of Mars

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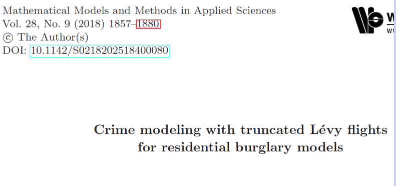
Abstract: The dust aerosols floating in the atmosphere of Mars cause an attenuation of the solar radiation traversing the atmosphere that cannot be modeled through the use of classical diffusion processes. However, the definition of a type of fractional diffusion equation offers a more accurate model for this dynamic and the second order moment of this equation allows one to establish a connection between the fractional equation and the Ångstrom law that models the attenuation of the solar radiation. In this work we consider both one and three dimensional wavelength-fractional diffusion equations, and we obtain the analytical solutions and numerical methods using two different approaches of the fractional derivative.



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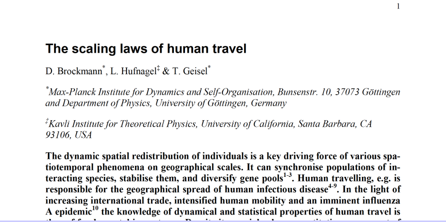
Crime modeling with truncated Lévy flights for residential burglary models

Application areas [3]



1

The scaling laws of human travel

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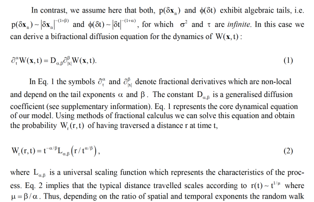
The dynamic spatial redistribution of individuals is a key driving force of various spatiotemporal phenomena on geographical scales. It can synchronise populations of interacting species, stabilise them, and diversify gene pools[1-3]. Human travelling, e.g. is responsible for the geographical spread of human infectious disease[4-9]. In the light of increasing international trade, intensified human mobility and an imminent influenza A epidemic[10] the knowledge of dynamical and statistical properties of human travel is



In contrast, we assume here that both, $p(\delta\mathbf{x}_n)$ and $\phi(\delta t)$ exhibit algebraic tails, i.e. $p(\delta\mathbf{x}_n) \sim |\delta\mathbf{x}_n|^{-(1+\beta)}$ and $\phi(\delta t) \sim |\delta t|^{-(1+\alpha)}$, for which σ^2 and τ are *infinite*. In this case we can derive a bifractional diffusion equation for the dynamics of $W(\mathbf{x},t)$:

$$\partial_t^\alpha W(\mathbf{x},t) = D_{\alpha,\beta}\partial_{|x|}^\beta W(\mathbf{x},t). \qquad (1)$$

In Eq. 1 the symbols ∂_t^α and $\partial_{|x|}^\beta$ denote fractional derivatives which are non-local and depend on the tail exponents α and β. The constant $D_{\alpha,\beta}$ is a generalised diffusion coefficient (see supplementary information). Eq. 1 represents the core dynamical equation of our model. Using methods of fractional calculus we can solve this equation and obtain the probability $W_r(r,t)$ of having traversed a distance r at time t,

$$W_r(r,t) = t^{-\alpha/\beta} L_{\alpha,\beta}\left(r/t^{\alpha/\beta}\right), \qquad (2)$$

where $L_{\alpha,\beta}$ is a universal scaling function which represents the characteristics of the process. Eq. 2 implies that the typical distance travelled scales according to $r(t) \sim t^{1/\mu}$ where $\mu = \beta/\alpha$. Thus, depending on the ratio of spatial and temporal exponents the random walk

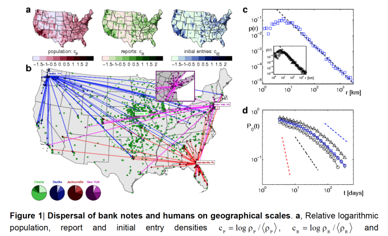
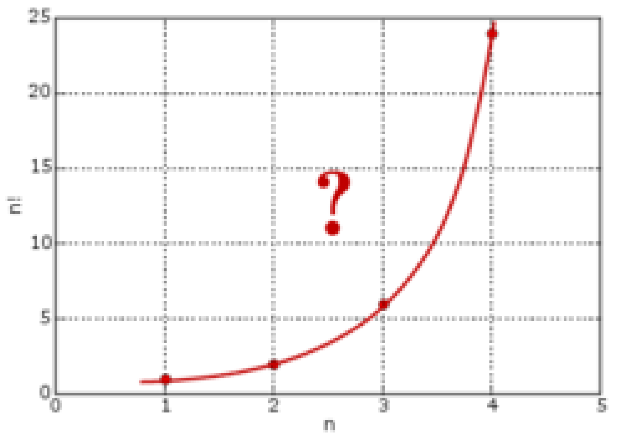


Figure 1| Dispersal of bank notes and humans on geographical scales. a, Relative logarithmic population, report and initial entry densities $c_P = \log \rho_P / \langle \rho_P \rangle$, $c_R = \log \rho_R / \langle \rho_R \rangle$ and

The Gamma-function $\Gamma(x)$ [1]



The Gamma-function $\Gamma(x)$ [2]

Euler 1730, Legendre 1809 $\Gamma(x)$, Gauss $\Pi(x)$:

$$\boxed{\Gamma(x) := \int_0^\infty t^{x-1}\mathrm{e}^{-t}\ dt = \int_0^1 [-\ln(t)]^{x-1} dt, x > 0}$$

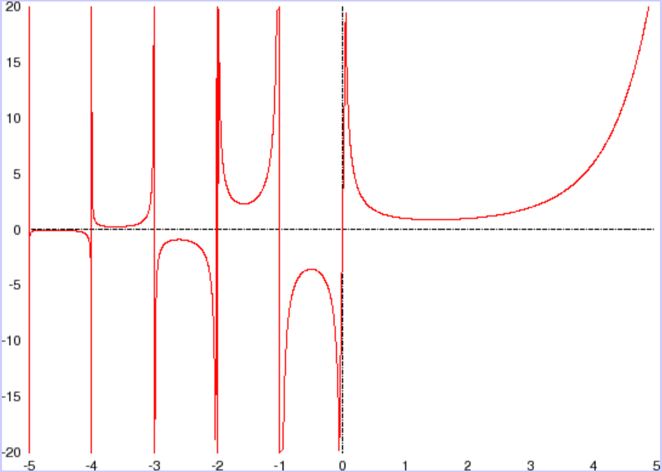
satisfies the functional equation:

$$\boxed{f(x+1) = x\ f(x),\ \ f(1) = 1,\ \ x > 0}$$

$$\Downarrow$$

$$\boxed{\Gamma(1) = 1,\ \ \Gamma(n+1) = n\Gamma(n) = n(n-1)\Gamma(n-1) = \ldots = n!}$$

The Gamma-function $\Gamma(x)$ [3]



The Gamma-function $\Gamma(x)$ [4]

The function $\Gamma(x)$ is not the unique solution of the functional equation. Other solutions are, e.g.:

$$\boxed{\begin{array}{l} \cos(2m\pi x)\Gamma(x),\ \ m \in \mathbb{N} \\ H(x) = \frac{1}{\Gamma(1-x)} \frac{d}{dx} \ln(\frac{\Gamma(\frac{1}{2}-\frac{1}{2}x)}{\Gamma(1-\frac{1}{2}x)}) \quad \text{Hadamard (1894)} \\ L(x) = \ldots \ \ \text{Luschny (2006)} \\ \textit{etcetera}\ldots \end{array}}$$

The Bohr-Mollerup theorem (1922): the Gamma function $\Gamma(x)$ is the unique solution of the functional equation, if we also demand that $f(x)$ is logarithmically convex.

A mysterious "contradiction" (?)

1)
$$y(x) = x^k \Rightarrow \frac{d^n y}{dx^n} = \frac{k!}{(k-n)!}x^{k-n} = \frac{\Gamma(k+1)}{\Gamma(k-n+1)}x^{k-n} \quad , k \geq n$$

$$\rightsquigarrow \frac{d^\alpha y}{dx^\alpha} = \frac{\Gamma(k+1)}{\Gamma(k-\alpha+1)}x^{k-\alpha} \quad , k \geq \alpha \in \mathbb{R}^{\geq 0}$$

2)
$$y(x) = \mathrm{e}^x \Rightarrow \frac{d^n y}{dx^n} = \mathrm{e}^x \rightsquigarrow \frac{d^\alpha y}{dx^\alpha} = \mathrm{e}^x = \sum_{k=0}^{\infty} \frac{x^k}{k!} =$$

$$\sum_{k=0}^{\infty} \frac{x^k}{\Gamma(k+1)}, \quad \alpha \in \mathbb{R}^{\geq 0} \quad [\star];$$

BUT , on the other hand:

$$y(x) = \mathrm{e}^x = \sum_{k=0}^{\infty} \frac{x^k}{k!} \Rightarrow \frac{d^n y}{dx^n} = \sum_{k=0}^{\infty} \frac{1}{k!}\frac{k!}{(k-n)!}x^{k-n} = \sum_{k=0}^{\infty} \frac{x^{k-n}}{(k-n)!}$$

$$\sum_{k=0}^{\infty} \frac{x^{k-n}}{\Gamma(k-n+1)}, \quad \rightsquigarrow \frac{d^\alpha y}{dx^\alpha} = \sum_{k=0}^{\infty} \frac{x^{k-\alpha}}{\Gamma(k-\alpha+1)} \neq [\star] \quad !?!$$

Cauchy-formula for repeated integration

$$\boxed{\begin{aligned}
&\mathcal{J}^0 f(x) = f(x)\\
&\mathcal{J}^1 f(x) = \textstyle\int_{-\infty}^{x} f(s)\ ds\\
&\mathcal{J}^2 f(x) = \textstyle\int_{-\infty}^{x} \mathcal{J}^1 f(s)\ ds\\
&\ldots\ldots.\\
&\mathcal{J}^n f(x) = \textstyle\int_{-\infty}^{x} \mathcal{J}^{n-1} f(s)\ ds
\end{aligned}}$$

for $f \in \tilde{S}(\mathbb{R})$, i.e. $P(x)\frac{d^k f}{dx^k} \to 0$ if $x \to -\infty$

Fractional integral of order $\alpha \geq 0$

$$\boxed{I^n f(x) := \frac{1}{(n-1)!}\int_{-\infty}^{x}(x-s)^{n-1}f(s)\;ds}\ \boxed{n! = \Gamma(n+1)}\ \text{for } n \in \mathbb{N}$$

It can be shown that: $\mathcal{J}^n f = I^n f, \quad n \in \mathbb{N}$.

Define for $\alpha \in \mathbb{R}^{\geq 0}$: $\boxed{\mathcal{J}^\alpha f(x) := \frac{1}{\Gamma(\alpha)}\int_{-\infty}^{x}\frac{f(s)}{(x-s)^{1-\alpha}}\;ds}$

Property: $\left\{ \begin{array}{l} \mathcal{J}^\alpha \mathcal{J}^\beta = \mathcal{J}^\beta \mathcal{J}^\alpha = \mathcal{J}^{\alpha+\beta} \quad \forall \alpha, \beta \geq 0 \\ \mathcal{J}^0 = \mathcal{I} \end{array} \right.$

("the semi-group property of fractional differ-integral operators")

Fractional derivative of order $\alpha < m$ (Riesz)

$$\alpha \in \mathbb{R}^{\geq 0} : \boxed{\mathcal{J}^{\alpha} f(x) := \frac{1}{\Gamma(\alpha)} \int_{-\infty}^{x} \frac{f(s)}{(x-s)^{1-\alpha}} \; ds}$$

Define the "Riesz"-derivative:

$$\boxed{\mathcal{D}_R^{\alpha} f(x) := \mathcal{J}^{m-\alpha}(\frac{d^m}{dx^m} f(x)), \quad m > \alpha, \quad f \in \tilde{S}(\mathbb{R})}$$

"Consistency" of Riesz-derivative

$$\mathcal{J}^{m-\alpha} f(x) = \frac{1}{\Gamma(m-\alpha)} \int_{-\infty}^{x} \frac{f(s)}{(x-s)^{1+\alpha-m}}\, ds, \quad m > \alpha, \quad f \in \tilde{S}(\mathbb{R})$$

$$= \chi_+^{m-\alpha} * f(x), \quad \text{where } \chi_+^{m-\alpha}(x) := \frac{1}{\Gamma(m-\alpha)} x^{m-\alpha-1} H(x)$$

$$\begin{aligned} \mathcal{D}_R^k f &= \mathcal{J}^{m-k}\left(\frac{d^m}{dx^m} f\right), \ m > k \\ &= \chi_+^{m-k} * \left(\frac{d^m}{dx^m} f\right) \\ &= \frac{d^k}{dx^k}\left[\left(\frac{d^{m-k}}{dx^{m-k}} \chi_+^{m-k}\right) * f\right] \\ &= \frac{d^k}{dx^k}[\delta * f] \\ &= \frac{d^k}{dx^k} f \end{aligned}$$

Fractional derivatives: Caputo & Riemann-Liouville

The "Caputo"-derivative:

$$\boxed{\mathcal{D}_C^{\alpha} f(x) := \mathcal{J}_0^{m-\alpha}(\frac{d^m}{dx^m} f(x)), \quad x > 0}$$

and the "Riemann-Liouville-derivative":

$$\boxed{\mathcal{D}_{RL}^{\alpha} f(x) := \frac{d^m}{dx^m}(\mathcal{J}_0^{m-\alpha}(f(x))), \quad x > 0}$$

Here: $\mathcal{J}_0^{\alpha} f(x) := \frac{1}{\Gamma(\alpha)} \int_0^x (x-s)^{\alpha-1} f(s)\ ds, \quad x > 0$

Note: $\mathcal{D}_C^{\alpha}(constant) = 0$ & $\mathcal{D}_{RL}^{\alpha}(constant) \sim x^{-\alpha} \neq 0$

"Consistency" of Caputo-derivative

For $f \in C^{m+1}([0,L]),\ \forall L > 0$:

$\mathcal{D}_C^{\alpha} f(x) =$

$$= \frac{1}{\Gamma(m-\alpha)} \int_0^x \frac{f^{(m)}(s)}{(x-s)^{1-(m-\alpha)}} ds$$
$$= \frac{1}{\Gamma(m-\alpha)} \{ -\frac{(x-s)^{m-\alpha}}{m-\alpha} f^{(m)}(s)|_{s=0}^{s=x} + \int_0^x \frac{(x-s)^{m-\alpha}}{m-\alpha} f^{(m+1)}(s) ds \}$$
$$= \frac{1}{\Gamma(m-\alpha+1)} \{ 0 + x^{m-\alpha} f^{(m)}(0) + \int_0^x (x-s)^{m-\alpha} f^{(m+1)}(s) ds \}$$

(take limit: $\alpha \in \mathbb{R} \to m \in \mathbb{N}$)

$$= \frac{1}{\Gamma(1)} \{ f^{(m)}(0) + \int_0^x f^{(m+1)}(s) ds \}$$
$$= f^{(m)}(0) + f^{(m)}(x) - f^{(m)}(0) = \frac{d^m f}{dx^m}(x)$$

"Caputo" vs "Riemann-Liouville" [1]

(Luchko & Gorenflo, 1999, th.2.3, p.213)

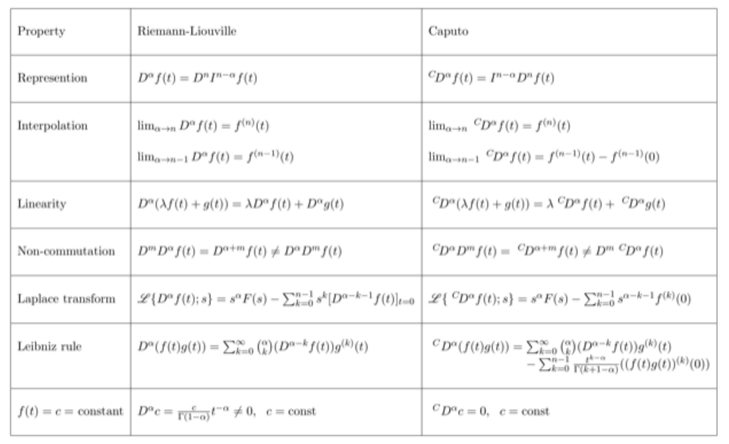
Let $f \in L^1([0,\infty)) \cap C^m([0,\infty))$ and $m-1 < \alpha \leq m$ for some $m \in \mathbb{N}$. Then:

$$\boxed{\mathcal{D}^{\alpha}_{RL} f(x) = \mathcal{D}^{\alpha}_{C} f(x) + \sum_{k=0}^{m-1} \frac{f^{(k)}(0^+)}{\Gamma(1+k-\alpha)} x^{k-\alpha} \quad (x>0)}$$

Notation: $f^{(k)}(0^+) = \lim_{x\downarrow 0} f^{(k)}(x)$

Corollary: $\boxed{\text{if } f^{(k)}(0^+) = 0,\ \ k = 0, 1, ..., m-1,\ \text{ then } \mathcal{D}^{\alpha}_{RL} = \mathcal{D}^{\alpha}_{C}}$

"Caputo" vs "Riemann-Liouville" [2]



Property	Riemann-Liouville	Caputo
Represention	$D^\alpha f(t) = D^n I^{n-\alpha} f(t)$	${}^C D^\alpha f(t) = I^{n-\alpha} D^n f(t)$
Interpolation	$\lim_{\alpha \to n} D^\alpha f(t) = f^{(n)}(t)$ $\lim_{\alpha \to n-1} D^\alpha f(t) = f^{(n-1)}(t)$	$\lim_{\alpha \to n} {}^C D^\alpha f(t) = f^{(n)}(t)$ $\lim_{\alpha \to n-1} {}^C D^\alpha f(t) = f^{(n-1)}(t) - f^{(n-1)}(0)$
Linearity	$D^\alpha(\lambda f(t) + g(t)) = \lambda D^\alpha f(t) + D^\alpha g(t)$	${}^C D^\alpha(\lambda f(t) + g(t)) = \lambda\, {}^C D^\alpha f(t) + {}^C D^\alpha g(t)$
Non-commutation	$D^m D^\alpha f(t) = D^{\alpha+m} f(t) \neq D^\alpha D^m f(t)$	${}^C D^\alpha D^m f(t) = {}^C D^{\alpha+m} f(t) \neq D^m\, {}^C D^\alpha f(t)$
Laplace transform	$\mathscr{L}\{D^\alpha f(t); s\} = s^\alpha F(s) - \sum_{k=0}^{n-1} s^k [D^{\alpha-k-1} f(t)]_{t=0}$	$\mathscr{L}\{{}^C D^\alpha f(t); s\} = s^\alpha F(s) - \sum_{k=0}^{n-1} s^{\alpha-k-1} f^{(k)}(0)$
Leibniz rule	$D^\alpha(f(t)g(t)) = \sum_{k=0}^{\infty} \binom{\alpha}{k} (D^{\alpha-k} f(t)) g^{(k)}(t)$	${}^C D^\alpha(f(t)g(t)) = \sum_{k=0}^{\infty} \binom{\alpha}{k} (D^{\alpha-k} f(t)) g^{(k)}(t)$ $- \sum_{k=0}^{n-1} \frac{t^{k-\alpha}}{\Gamma(k+1-\alpha)} ((f(t)g(t))^{(k)}(0))$
$f(t) = c =$ constant	$D^\alpha c = \frac{c}{\Gamma(1-\alpha)} t^{-\alpha} \neq 0, \quad c = \text{const}$	${}^C D^\alpha c = 0, \quad c = \text{const}$

A few other properties

$$\boxed{\mathcal{D}_C^{\alpha}(\mathcal{D}_C^{m} f(x)) = \mathcal{D}_C^{\alpha+m} f(x) \quad (m = 0, 1, 2, \ldots; m - 1 < \alpha < m)}$$

$$\boxed{\mathcal{D}_{RL}^{m}(\mathcal{D}_{RL}^{\alpha} f(x)) = \mathcal{D}_{RL}^{\alpha+m} f(x) \quad (m = 0, 1, 2, \ldots; m - 1 < \alpha < m)}$$

$$\boxed{\mathcal{D}_C^{m} \mathcal{J}^{m} = \mathcal{I}}$$

$$\boxed{\begin{array}{l} \mathcal{D}_C^{\alpha}(\mathcal{D}_C^{m} f(x)) = \mathcal{D}_C^{m}(\mathcal{D}_C^{\alpha} f(x)) = \mathcal{D}_C^{\alpha+m} f(x), \\ \text{IF } f^{(s)}(0) = 0, \text{ for } s = n, n+1, \ldots, m; m = 0, 1, \ldots \ (m - 1 < \alpha < m) \end{array}}$$

A straightforward discretization for $\mathcal{D}_C^\alpha$ $(1 < \alpha < 2)$

$$\begin{aligned}
&\mathcal{D}_C^\alpha u\big|_{x_i}\\
&\quad = \frac{1}{\Gamma(2-\alpha)} \int_0^{x_i} \frac{u''(s)}{(x_i-s)^{\alpha-1}}\, ds\\
&\quad \approx \frac{1}{\Gamma(3-\alpha)} \sum_{j=1}^{i-1} \left\{x_{j+1}^{2-\alpha} - x_j^{2-\alpha}\right\} \frac{u_{i-j+1}-2u_{i-j}+u_{i-j-1}}{h^2}\\
&\quad = \frac{1}{\Gamma(3-\alpha)} \sum_{j=1}^{i-1} \left\{\frac{j^{2-\alpha}-(j-1)^{2-\alpha}}{h^{2-\alpha}}\right\}\left\{\frac{u_{i-j+1}-2u_{i-j}+u_{i-j-1}}{h^2}\right\}\\
&\quad = \frac{1}{\Gamma(3-\alpha)h^\alpha} \sum_{j=1}^{i-1} \{j^{2-\alpha} - (j-1)^{2-\alpha}\}\{u_{i-j+1} - 2u_{i-j} + u_{i-j-1}\}
\end{aligned}$$

Grünwald-Letnikov-definition [1]

$$\boxed{\begin{array}{l} f'(x) = \lim_{h\to 0} \frac{f(x+h)-f(x)}{h} \\ f''(x) = \lim_{h_1\to 0} \frac{\lim_{h_2\to 0} \frac{f(x+h_1+h_2)-f(x+h_1)}{h_2} - \lim_{h_2\to 0} \frac{f(x+h_2)-f(x)}{h_2}}{h_1} \end{array}}$$

Take $h = h_1 = h_2 \Rightarrow f''(x) = \lim_{h\to 0} \frac{f(x+2h)-2f(x+h)+f(x)}{h^2}$

By induction:

$$\boxed{f^{(n)}(x) = \lim_{h\to 0} \frac{1}{h^n} \sum_{m=0}^{n} (-1)^m \left(\begin{array}{c} n \\ m \end{array} \right) f(x+mh), \;\; n \in \mathbb{N}}$$

Grünwald-Letnikov-definition [2]

$$f^{(n)}(x) = \lim_{h\to 0} \frac{1}{h^n} \sum_{m=0}^{n} (-1)^m \left(\begin{array}{c} n \\ m \end{array} \right) f(x+mh), \;\; n \in \mathbb{N}$$

Note: $\left(\begin{array}{c} n \\ m \end{array} \right) = \frac{n!}{m!(n-m)!}$, replace "!"-terms by "Γ"-values

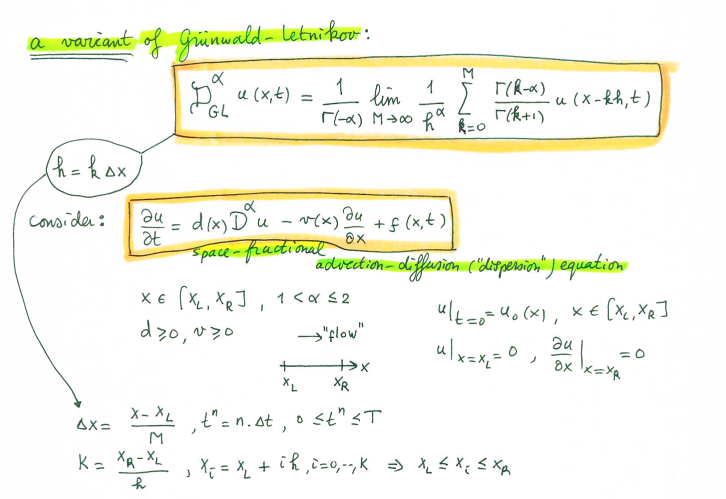
Define: $\boxed{\mathcal{D}^{\alpha}_{GL} f(x) = \lim_{h\to 0} \frac{1}{h^{\alpha}} \sum_{m=0}^{[\alpha]} (-1)^m \frac{\Gamma(\alpha+1)}{m!\Gamma(\alpha-m+1)} f(x+mh)}$

Podlubny, 1999:

$$f \in C^{m+1}_{0-}(\mathbf{R}^{\geq 0}) := \{f \in C^{m+1}([0,\infty)) \;\&\; f(x) = 0 \text{ for } x \leq 0\}$$

$$\Rightarrow \qquad \mathcal{D}^{\alpha}_{GL} f(x) = \mathcal{D}^{\alpha}_{RL} f(x) = \mathcal{D}^{\alpha}_{C} f(x) = \mathcal{D}^{\alpha}_{R} f(x)$$

Grünwald-Letnikov-definition [3]



a variant of Grünwald-Letnikov:

$$\boxed{{}_{GL}\mathcal{D}^{\alpha} u(x,t) = \frac{1}{\Gamma(-\alpha)} \lim_{M\to\infty} \frac{1}{h^{\alpha}} \sum_{k=0}^{M} \frac{\Gamma(k-\alpha)}{\Gamma(k+1)} u(x-kh,t)}$$

$h = k\,\Delta x$

Consider: $\boxed{\frac{\partial u}{\partial t} = d(x)\,\mathcal{D}^{\alpha} u - v(x)\frac{\partial u}{\partial x} + f(x,t)}$

space-fractional advection-diffusion ("dispersion") equation

$x \in [x_L, x_R]$, $1 < \alpha \leq 2$

$d \geq 0$, $v \geq 0$

$\longrightarrow$ "flow"

x_L x_R x

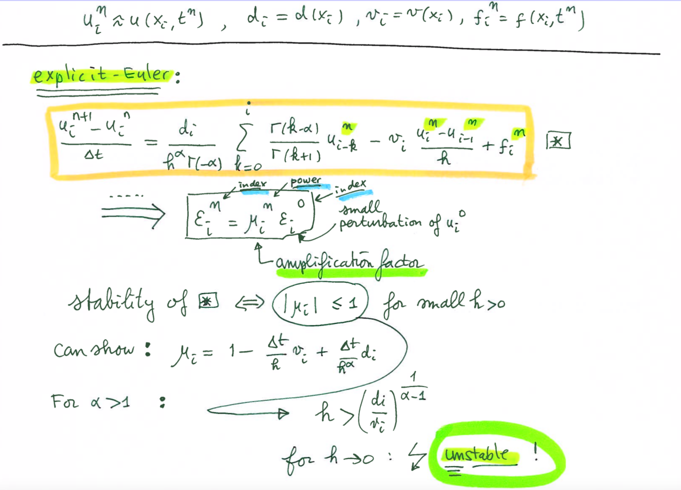
$u|_{t=0} = u_0(x)$, $x \in [x_L, x_R]$

$u|_{x=x_L} = 0$, $\frac{\partial u}{\partial x}\Big|_{x=x_R} = 0$

$\Delta x = \frac{x - x_L}{M}$, $t^n = n.\Delta t$, $0 \leq t^n \leq T$

$K = \frac{x_R - x_L}{h}$, $x_i = x_L + ih$, $i = 0,..,K$ $\Rightarrow$ $x_L \leq x_i \leq x_R$

Grünwald-Letnikov-definition [4]



$u_i^n \approx u(x_i,t^n)$, $d_i = d(x_i)$, $v_i = v(x_i)$, $f_i^n = f(x_i,t^n)$

---

explicit-Euler:

$$\boxed{\frac{u_i^{n+1}-u_i^n}{\Delta t} = \frac{d_i}{h^\alpha \Gamma(-\alpha)} \sum_{k=0}^{i} \frac{\Gamma(k-\alpha)}{\Gamma(k+1)} u_{i-k}^n - v_i \frac{u_i^n - u_{i-1}^n}{h} + f_i^n} \quad \boxed{*}$$

$$\ldots\ldots \Longrightarrow \boxed{\varepsilon_i^n = \mu_i^n \varepsilon_i^0}$$

index power index

small perturbation of u_i^0

amplification factor

stability of $\boxed{*}$ $\Longleftrightarrow$ $|\mu_i| \le 1$ for small $h>0$

Can show: $\mu_i = 1 - \frac{\Delta t}{h} v_i + \frac{\Delta t}{h^\alpha} d_i$

For $\alpha > 1$: $\longrightarrow$ $h > \left(\frac{d_i}{v_i}\right)^{\frac{1}{\alpha-1}}$

for $h \to 0$: ↯ unstable !

Grünwald-Letnikov-definition [5]

implicit-Euler:

$$\boxed{\frac{u_i^{n+1}-u_i^{n}}{\Delta t} = \frac{d_i}{h^{\alpha}} \sum_{k=0}^{i} \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)} u_{i-k}^{n+1} - v_i \frac{u_i^{n+1}-u_{i-1}^{n+1}}{h} + f_i^{n+1}}$$

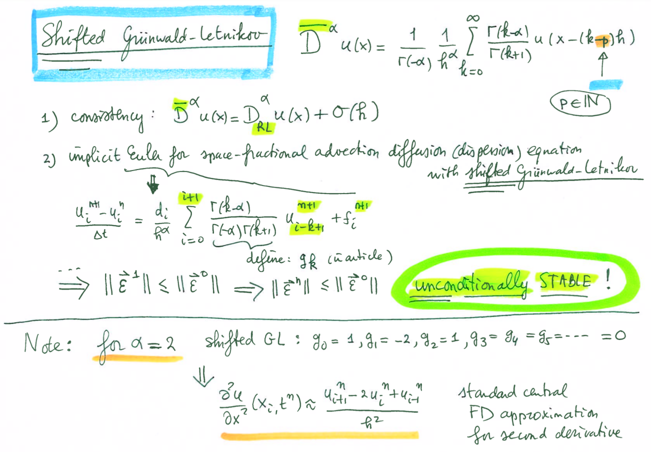
$$\overset{\cdots}{\Longrightarrow} \begin{cases} \varepsilon_i^{\overset{\text{index}}{n}} = \tilde{\mu}_i^{\overset{\text{power}}{n}} \, \varepsilon_i^{\overset{\text{index}}{0}} \\ \tilde{\mu}_i = \dfrac{1}{1 + \dfrac{v_i \Delta t}{h} - \dfrac{d_i \Delta t}{h^{\alpha}}} \end{cases}$$

Stability for $|\tilde{\mu}_i| \leq 1$

However, ∀ h sufficiently small : $|\tilde{\mu}_i| > 1$

UN stable !!

Grünwald-Letnikov-definition [6]



Shifted Grünwald-Letnikov

$$\overline{D}^{\alpha} u(x) = \frac{1}{\Gamma(-\alpha)} \frac{1}{h^{\alpha}} \sum_{k=0}^{\infty} \frac{\Gamma(k-\alpha)}{\Gamma(k+1)} u(x-(k-\underset{\uparrow}{p})h)$$

$p \in \mathbb{N}$

1) consistency: $\overline{D}^{\alpha} u(x) = D^{\alpha}_{RL} u(x) + O(h)$

2) implicit Euler for space-fractional advection diffusion (dispersion) equation with shifted Grünwald-Letnikov

$$\Downarrow$$

$$\frac{u_i^{n+1}-u_i^{n}}{\Delta t} = \frac{d_i}{h^{\alpha}} \sum_{i=0}^{i+1} \underbrace{\frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)}}_{\text{define: } g_k \text{ (in article)}} u_{i-k+1}^{n+1} + f_i^{n+1}$$

$$\overset{---}{\Longrightarrow} \|\vec{\varepsilon}^{\,1}\| \leq \|\vec{\varepsilon}^{\,0}\| \Longrightarrow \|\vec{\varepsilon}^{\,n}\| \leq \|\vec{\varepsilon}^{\,0}\|$$

unconditionally STABLE !

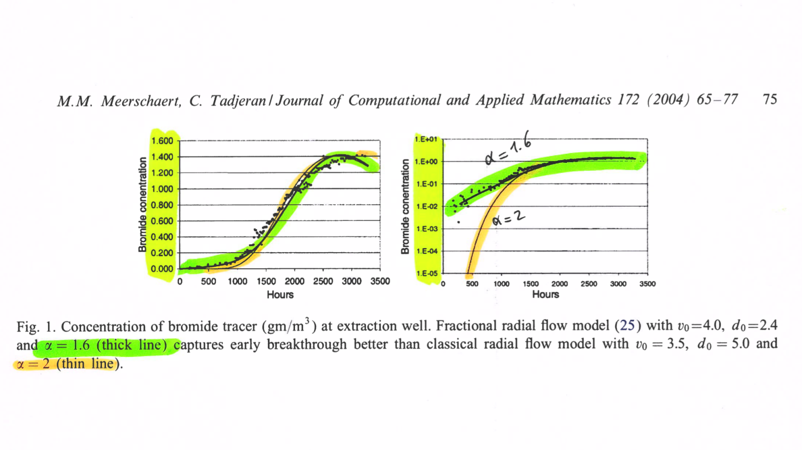
Note: for $\alpha = 2$ shifted GL : $g_0 = 1, g_1 = -2, g_2 = 1, g_3 = g_4 = g_5 = \cdots = 0$

$$\Downarrow$$

$$\frac{\partial^2 u}{\partial x^2}(x_i, t^n) \approx \frac{u_{i+1}^{n} - 2u_i^{n} + u_{i-1}^{n}}{h^2}$$

standard central FD approximation for second derivative

Grünwald-Letnikov-definition [7]



M.M. Meerschaert, C. Tadjeran / Journal of Computational and Applied Mathematics 172 (2004) 65–77 75

Fig. 1. Concentration of bromide tracer (gm/m^3) at extraction well. Fractional radial flow model (25) with v_0=4.0, d_0=2.4 and $\alpha = 1.6$ (thick line) captures early breakthrough better than classical radial flow model with $v_0 = 3.5$, $d_0 = 5.0$ and $\alpha = 2$ (thin line).

Fourier's definition of a fractional derivative

Fourier, 1822:

$$f(x) = \frac{1}{2\pi} \int\int_{\mathbb{R}^2} f(\gamma) \cos(p(x-\gamma))\ dp\ d\gamma$$

$\Rightarrow$

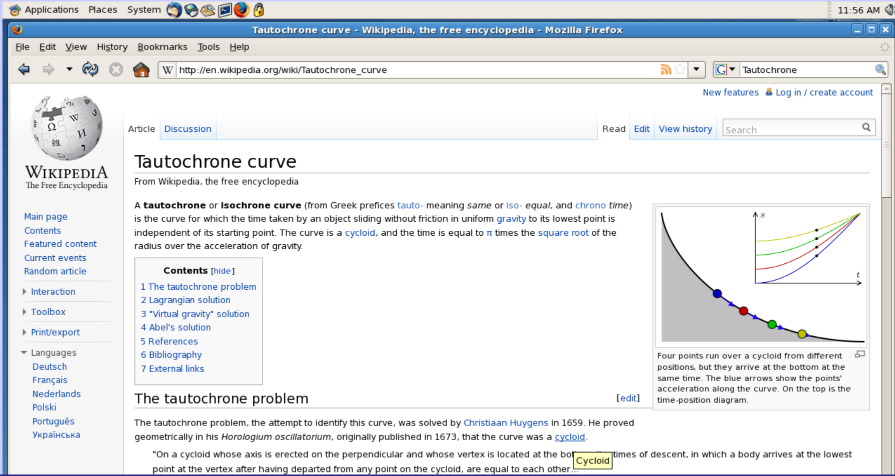
$$\frac{d^n f}{dx^n}(x) = \frac{1}{2\pi} \int\int_{\mathbb{R}^2} f(\gamma) p^n \cos(p(x-\gamma) + \frac{n\pi}{2})\ dp\ d\gamma, \quad n \in \mathbb{N}$$

$\rightsquigarrow$

$$\frac{d^\alpha f}{dx^\alpha}(x) = \frac{1}{2\pi} \int\int_{\mathbb{R}^2} f(\gamma) p^\alpha \cos(p(x-\gamma) + \frac{\alpha\pi}{2})\ dp\ d\gamma, \quad \alpha \in \mathbb{R}$$

... ..., Weyl, Marchaud, Riesz, pointwise Liouville-Grünwald, ...

An application: the tautochrone curve



Tautochrone curve

From Wikipedia, the free encyclopedia

A **tautochrone** or **isochrone curve** (from Greek prefixes tauto- meaning *same* or iso- *equal*, and chrono *time*) is the curve for which the time taken by an object sliding without friction in uniform gravity to its lowest point is independent of its starting point. The curve is a cycloid, and the time is equal to π times the square root of the radius over the acceleration of gravity.

Contents [hide]

Four points run over a cycloid from different positions, but they arrive at the bottom at the same time. The blue arrows show the points' acceleration along the curve. On the top is the time-position diagram.

The tautochrone problem

[edit]

The tautochrone problem, the attempt to identify this curve, was solved by Christiaan Huygens in 1659. He proved geometrically in his *Horologium oscillatorium*, originally published in 1673, that the curve was a cycloid.

> "On a cycloid whose axis is erected on the perpendicular and whose vertex is located at the bot times of descent, in which a body arrives at the lowest point at the vertex after having departed from any point on the cycloid, are equal to each other...

The tautochrone: Abel's mechanical problem

Abel, 1823 (integral equation)

$$\frac{1}{\Gamma(\alpha)} \int_0^x \frac{y(s)}{(x-s)^{1-\alpha}}\, ds = h(x), \quad 0 < \alpha < 1$$

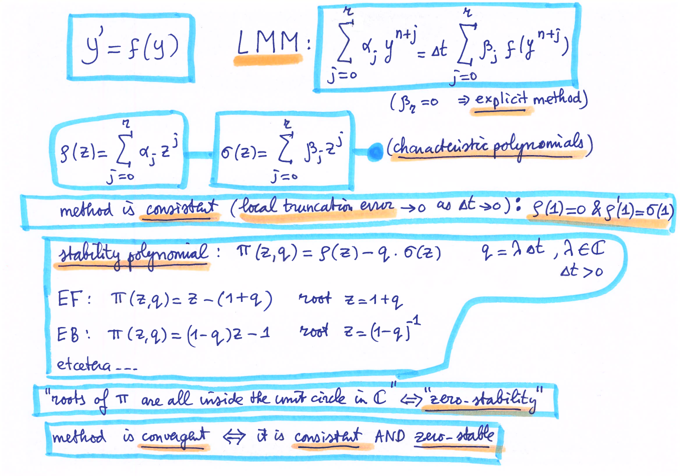
$\Rightarrow$

$$y(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_0^x \frac{h(s)}{(x-s)^{\alpha}}\, ds = \mathcal{D}^{\alpha}_{RL} h(x)$$

PART 2

Boundary-value methods

Stability regions [1]



$y' = f(y)$

LMM: $\sum_{j=0}^{r} \alpha_j y^{n+j} = \Delta t \sum_{j=0}^{r} \beta_j f(y^{n+j})$

($\beta_r = 0 \Rightarrow$ explicit method)

$\rho(z) = \sum_{j=0}^{r} \alpha_j z^j$ $\sigma(z) = \sum_{j=0}^{r} \beta_j z^j$ (characteristic polynomials)

method is consistant (local truncation error → 0 as $\Delta t \to 0$): $\rho(1)=0$ & $\rho'(1)=\sigma(1)$

stability polynomial: $\pi(z,q) = \rho(z) - q \cdot \sigma(z)$ $q = \lambda \Delta t$, $\lambda \in \mathbb{C}$, $\Delta t > 0$

EF: $\pi(z,q) = z - (1+q)$ root $z = 1+q$

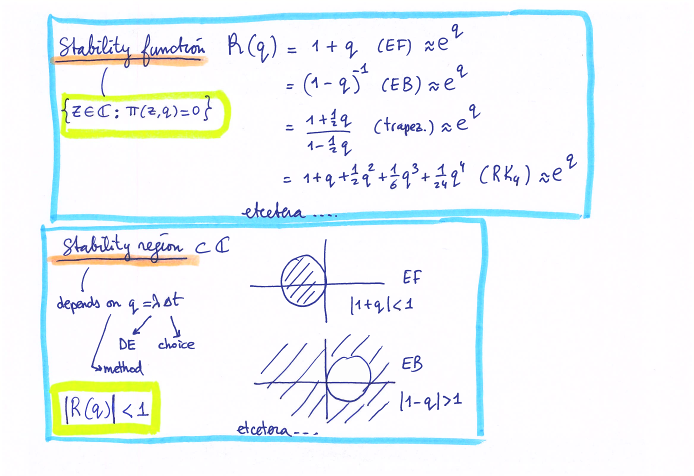
EB: $\pi(z,q) = (1-q)z - 1$ root $z = (1-q)^{-1}$

etcetera ...

"roots of π are all inside the unit circle in $\mathbb{C}$" $\Leftrightarrow$ "zero-stability"

method is convergent $\Leftrightarrow$ it is consistant AND zero-stable

Stability regions [2]



Stability function

$\boxed{\{z \in \mathbb{C} : \pi(z,q)=0\}}$

$$R(q) = 1+q \quad (EF) \approx e^{q}$$

$$= (1-q)^{-1} \quad (EB) \approx e^{q}$$

$$= \frac{1+\frac{1}{2}q}{1-\frac{1}{2}q} \quad (\text{trapez.}) \approx e^{q}$$

$$= 1+q+\frac{1}{2}q^2+\frac{1}{6}q^3+\frac{1}{24}q^4 \quad (RK_4) \approx e^{q}$$

etcetera ....

Stability region $\subset \mathbb{C}$

depends on $q = \lambda \Delta t$

DE choice

method

$\boxed{|R(q)| < 1}$

EF

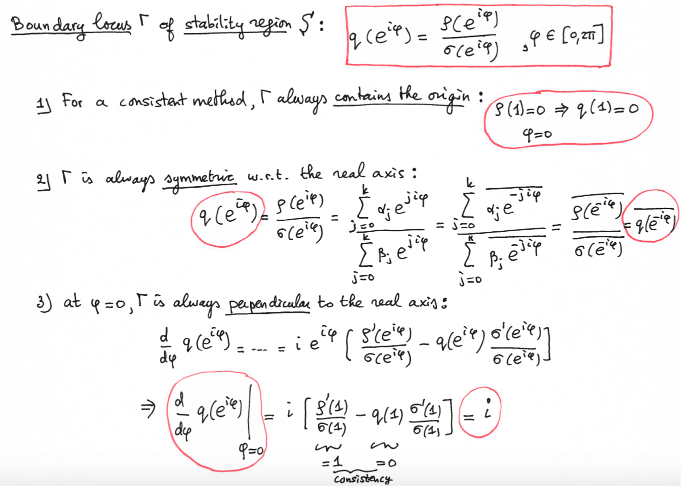
$|1+q|<1$

EB

$|1-q|>1$

etcetera ---

Stability regions [3]



Boundary locus Γ of stability region S:

$$\boxed{q(e^{i\varphi}) = \frac{\rho(e^{i\varphi})}{\sigma(e^{i\varphi})}, \ \varphi \in [0,2\pi]}$$

1) For a consistent method, Γ always contains the origin:

$$\rho(1)=0 \Rightarrow q(1)=0$$
$$\varphi=0$$

2) Γ is always symmetric w.r.t. the real axis:

$$q(e^{i\varphi}) = \frac{\rho(e^{i\varphi})}{\sigma(e^{i\varphi})} = \frac{\sum_{j=0}^{k} \alpha_j e^{ji\varphi}}{\sum_{j=0}^{k} \beta_j e^{ji\varphi}} = \frac{\sum_{j=0}^{k} \alpha_j \overline{e^{-ji\varphi}}}{\sum_{j=0}^{k} \beta_j \overline{e^{-ji\varphi}}} = \frac{\overline{\rho(e^{-i\varphi})}}{\overline{\sigma(e^{-i\varphi})}} = \overline{q(e^{-i\varphi})}$$

3) at $\varphi=0$, Γ is always perpendicular to the real axis:

$$\frac{d}{d\varphi} q(e^{i\varphi}) = \cdots = i e^{i\varphi}\left[\frac{\rho'(e^{i\varphi})}{\sigma(e^{i\varphi})} - q(e^{i\varphi})\frac{\sigma'(e^{i\varphi})}{\sigma(e^{i\varphi})}\right]$$

$$\Rightarrow \left.\frac{d}{d\varphi} q(e^{i\varphi})\right|_{\varphi=0} = i\left[\underbrace{\underbrace{\frac{\rho'(1)}{\sigma(1)}}_{=1} - \underbrace{q(1)}_{=0}}_{\text{consistency}}\frac{\sigma'(1)}{\sigma(1)}\right] = i$$

Stability regions [4]

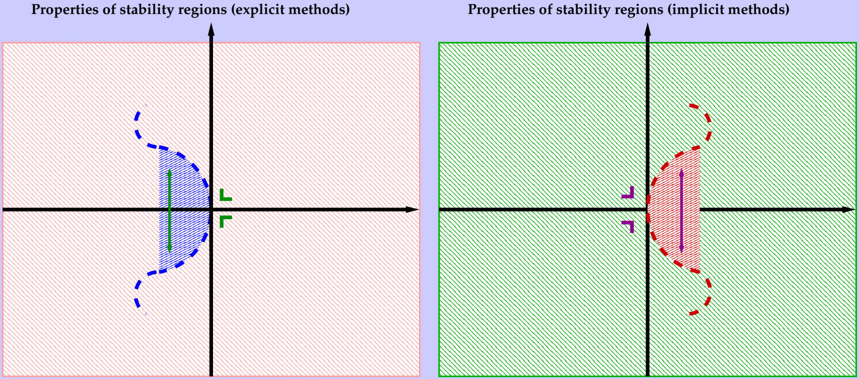
Theorem 1:

The angle of the boundary locus of a stability region with the real axis at $z = 0$ in the complex plane is 90^0. This holds for all explicit and all implicit methods.

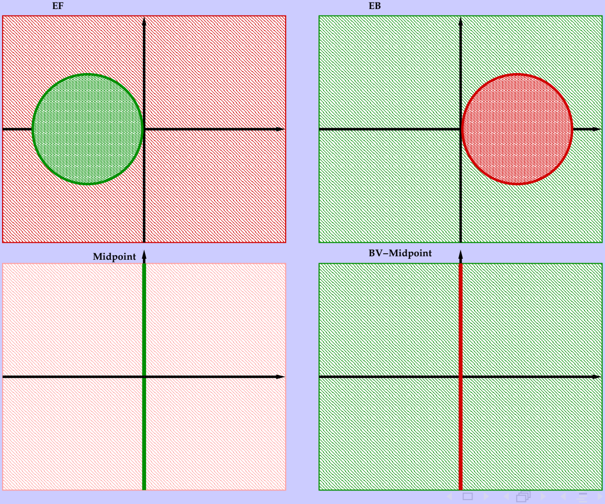
Theorem 2:

The stability region is symmetric around the real axis in the complex plane. This holds for all explicit and all implicit methods.

Stability regions [5]



Stability regions [6]



Boundary-value methods [1]

History:

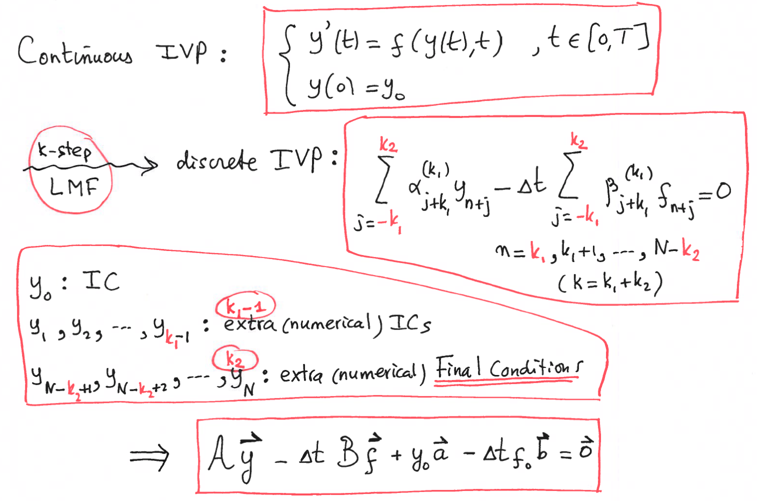
- Fox & Goodwin 1948, Loud 1948
- Allen & Severn 1951, Fox & Miller 1951, Todd 1952
- Dahlquist 1952, Miller 1952, Fox 1953
- Dahlquist 1963, Usmani 1965, Gautschi 1965, Olver 1967

- Carasso & Parter 1970, Cryer 1972, Olver & Sookne 1972
- Rolfes 1981
- Axelsson & Verwer 1985

- Lopez & Trigiante 1993, Amodio, Mazzia & Trigiante 1993
- Brugnano & Trigiante 1998
- Sun & Zhang 2003, Iavernaro et al 2005, Aceto & Trigiante 2007

😐 😐 😐 Zegeling & van Spengler 2022

Boundary-value methods [2]



Continuous IVP : $\boxed{\begin{cases} y'(t) = f(y(t),t) \quad , t \in [0,T] \\ y(0) = y_0 \end{cases}}$

k-step LMF $\rightsquigarrow$ discrete IVP : $\boxed{\begin{array}{c} \sum_{j=-k_1}^{k_2} \alpha^{(k_1)}_{j+k_1} y_{n+j} - \Delta t \sum_{j=-k_1}^{k_2} \beta^{(k_1)}_{j+k_1} f_{n+j} = 0 \\ n = k_1, k_1+1, \dots, N-k_2 \\ (k = k_1 + k_2) \end{array}}$

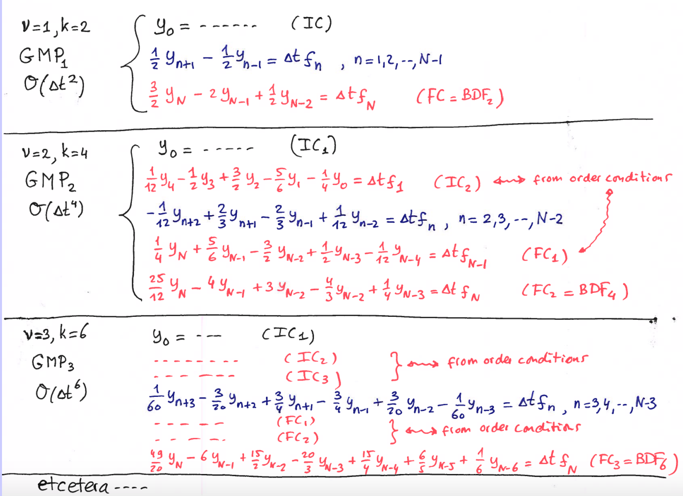
y_0 : IC

$y_1, y_2, \dots, y_{k_1-1}$: $\overset{k_1-1}{\text{extra}}$ (numerical) ICs

$y_{N-k_2+1}, y_{N-k_2+2}, \dots, \overset{k_2}{y_N}$: extra (numerical) Final Conditions

$$\Longrightarrow \boxed{A\vec{y} - \Delta t\, B\vec{f} + y_0\vec{a} - \Delta t\, f_0\vec{b} = \vec{0}}$$

Boundary-value methods [3]



$\nu=1, k=2$
GMP$_1$
$\mathcal{O}(\Delta t^2)$

$$\begin{cases} y_0 = - - - - - - & (IC) \\ \frac{1}{2} y_{n+1} - \frac{1}{2} y_{n-1} = \Delta t f_n , & n = 1,2,--,N-1 \\ \frac{3}{2} y_N - 2 y_{N-1} + \frac{1}{2} y_{N-2} = \Delta t f_N & (FC = BDF_2) \end{cases}$$

$\nu=2, k=4$
GMP$_2$
$\mathcal{O}(\Delta t^4)$

$$\begin{cases} y_0 = - - - - - & (IC_1) \\ \frac{1}{12} y_4 - \frac{1}{2} y_3 + \frac{3}{2} y_2 - \frac{5}{6} y_1 - \frac{1}{4} y_0 = \Delta t f_1 & (IC_2) \leftrightsquigarrow \text{from order conditions} \\ -\frac{1}{12} y_{n+2} + \frac{2}{3} y_{n+1} - \frac{2}{3} y_{n-1} + \frac{1}{12} y_{n-2} = \Delta t f_n , & n = 2,3,--,N-2 \\ \frac{1}{4} y_N + \frac{5}{6} y_{N-1} - \frac{3}{2} y_{N-2} + \frac{1}{2} y_{N-3} - \frac{1}{12} y_{N-4} = \Delta t f_{N-1} & (FC_1) \\ \frac{25}{12} y_N - 4 y_{N-1} + 3 y_{N-2} - \frac{4}{3} y_{N-2} + \frac{1}{4} y_{N-3} = \Delta t f_N & (FC_2 = BDF_4) \end{cases}$$

$\nu=3, k=6$
GMP$_3$
$\mathcal{O}(\Delta t^6)$

$y_0 = - - -$ (IC_1)

$- - - - - - - - -$ (IC_2)
$- - - - - - -$ (IC_3)
$\Big\} \rightsquigarrow$ from order conditions

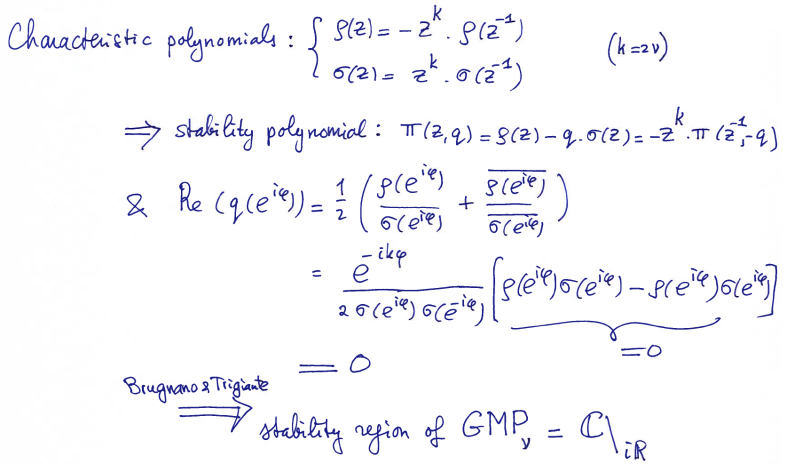
$\frac{1}{60} y_{n+3} - \frac{3}{20} y_{n+2} + \frac{3}{4} y_{n+1} - \frac{3}{4} y_{n-1} + \frac{3}{20} y_{n-2} - \frac{1}{60} y_{n-3} = \Delta t f_n , \quad n = 3,4,--,N-3$

$- - - - - -$ (FC_1)
$- - - - -$ (FC_2)
$\Big\} \rightsquigarrow$ from order conditions

$\frac{49}{20} y_N - 6 y_{N-1} + \frac{15}{2} y_{N-2} - \frac{20}{3} y_{N-3} + \frac{15}{4} y_{N-4} + \frac{6}{5} y_{N-5} + \frac{1}{6} y_{N-6} = \Delta t f_N \quad (FC_3 = BDF_6)$

etcetera - - - -

Boundary-value methods [4]



Characteristic polynomials: $\begin{cases} \rho(z) = -z^k \cdot \rho(z^{-1}) \\ \sigma(z) = z^k \cdot \sigma(z^{-1}) \end{cases}$ $(k = 2\nu)$

$\Rightarrow$ stability polynomial: $\pi(z,q) = \rho(z) - q \cdot \sigma(z) = -z^k \cdot \pi(z^{-1}, -q)$

$$\& \quad \mathrm{Re}\,(q(e^{i\varphi})) = \frac{1}{2}\left(\frac{\rho(e^{i\varphi})}{\sigma(e^{i\varphi})} + \frac{\overline{\rho(e^{i\varphi})}}{\overline{\sigma(e^{i\varphi})}}\right)$$

$$= \frac{e^{-ik\varphi}}{2\sigma(e^{i\varphi})\sigma(e^{-i\varphi})}\Big[\underbrace{\rho(e^{i\varphi})\sigma(e^{i\varphi}) - \rho(e^{i\varphi})\sigma(e^{i\varphi})}_{=0}\Big]$$

$$= 0$$

$$\xrightarrow{\text{Brugnano \& Trigiante}} \text{stability region of } GMP_\nu = \mathbb{C}\backslash_{i\mathbb{R}}$$

A semi-stable ODE [1]

$$\begin{cases} \dot{u}(t) = \cos(t)\; u(t), & t \in [0, T] \\ u(0) = 1 \end{cases}$$

with exact solution $u(t) = e^{\sin(t)}$

Note: $\{\cos(t)\}_{t\in\mathbb{R}} \not\subset \mathcal{S}_{\mathcal{EF}}$ and $\not\subset \mathcal{S}_{\mathcal{EB}}$, but $\subset \mathcal{S}_{\mathcal{BV}mp} = \mathbb{C} \setminus (i\;\mathbb{R})$

Method 1: Forward in time (explicit):

$$\begin{cases} u_0 = 1 \\ u_{n+1} = [1 + \Delta t \cos(t_n)]u_n, & n = 0, 1, ..., N-1 \\ t_{n+1} = t_n + \Delta t, \quad N = \frac{T}{\Delta t} \end{cases}$$

A semi-stable ODE [2]

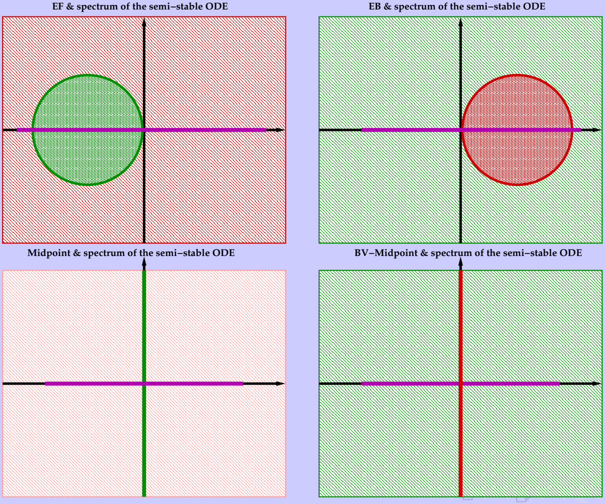
Method 2: Backward in time (implicit):

$$\begin{cases} u_0 = 1 \\ u_{n+1} = \frac{1}{1-\Delta t\cos(t_{n+1})} u_n, \quad n = 0, 1, ..., N-1 \\ t_{n+1} = t_n + \Delta t, \quad N = \frac{T}{\Delta t} \end{cases}$$

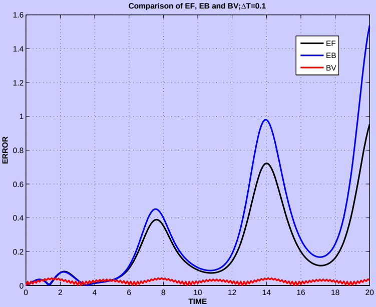
Method 3: Boundary-Value Method (midpoint + EB):

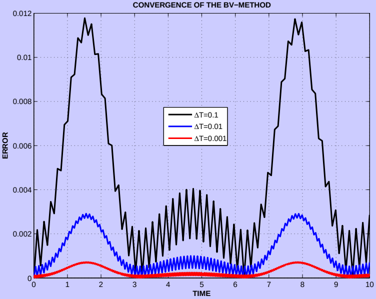
$$\begin{cases} u_0 = 1, \\ u_{n+1} - u_{n-1} - 2\Delta t \cos(t_n) u_n = 0, \quad n = 1, ..., N-1 \\ u_N - u_{N-1} - \Delta t \cos(T) u_N = 0 \\ t_{n+1} = t_n + \Delta t, \quad N = \frac{T}{\Delta t} \end{cases}$$

A semi-stable ODE [3]



A semi-stable ODE [4]





FT vs BT vs BV-method (midpoint +EB)

A semi-stable ODE [5]

Why does this work? Consider the test equation:

$$\begin{cases} y'(t) = \lambda y(t) & t \in [0, T] \\ y(0) = y_0 \end{cases}$$

2nd-order explicit midpoint method (with BDF2 final condition):

$$\begin{cases} \frac{y_{n+1} - y_{n-1}}{2\Delta t} = \lambda y_n, \ \ n = 1, 2, 3, ..., N-1 \\ \\ \frac{3y_N - 4y_{N-1} + y_{N-2}}{2\Delta t} = \lambda y_N \\ \\ t_{n+1} = t_n + \Delta t, \quad N = \frac{T}{\Delta t} \end{cases}$$

⇒ <u>forward</u> recurrence relation:

$y_{n+1} - 2\lambda\Delta t y_n - y_{n-1} = 0, \quad n = 1, 2, ...$

A semi-stable ODE [6]

$\Rightarrow$ characteristic polynomial: $r^2 - 2\lambda\Delta t\ r - 1 = 0$
and two roots:

$$\begin{cases} r_1 = \lambda\Delta t - \sqrt{1 + (\lambda\Delta t)^2}, & \rightarrow\ |r_1| < 1 \\ r_2 = \lambda\Delta t + \sqrt{1 + (\lambda\Delta t)^2} & \rightarrow\ |r_2| > 1 \end{cases}$$

We have a stable (forward) recurrence, if $|r_{1,2}| < 1$
and a stable (backward) recurrence, if $|r_{1,2}| > 1$

$\Rightarrow$ the above method is *un*stable!

A semi-stable ODE [7]

However... define the forward shift operator: $Ey_{n-1} = y_n$ $\Rightarrow E^2 y_{n-1} = Ey_n = y_{n+1}$. We can rewrite/decompose the above method (in the sense of a BV method) as

$$(E - r_1 I)(E - r_2 I) y_{n-1} = 0$$

or split:

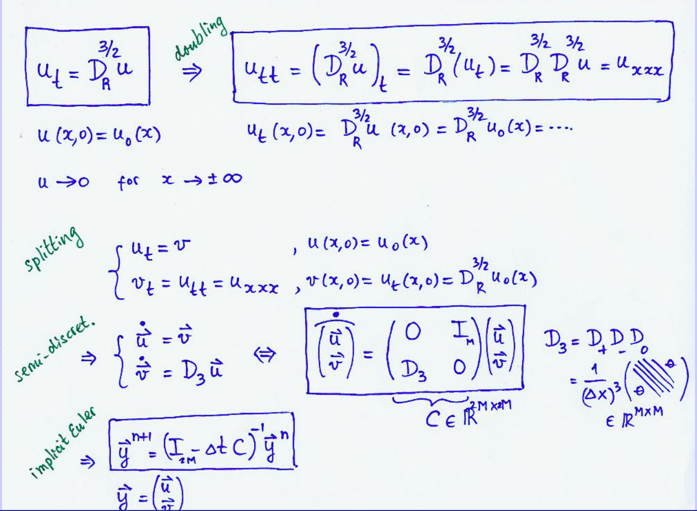
$$\begin{cases} (E - r_1 I) z_n = 0 \\ (E - r_2 I) y_{n-1} = z_n \end{cases}$$

rewritten as:

$$\begin{cases} z_{n+1} = r_1 z_n \quad \text{(a forward recurrence for } z_n \text{ with } |r_1| < 1) \\ y_n = r_2 y_{n-1} + z_n \quad \text{(a backward recurrence for } y_n \text{ with } |r_2| > 1) \end{cases}$$

$\Rightarrow$ the full recurrence method, seen as a BV method, is *unconditionally* stable!

Doubling-splitting for $\alpha = \frac{3}{2}$ [1]



$$\boxed{u_t = D_R^{3/2} u} \quad \overset{\text{doubling}}{\Rightarrow} \quad \boxed{u_{tt} = \left(D_R^{3/2} u\right)_t = D_R^{3/2}(u_t) = D_R^{3/2} D_R^{3/2} u = u_{xxx}}$$

$$u(x,0) = u_0(x) \qquad u_t(x,0) = D_R^{3/2} u\,(x,0) = D_R^{3/2} u_0(x) = \cdots$$

$$u \to 0 \quad \text{for} \quad x \to \pm\infty$$

splitting

$$\begin{cases} u_t = v & , u(x,0) = u_0(x) \\ v_t = u_{tt} = u_{xxx} & , v(x,0) = u_t(x,0) = D_R^{3/2} u_0(x) \end{cases}$$

semi-discret.

$$\Rightarrow \begin{cases} \dot{\vec{u}} = \vec{v} \\ \dot{\vec{v}} = D_3 \vec{u} \end{cases} \Leftrightarrow \underbrace{\boxed{\dot{\begin{pmatrix} \vec{u} \\ \vec{v} \end{pmatrix}} = \begin{pmatrix} 0 & I_M \\ D_3 & 0 \end{pmatrix} \begin{pmatrix} \vec{u} \\ \vec{v} \end{pmatrix}}}_{C \in \mathbb{R}^{2M \times 2M}} \qquad D_3 = D_+ D_- D_0 = \frac{1}{(\Delta x)^3} \begin{pmatrix} \ddots & \ddots & 0 \\ 0 & \ddots & \ddots \end{pmatrix} \in \mathbb{R}^{M \times M}$$

implicit Euler

$$\Rightarrow \boxed{\vec{y}^{\,n+1} = \left(I_{2M} - \Delta t\, C\right)^{-1} \vec{y}^{\,n}}$$

$$\vec{y} = \begin{pmatrix} \vec{u} \\ \vec{v} \end{pmatrix}$$

Doubling-splitting for $\alpha = \frac{3}{2}$ [2]

Second-order approximation of u_{xxx} at x_i:

$$D_3 = \frac{1}{2(\Delta x)^3} \begin{pmatrix} 0 & -2 & 1 & 0 & \dots & \dots & 0 \\ 2 & 0 & -2 & 1 & 0 & \dots & 0 \\ -1 & 2 & 0 & -2 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & -1 & 2 & 0 & -2 & 1 \\ 0 & \dots & 0 & -1 & 2 & 0 & -2 \\ 0 & \dots & \dots & 0 & -1 & 2 & 0 \end{pmatrix}$$

Doubling-splitting for $\alpha = \frac{3}{2}$ [3]

Boundary-value methods:

⋆ Allen & Severn 1951, Miller 1952, Fox 1953, Carasso & Parter 1970

⋆ Axelsson & Verwer 1985, Brugnano & Trigiante 1998

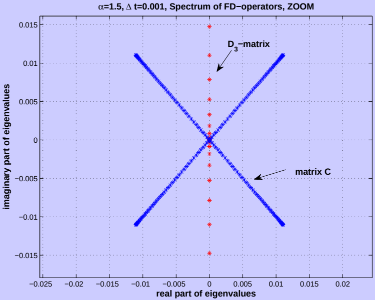
Boundary-value approximation:

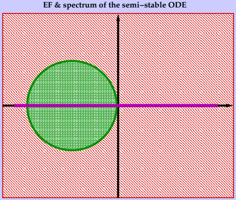
$$\begin{cases} \vec{y}^0 = \vec{y}_0 \\ \vec{y}^{n+1} - 2\Delta t C \vec{y}^n - \vec{y}^{n-1} = \vec{0}, \quad n = 1, ..., N-1 \\ \vec{y}^N - \Delta t C \vec{y}^N - \vec{y}^{N-1} = \vec{0} \end{cases}$$

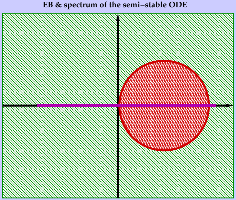
with $t_{n+1} = t_n + \Delta t, \quad N = \frac{T}{\Delta t}$.

$$\Rightarrow \boxed{M\vec{\eta} = \vec{b}}$$

Eigenvalue distribution & stability regions







A dispersive-wave equation [1]

$$\begin{cases} u_{tt} = u_{xxx}, \quad (x,t) \in [0,1] \times [0,0.3] \\ u(x,0) = \sin(2\pi x), \quad u_t(x,0) = 0 \ \ \text{\& periodic BCs} \end{cases}$$

with exact solution

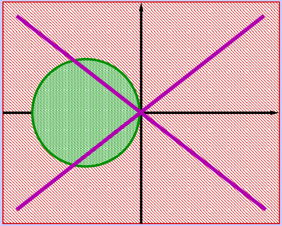
$$u(x,t) = \frac{1}{2}[\mathrm{e}^{2\pi^{\frac{3}{2}}t} \sin(2\pi x - 2\pi^{\frac{3}{2}} t) + \mathrm{e}^{-2\pi^{\frac{3}{2}}t} \sin(2\pi x + 2\pi^{\frac{3}{2}} t)]$$

Application areas:

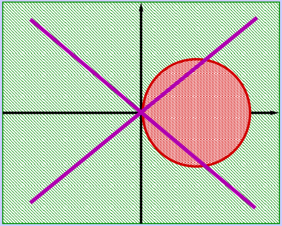
hydrodynamics, ‘Harry Dym equation’, potential theory, ...

A dispersive-wave equation [2]

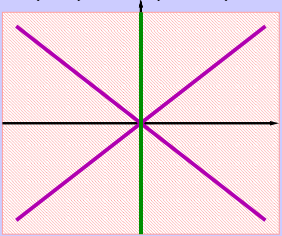
EF & spectrum of the dispersive wave equation



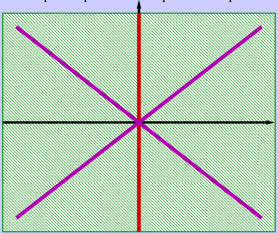
EB & spectrum of the dispersive wave equation



Midpoint & spectrum of the dispersive wave equation



BV–Midpoint & spectrum of the dispersive wave equation



A dispersive-wave equation [3]

BV-method:

$$\begin{cases} \vec{y}_0 = \dots \qquad \text{(IC)} \\ \vec{y}_{n+1} = \vec{y}_{n-1} + 2\Delta t C \vec{y}_n, \;\; n = 1, \dots, N-1 \qquad \text{(MP)} \\ \vec{y}_N = \vec{y}_{N-1} + \Delta t C \vec{y}_N \quad \text{(EB final condition)} \end{cases}$$

with $C := \begin{pmatrix} \mathcal{O} & \mathcal{I} \\ \mathcal{D}_3 & \mathcal{O} \end{pmatrix}$

Note: $\sigma(C) \subset \sqrt{i}\;\mathbb{R} \not\subset \mathcal{S}_{\mathcal{EF}}$ and $\not\subset \mathcal{S}_{\mathcal{EB}}$, but $\subset \mathcal{S}_{\mathcal{BV}mp} = \mathbb{C} \setminus (i\;\mathbb{R})$

A dispersive-wave equation [4]

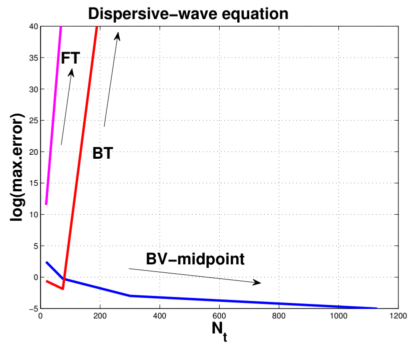
Maximum error at $t = 0.3$ and cpu-time in seconds:

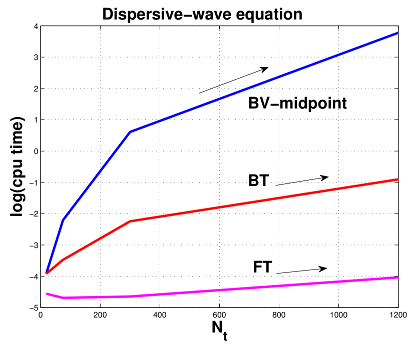
$\Delta x = 0.0125$	BV_{er}	BV_{ti}	FT_{er}	FT_{ti}	BT_{er}	BT_{ti}
$\Delta t = 0.01600$	11.5146	0.02	$\mathcal{O}(10^5)$	0.0105	0.5532	0.0199
$\Delta t = 0.00400$	0.7859	0.11	$\mathcal{O}(10^{19})$	0.0092	0.1528	0.0310
$\Delta t = 0.00100$	0.0508	1.84	$\mathcal{O}(10^{71})$	0.0096	$\mathcal{O}(10^{35})$	0.1061
$\Delta t = 0.00025$	0.0056	43.71	$\mathcal{O}(10^{86})$	0.0177	$\mathcal{O}(10^{104})$	0.4053

Maximum error at $t = 0.3$:

BV-method	$\Delta x = 0.2$	$\Delta x = 0.1$	$\Delta x = 0.05$	$\Delta x = 0.025$
$\Delta t = 0.0020$	0.9104	0.3628	0.2170	0.2012
$\Delta t = 0.0010$	0.8462	0.2859	0.0891	0.0561
$\Delta t = 0.0005$	0.8305	0.2648	0.0650	0.0223
$\Delta t = 0.0025$	0.8265	0.2598	0.0611	0.0160

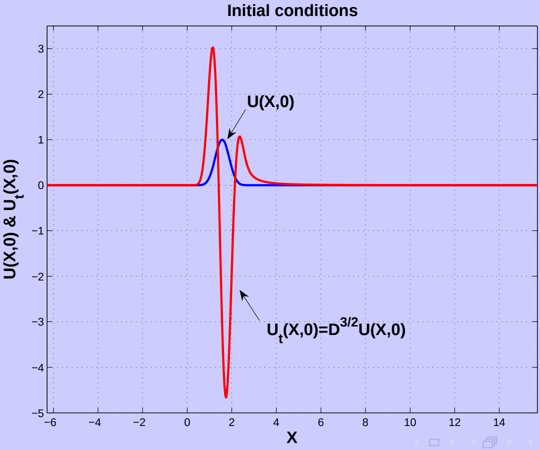
A dispersive-wave equation [5]



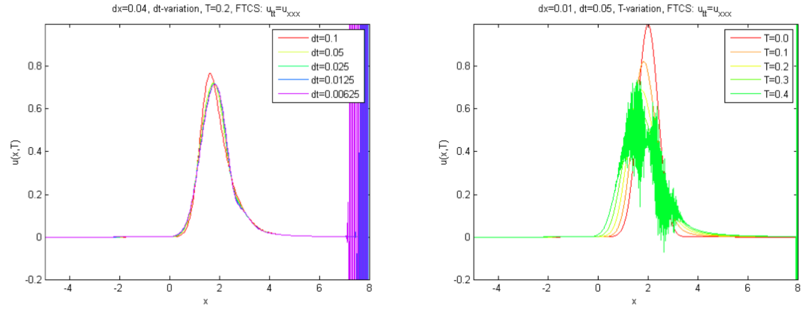


A space-fractional heat equation [1]

Fractional order $\alpha = \frac{3}{2}$ & initial conditions:

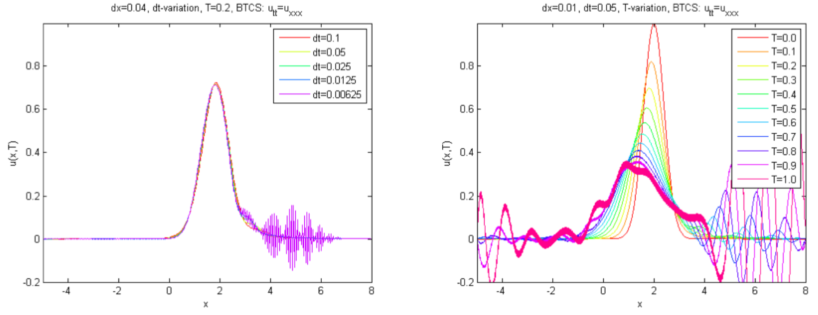


A space-fractional heat equation [2]



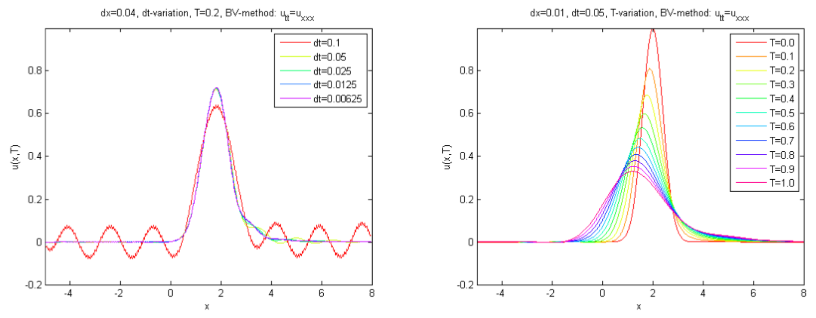
Forward in time (EF)

A space-fractional heat equation [3]



Backward in time (EB)

A space-fractional heat equation [4]



Boundary-Value Method (BVM); midpoint + EB final condition

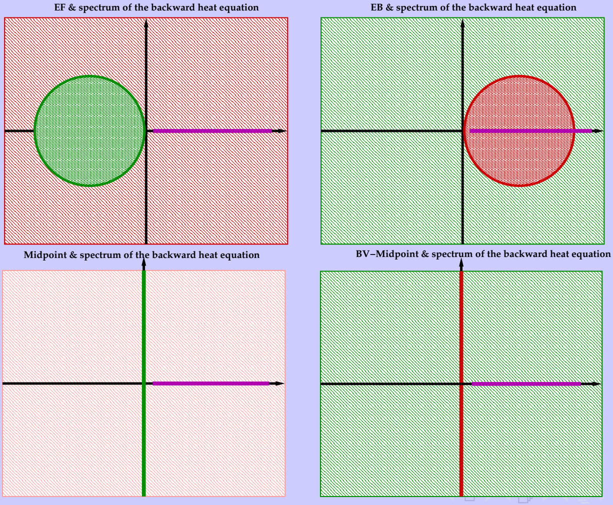
A backward heat equation [1]

$$\begin{cases} u_t = -u_{xx}, \quad (x,t) \in [0,1] \times [0,0.3] \\ u(x,0) = \sin(\pi x), \quad u(0,t) = u(1,t) = 0 \end{cases}$$

with exact solution

$$u(x,t) = \mathrm{e}^{\pi^2 t} \sin(\pi x)$$

A backward heat equation [2]



A backward heat equation [3]

Maximum error of FTCS and BTCS at $t = 0.3$ and cpu-time:

FTCS	$\Delta x = 0.1$	*sec*	$\Delta x = 0.05$	*sec*	$\Delta x = 0.025$	*sec*
$\Delta t = 0.02$	0.91	$\mathcal{O}(10^{-4})$	0.86	$\mathcal{O}(10^{-4})$	$\mathcal{O}(10^{2})$	$\mathcal{O}(10^{-4})$
$\Delta t = 0.01$	0.63	$\mathcal{O}(10^{-4})$	$\mathcal{O}(10^{7})$	$\mathcal{O}(10^{-4})$	$\mathcal{O}(10^{17})$	$\mathcal{O}(10^{-4})$
$\Delta t = 0.005$	4.56	$\mathcal{O}(10^{-4})$	$\mathcal{O}(10^{20})$	$\mathcal{O}(10^{-4})$	$\mathcal{O}(10^{42})$	$\mathcal{O}(10^{-4})$
$\Delta t = 0.0025$	$\mathcal{O}(10^{6})$	$\mathcal{O}(10^{-4})$	$\mathcal{O}(10^{38})$	$\mathcal{O}(10^{-4})$	$\mathcal{O}(10^{80})$	$\mathcal{O}(10^{-4})$

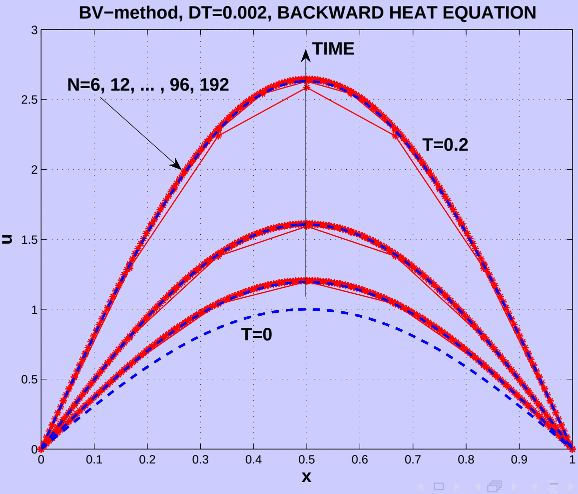
BTCS	$\Delta x = 0.1$	*sec*	$\Delta x = 0.05$	*sec*	$\Delta x = 0.025$	*sec*
$\Delta t = 0.02$	1.20	$\mathcal{O}(10^{-4})$	1.29	$\mathcal{O}(10^{-4})$	1.32	$\mathcal{O}(10^{-4})$
$\Delta t = 0.01$	0.55	$\mathcal{O}(10^{-4})$	13.79	$\mathcal{O}(10^{-4})$	2.98	$\mathcal{O}(10^{-3})$
$\Delta t = 0.005$	$\mathcal{O}(10^{-16})$	$\mathcal{O}(10^{-4})$	$\mathcal{O}(10^{13})$	$\mathcal{O}(10^{-3})$	$\mathcal{O}(10^{10})$	$\mathcal{O}(10^{-3})$
$\Delta t = 0.0025$	$\mathcal{O}(10^{110})$	$\mathcal{O}(10^{-4})$	$\mathcal{O}(10^{65})$	$\mathcal{O}(10^{-3})$	$\mathcal{O}(10^{54})$	$\mathcal{O}(10^{-3})$

A backward heat equation [4]

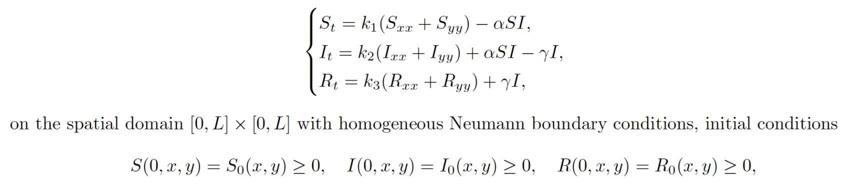
Maximum error of BVM at $t = 0.3$ and cpu-time:

BVM	$\Delta x = 0.1$	*sec*	$\Delta x = 0.05$	*sec*	$\Delta x = 0.025$	*sec*
$\Delta t = 0.015$	58.75	0.005	53.21	0.009	52.04	0.021
$\Delta t = 0.0075$	11.73	0.017	13.32	0.035	13.75	0.076
$\Delta t = 0.00375$	1.82	0.063	2.32	0.130	2.45	0.272
$\Delta t = 0.001875$	0.096	0.243	0.47	0.500	0.57	1.111

A backward heat equation [5]



(backward) SIR-model [1]



$$\begin{cases} S_t = k_1(S_{xx} + S_{yy}) - \alpha S I, \\ I_t = k_2(I_{xx} + I_{yy}) + \alpha S I - \gamma I, \\ R_t = k_3(R_{xx} + R_{yy}) + \gamma I, \end{cases}$$

on the spatial domain $[0, L] \times [0, L]$ with homogeneous Neumann boundary conditions, initial conditions

$$S(0,x,y) = S_0(x,y) \geq 0, \quad I(0,x,y) = I_0(x,y) \geq 0, \quad R(0,x,y) = R_0(x,y) \geq 0,$$

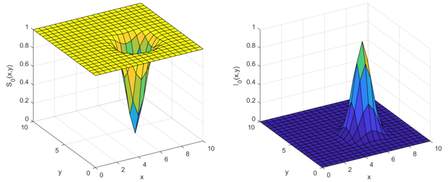


Figure 4.3: The initial density of the susceptible compartment $S_0(x, y)$ on the left and the initial density of the infected compartment $I_0(x, y)$ on the right, represented on the uniform discretization of the spatial domain defined by $\Delta x = \Delta y = \frac{1}{2}$.

(backward) SIR-model [2]

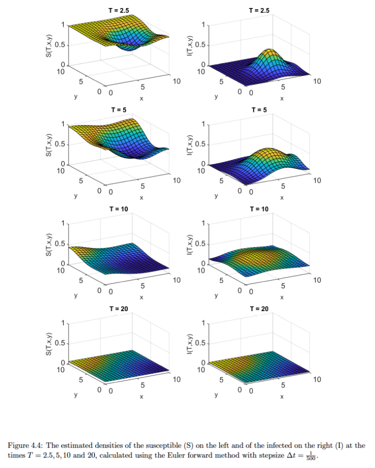
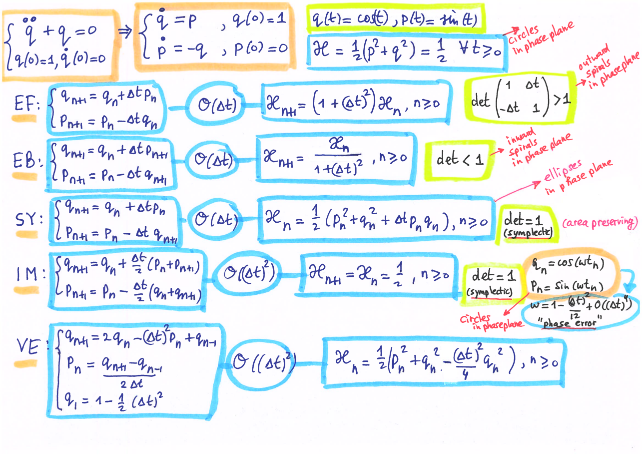


Figure 4.4: The estimated densities of the susceptible (S) on the left and of the infected on the right (I) at the times $T = 2.5, 5, 10$ and 20, calculated using the Euler forward method with stepsize $\Delta t = \frac{1}{500}$.

Periodicity [1]



$$\begin{cases}\ddot{q}+q=0\\ q(0)=1,\ \dot{q}(0)=0\end{cases} \Rightarrow \begin{cases}\dot{q}=p, & q(0)=1\\ \dot{p}=-q, & p(0)=0\end{cases}$$

$q(t)=\cos(t),\ p(t)=\sin(t)$

$\mathcal{H}=\frac{1}{2}(p^2+q^2)=\frac{1}{2}\ \forall t\geq 0$ → circles in phase plane

EF: $\begin{cases}q_{n+1}=q_n+\Delta t\,p_n\\ p_{n+1}=p_n-\Delta t\,q_n\end{cases}$ — $\mathcal{O}(\Delta t)$ — $\mathcal{H}_{n+1}=(1+(\Delta t)^2)\mathcal{H}_n,\ n\geq 0$ — $\det\begin{pmatrix}1 & \Delta t\\ -\Delta t & 1\end{pmatrix}>1$ → outward spirals in phaseplane

EB: $\begin{cases}q_{n+1}=q_n+\Delta t\,p_{n+1}\\ p_{n+1}=p_n-\Delta t\,q_{n+1}\end{cases}$ — $\mathcal{O}(\Delta t)$ — $\mathcal{H}_{n+1}=\dfrac{\mathcal{H}_n}{1+(\Delta t)^2},\ n\geq 0$ — $\det<1$ → inward spirals in phase plane

SY: $\begin{cases}q_{n+1}=q_n+\Delta t\,p_n\\ p_{n+1}=p_n-\Delta t\,q_{n+1}\end{cases}$ — $\mathcal{O}(\Delta t)$ — $\mathcal{H}_n=\frac{1}{2}(p_n^2+q_n^2+\Delta t\,p_n q_n),\ n\geq 0$ → ellipses in phase plane — $\det=1$ (symplectic) (area preserving)

IM: $\begin{cases}q_{n+1}=q_n+\frac{\Delta t}{2}(p_n+p_{n+1})\\ p_{n+1}=p_n-\frac{\Delta t}{2}(q_n+q_{n+1})\end{cases}$ — $\mathcal{O}((\Delta t)^2)$ — $\mathcal{H}_{n+1}=\mathcal{H}_n=\frac{1}{2},\ n\geq 0$ — $\det=1$ (symplectic) → circles in phaseplane

$q_n=\cos(\omega t_n)$

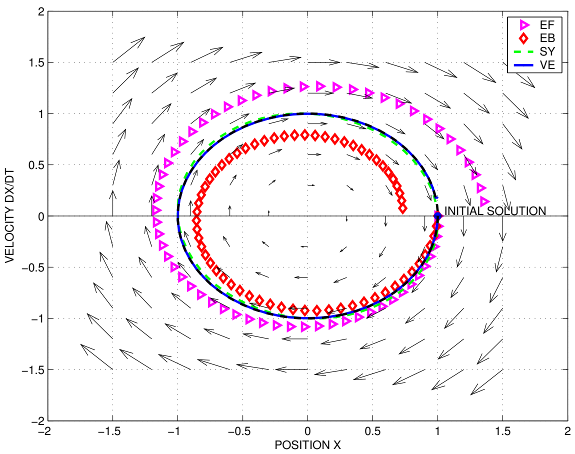
$p_n=\sin(\omega t_n)$

$\omega=1-\frac{(\Delta t)^2}{12}+O((\Delta t)^4)$ "phase error"

VE: $\begin{cases}q_{n+1}=2q_n-(\Delta t)^2p_n+q_{n-1}\\ p_n=\dfrac{q_{n+1}-q_{n-1}}{2\Delta t}\\ q_1=1-\frac{1}{2}(\Delta t)^2\end{cases}$ — $\mathcal{O}((\Delta t)^2)$ — $\mathcal{H}_n=\frac{1}{2}\left(p_n^2+q_n^2-\frac{(\Delta t)^2}{4}q_n^2\right),\ n\geq 0$

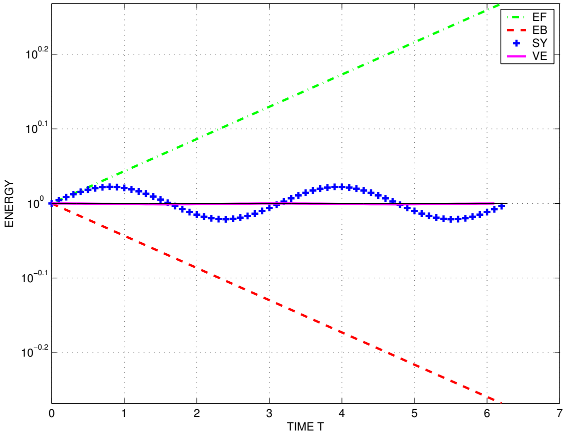
Periodicity [2]

Phase plane solutions for four traditional time-integrators:



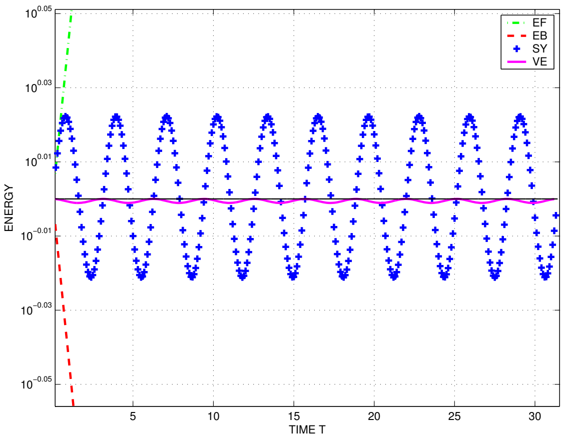
Periodicity [3a]

Total energy for these four time-integrators:

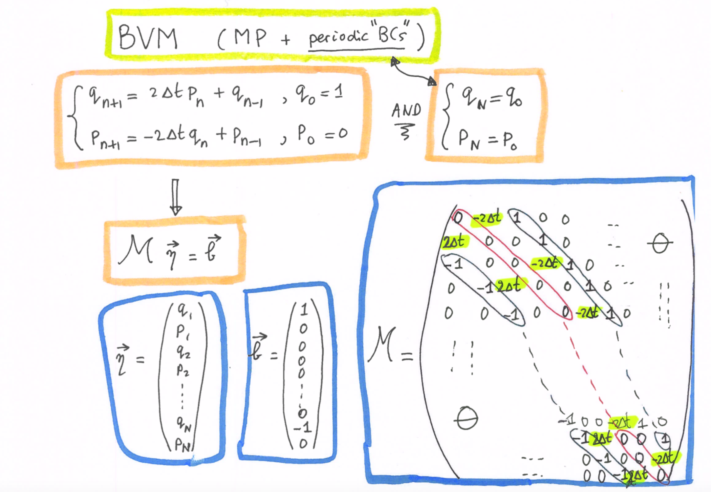


Periodicity [3b]

Total energy (close up):



Periodicity [4]



BVM (MP + periodic "BCs")

$$\left\{\begin{array}{ll} q_{n+1} = 2\Delta t\, p_n + q_{n-1}, & q_0 = 1 \\ p_{n+1} = -2\Delta t\, q_n + p_{n-1}, & p_0 = 0 \end{array}\right. \quad \text{AND} \quad \left\{\begin{array}{l} q_N = q_0 \\ p_N = p_0 \end{array}\right.$$

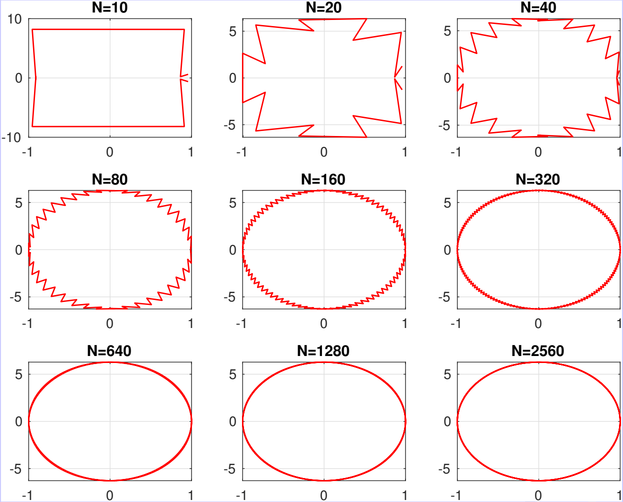
$$\Downarrow$$

$$\mathcal{M}\vec{\eta} = \vec{b}$$

$$\vec{\eta} = \begin{pmatrix} q_1 \\ p_1 \\ q_2 \\ p_2 \\ \vdots \\ q_N \\ p_N \end{pmatrix} \qquad \vec{b} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ -1 \\ 0 \end{pmatrix}$$

$$\mathcal{M} = \begin{pmatrix} 0 & -2\Delta t & 1 & 0 & 0 & \cdots & & & & \Theta \\ 2\Delta t & 0 & 0 & 1 & 0 & \cdots & & & & \\ -1 & 0 & 0 & -2\Delta t & 1 & 0 & \cdots & & & \vdots \\ 0 & -1 & 2\Delta t & 0 & 0 & 1 & 0 & \cdots & & \vdots \\ 0 & 0 & -1 & 0 & 0 & -2\Delta t & 1 & 0 & & \vdots \\ \vdots & \vdots & & \ddots & & \ddots & & \ddots & & \\ & & & -1 & 0 & 0 & -2\Delta t & 1 & 0 & \\ \Theta & & & & -1 & 2\Delta t & 0 & 0 & 1 & \\ & & & \cdots & 0 & -1 & 0 & 0 & -2\Delta t & \\ & & & \cdots & 0 & 0 & -1 & 2\Delta t & 0 & \end{pmatrix}$$

Periodicity [5]



Periodicity [6]