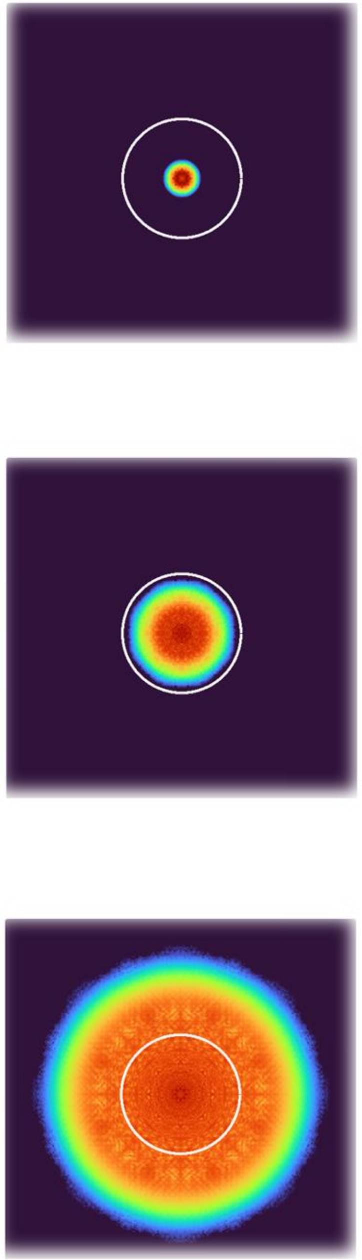

An algorithm for verified computation of semigroups

Matthew J. Colbrook
University of Cambridge

IMA Leslie Fox Prize Meeting, 26 June 2023

Based on: C. "*Computing semigroups with error control.*" SINUM 60.1 (2022): 396-422.

*"The **INFINITE**! No other question has ever moved so profoundly the spirit of humankind; no other idea has so fruitfully stimulated the intellect; yet no other concept stands in greater need of clarification."* — David Hilbert (1925)

solve-then-discretise

The problem

generator: linear operator
(typically unbounded)

initial condition

$$\frac{\mathrm{d}u}{\mathrm{d}t} = Au, \qquad u(0) = u_0 \in \mathcal{H}$$

infinite-dimensional
Hilbert space
inner product $\langle \cdot, \cdot \rangle$

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GOAL: Compute $u(t)$
- **For arbitrary A.**
- **For arbitrary u_0.**
- **To any desired accuracy.**

Error control:
verifiable computation

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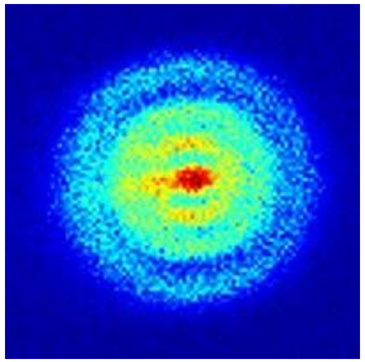
E.g., time-dependent PDEs, such as Schrödinger equation



Orbital of excited hydrogen

$$\frac{\partial \psi}{\partial t} = i(\Delta - V)\psi, \qquad \psi \in L^2(\mathbb{R}^d),$$

inf discrete systems, higher-order time derivatives, etc.

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Error control: verifiable computation

Julian Schwinger
(Nobel Prize in Physics 1965)

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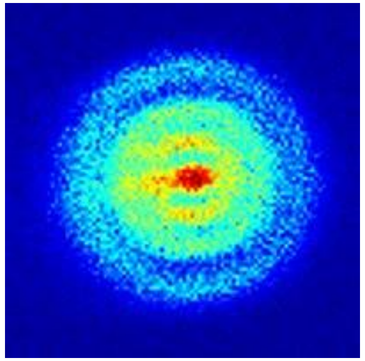

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- Schwinger, *"Unitary operator bases,"* **Proceedings of the National Academy of Sciences**, 1960.
- Weyl, *"The theory of groups and quantum mechanics,"* **Dover**, 1931.
- Digernes, Varadarajan, Varadhan, *"Finite approximations to quantum systems,"* **Rev. Math. Phys.**, 1994.

Common paradigm: discretise-then-solve

$$A \to \mathbb{A} \in \mathbb{C}^{n \times n}$$

- **Domain truncation and absorbing boundary conditions.**
  - Engquist, Majda, *“Absorbing boundary conditions for numerical simulation of waves,”* PNAS, 1977.
- **Exponential integrators and splitting methods.**
  - Hochbruck, Ostermann, *“Exponential integrators,”* Acta Numerica, 2010.
  - Jahnke, Lubich, *“Error bounds for exponential operator splittings,"* BIT Numer. Math., 2000.
  - McLachlan, Quispel, *“Splitting methods,”* Acta Numerica, 2002.
- **Finite differences and generalised Sobolev-type norms.**
  - Jovanović, Süli, *“Analysis of finite difference schemes for linear partial differential equations with generalized solutions,”* Springer Science & Business Media, 2013.
- **Rational approximations with time-stepping.**
  - Crouzeix, Larsson, Piskarev, Thomée, *“The stability of rational approximations of analytic semigroups,”* BIT Numer. Math., 1993.
- **Variational/projection methods.**
  - Lasser, Lubich, *“Computing quantum dynamics in the semiclassical regime,”* Acta Numerica, 2020.
  - Dirac, *“Note on exchange phenomena in the Thomas atom,”* Proc. Cambridge Phil. Soc. 1930.

Common paradigm: discretise-then-solve

$$A \to \mathbb{A} \in \mathbb{C}^{n \times n}$$

Challenges:

- **Unbounded** $\boldsymbol{A}$ (e.g., for splitting methods).
- Bound error from $A \to \mathbb{A}$.
- PDEs on **unbounded domains**:
  - Truncate physical domain.
  - Discretise operator restricted to truncated domain.

Can we rigorously deal with domain truncation?

- Often need to show decay and/or regularity of $u(t)$.
- Can be more difficult to study $\mathbb{A}$ than A (e.g., bounding evals of $\mathbb{A}$)!

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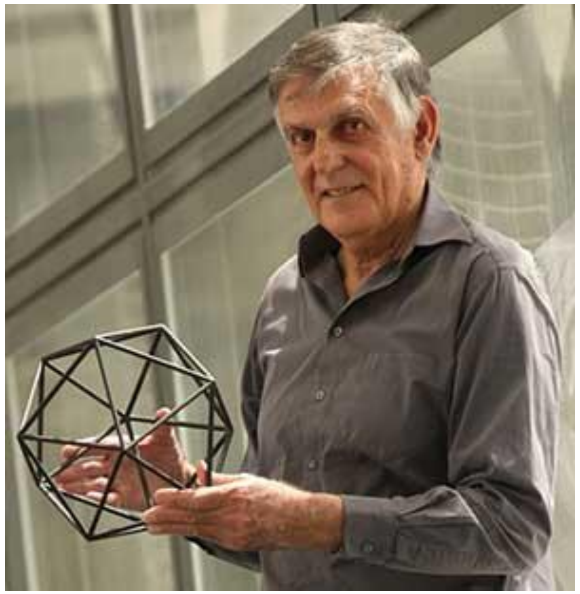
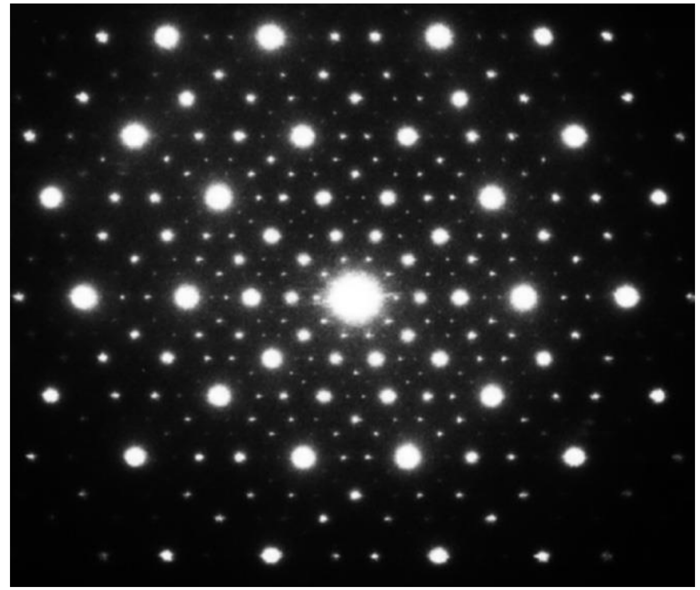
Theme of talk: solve-then-discretise

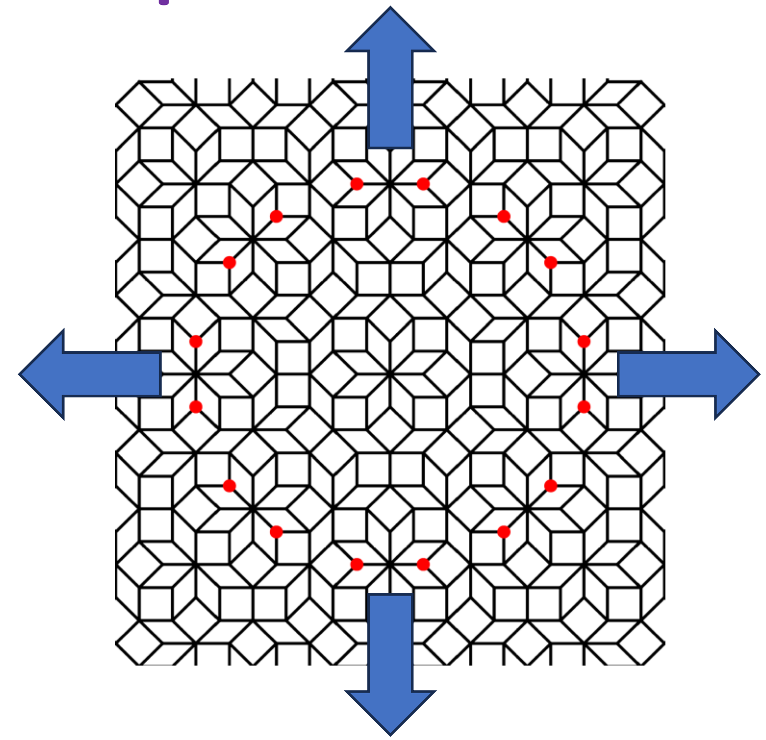
Example where standard paradigm fails: aperiodic media



Dan Shechtman
(Nobel Prize in Chemistry 2011 for
"a paradigm shift within chemistry")



$Al_{63}Cu_{24}Fe_{13}$, icosahedrite.
Bindi, Steinhardt, Yao, Lu,
"Natural quasicrystals," **Science**, 2009.

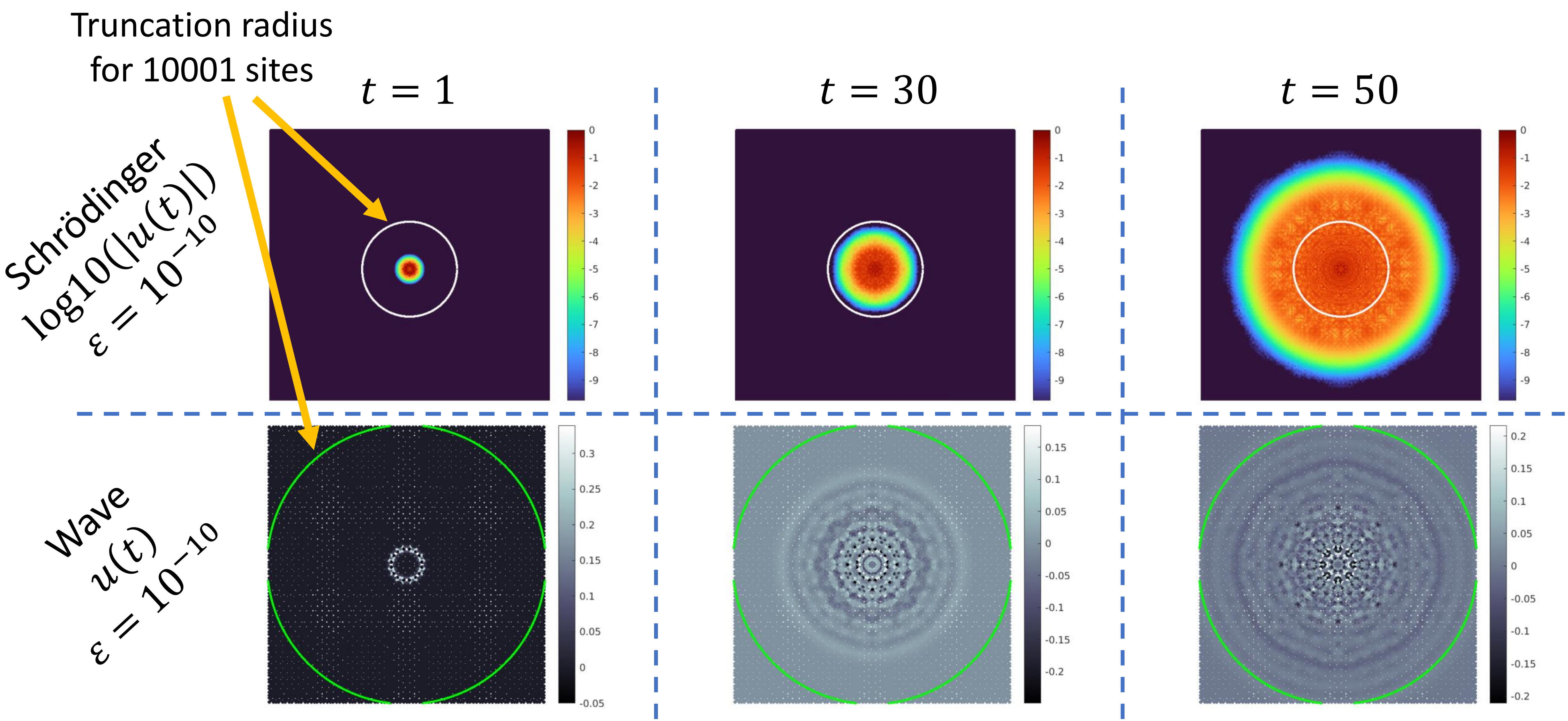


Aperiodic infinite
Ammann-Beenker tile

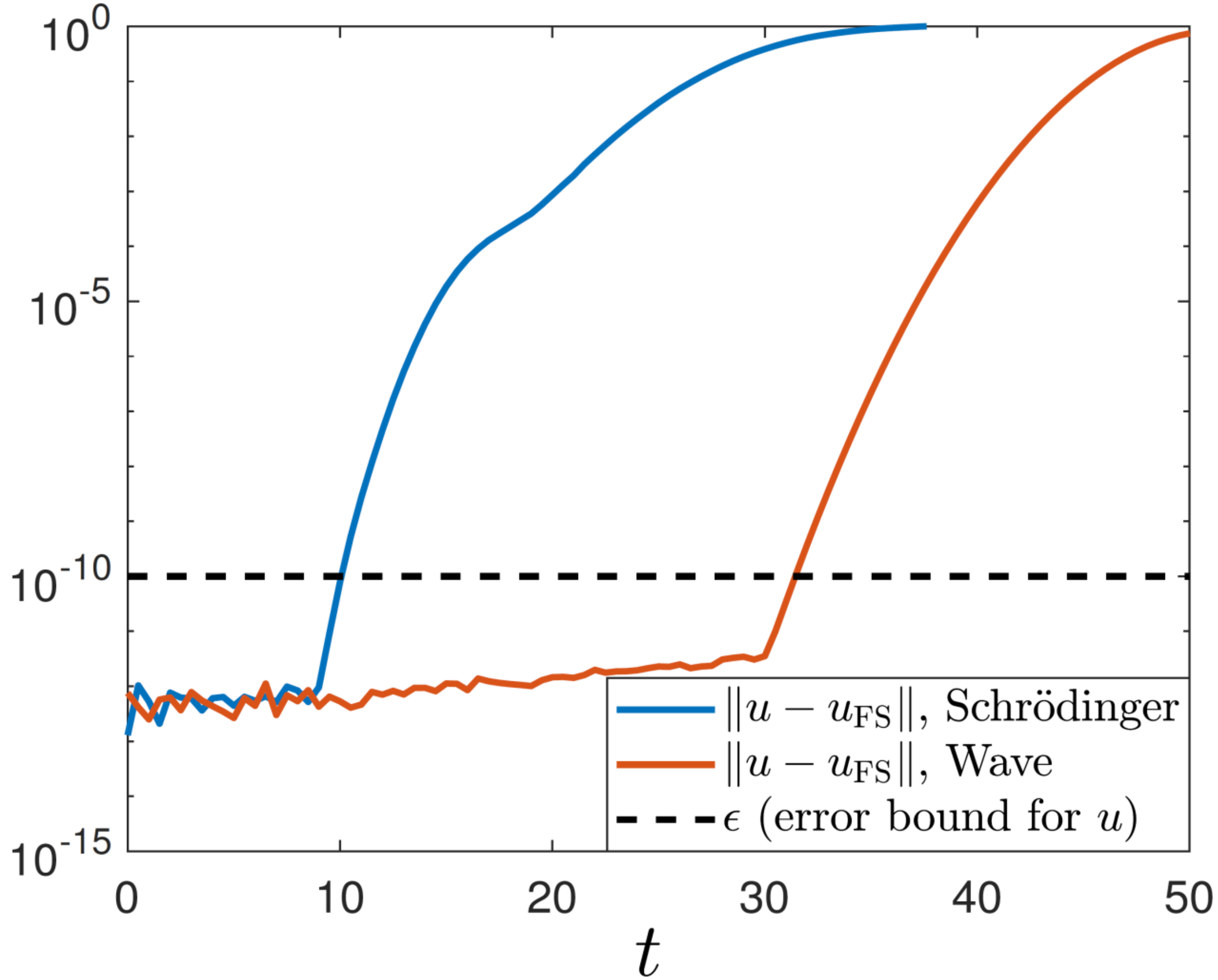
Schrödinger: $\frac{\partial u}{\partial t} = i\Delta u,$ Wave: $\frac{\partial^2 u}{\partial t^2} = \Delta u,$ u_0 localised at red dots

Aperiodicity $\Longrightarrow$ interesting physics ***BUT*** computations difficult.

Solutions computed using method of this talk



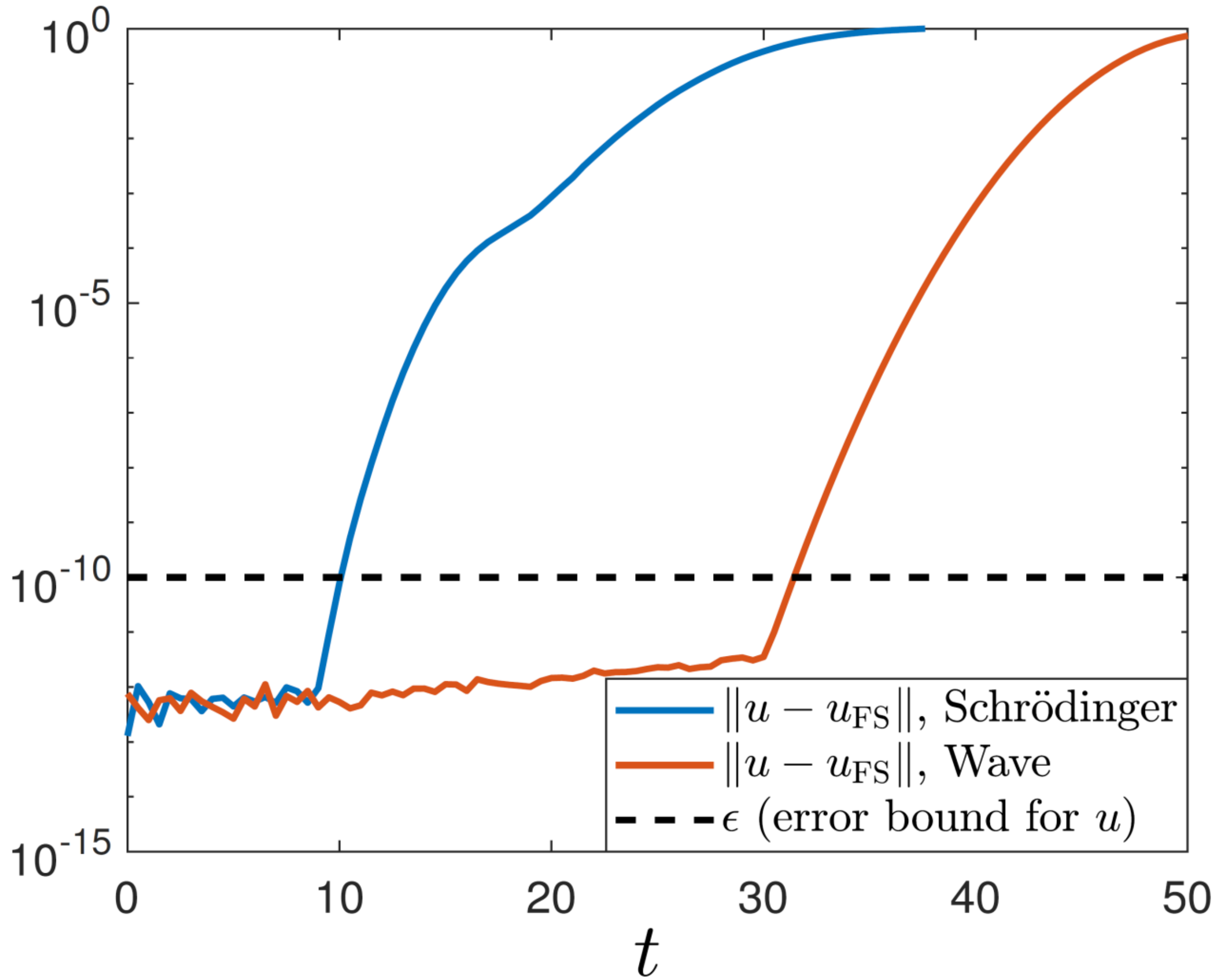
Comparison with naïve truncation



$u_{\rm FS}$: naïve truncation to 10001 sites

u: computed solution, error $< 10^{-10}$

Comparison with naïve truncation



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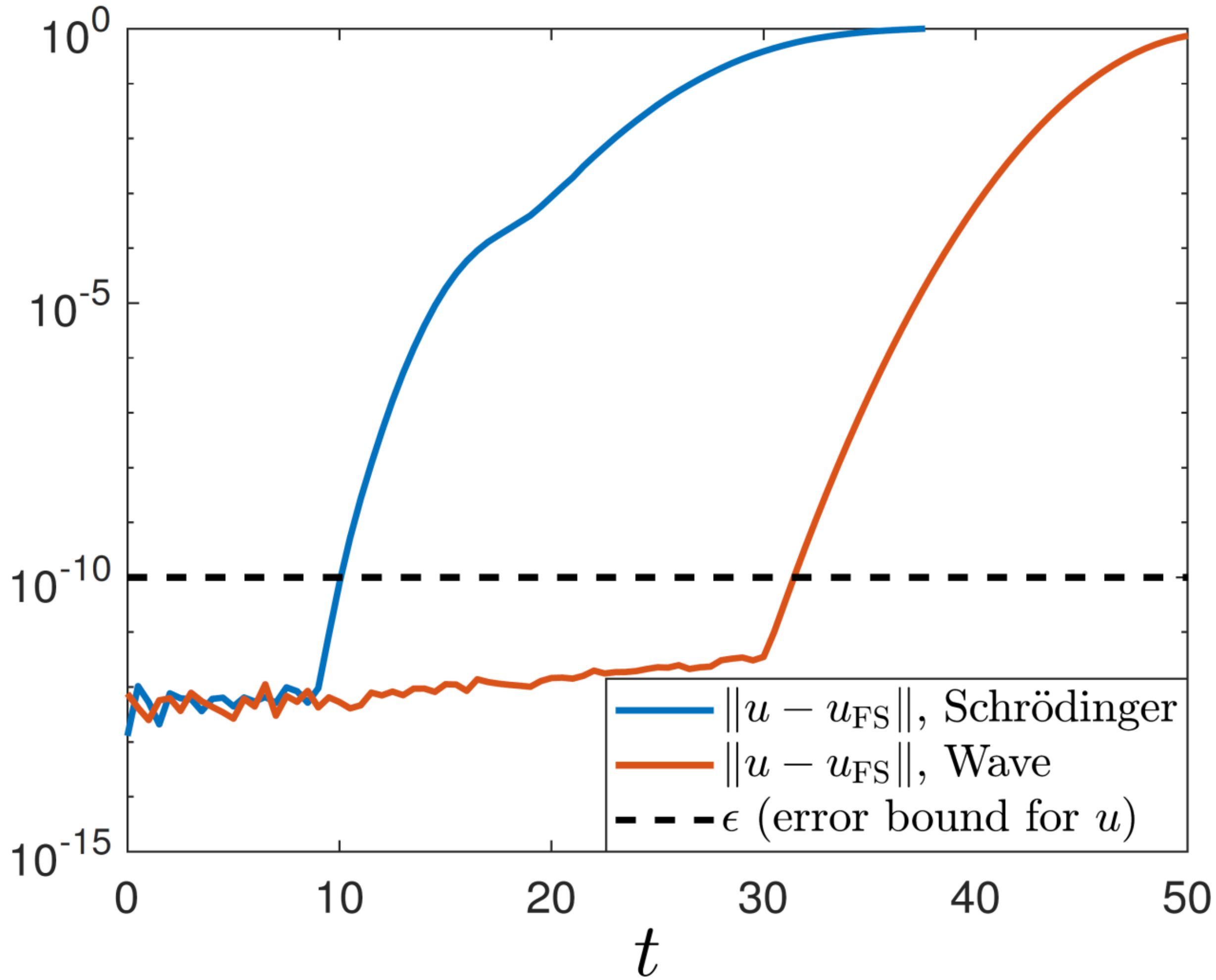
How do we compute u with error guarantee?

Comparison with naïve truncation



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How do we compute u with error guarantee?

solve-then-discretise $\Longrightarrow$ **Adaptive truncation!**

Why this is NOT just a matrix exponential

Strongly continuous semigroup

$$\frac{\mathrm{d}u}{\mathrm{d}t} = Au, \qquad u(0) = u_0 \in \mathcal{H} \qquad (\ddagger)$$

Hille-Yosida Theorem: ($\ddagger$) well-posed if and only if A closed densely defined, and there exists $\omega \in \mathbb{R}$, $M > 0$ such that

$$(1) \quad \mathrm{Sp}(A) \coloneqq \{z \in \mathbb{C}: A - zI \text{ not invertible}\} \subseteq \{z \in \mathbb{C}: \mathrm{Re}(z) \leq \omega\},$$

$$(2) \quad \text{if} \quad \mathrm{Re}(z) > \omega \quad \text{then} \quad \|(A - zI)^{-n}\| \leq \frac{M}{(\mathrm{Re}(z) - \omega)^n} \qquad \forall n \in \mathbb{N}$$

$$(\implies \|u(t)\| \leq M\exp(\omega t)\|u_0\| \ )$$

Einar Hille

Assume ($\ddagger$) well-posed and we know suitable ω and M.

(later: ways to compute these in practice)

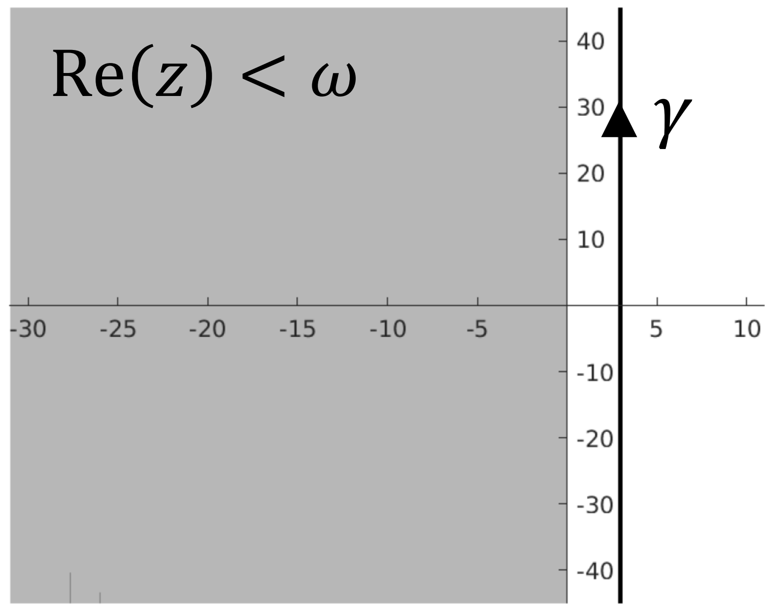
Kōsaku Yosida

- Hille, Phillips, *"Functional analysis and semi-groups,"* **Vol. 31. American Mathematical Soc.**, 1996.
- Pazy, *"Semigroups of linear operators and applications to partial differential equations,"* **Vol. 44. Springer Science & Business Media**, 2012.

Why this is NOT just a matrix exponential

$$\frac{\mathrm{d}u}{\mathrm{d}t} = Au, \qquad u(0) = u_0 \in \mathcal{H}$$

z plane



First attempt: Laplace transform

$$\hat{u}(z) = \int_0^\infty e^{-zs} u(s)\mathrm{d}s = -(A - zI)^{-1} u_0$$

$$u(t) \overset{?}{=} \left[\frac{-1}{2\pi i}\int_\gamma e^{zt}\,(A - zI)^{-1}\mathrm{d}z\right] u_0$$

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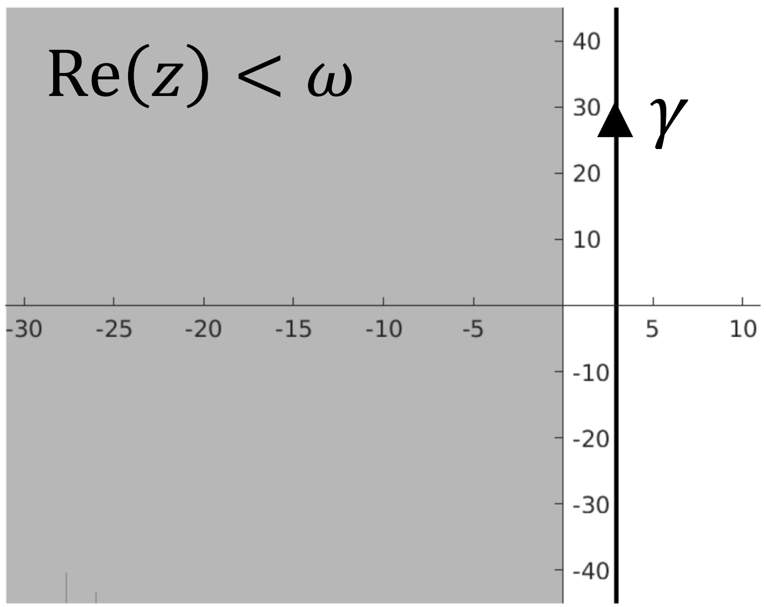

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Problems:

- Integrand need not decay at ∞.
- How to compute $(A - zI)^{-1}$?
- How to bound approximation error (e.g., quadrature)?

Open problem for general $\mathcal{H}$

Does there exist a **universal** algorithm with

INPUT:

- Generator A,
- Time $t > 0$,
- Arbitrary initial condition $u_0 \in \mathcal{H}$,
- Error tolerance $\varepsilon > 0$.

OUTPUT: Approximation of $u(t)$ with error $\leq \varepsilon$ in $\mathcal{H}$?

E.g., for PDEs on $\mathcal{H} = L^2(\mathbb{R}^d)$.

Minimal assumptions on A and u_0.

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Minimal assumptions on A and u_0.

$\boxed{\text{solve-then-discretise}}$

Two parts

- General strongly continuous semigroups.

  E.g., Schrödinger equations, wave equations.

- Analytic semigroups and inverse Laplace transforms.

  E.g., diffusion equations.

$\boxed{\text{solve-then-discretise}}$

$\mathcal{H} = l^2(\mathbb{N})$

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, \qquad A\left(\sum_{k=1}^{\infty} x_k e_k\right) = \sum_{j=1}^{\infty}\left(\sum_{k=1}^{\infty} a_{jk} x_k\right) e_j$$

canonical basis of $l^2(\mathbb{N})$

Input: (A, u_0, t, ε), $A, u_0 \in l^2(\mathbb{N})$, $t > 0$, $\varepsilon > 0$.

Can access (or approximate with error control):

- Matrix evaluations $\langle Ae_k, e_j \rangle, \langle Ae_k, Ae_j \rangle \quad \forall\, j, k \in \mathbb{N}$.
- Coefficients $\langle u_0, u_0 \rangle, \langle u_0, e_j \rangle \quad \forall\, j \in \mathbb{N}$.

Theorem: $\exists$ **universal** algorithm $\Gamma_{l^2(\mathbb{N})}$ using above input such that

$$\left\| \Gamma_{l^2(\mathbb{N})}(A, u_0, t, \varepsilon) - u(t) \right\|_{l^2(\mathbb{N})} \leq \varepsilon.$$

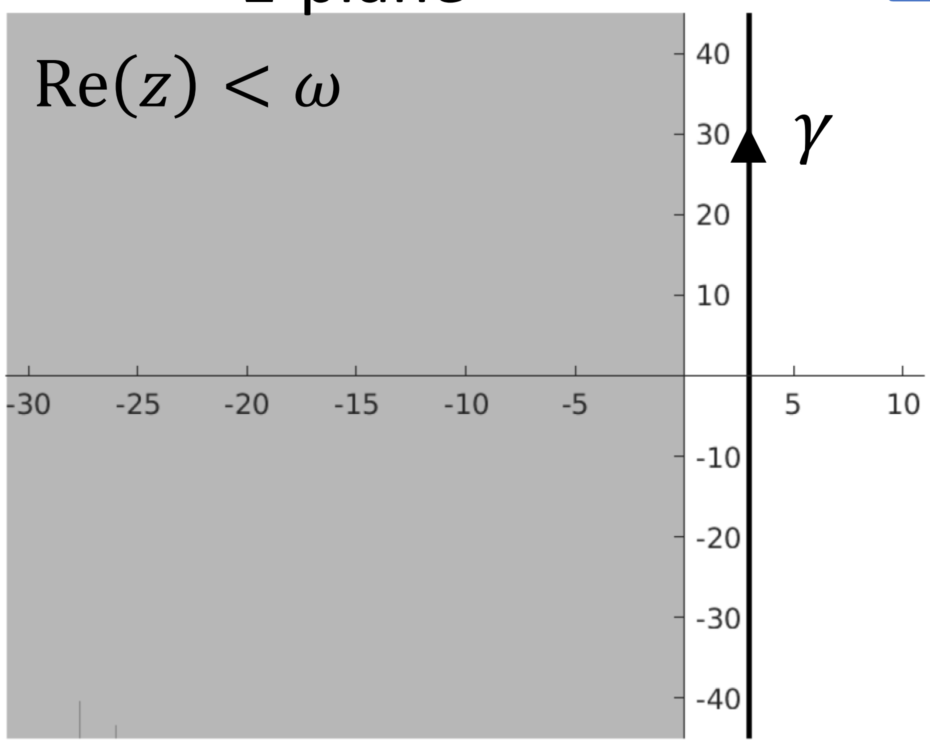
How?

Integrable!

- **Regularisation:**

$$u(t) = (A - (\omega + 2)I)^2 \underbrace{\left[\frac{-1}{2\pi i} \int_{\omega+1-i\infty}^{\omega+1+i\infty} \frac{e^{zt}(A - zI)^{-1}}{(z - (\omega + 2))^2} \mathrm{d}z\right]}_{B} u_0.$$

z plane



solve

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- **Hille-Yosida** controls error

$$u_0 \approx \sum_{j=1}^{M} \langle u_0, e_j\rangle\, e_j, \qquad \exp(At)\, u_0 \approx \sum_{j=1}^{M} \langle u_0, e_j\rangle \exp(At)\, e_j.$$

- **Commutativity**: $ABe_j = BAe_j$ … reduction to computing Be_j.
- **Quadrature** (Hille-Yosida controls error), reduction to computing

$$z \mapsto (A - zI)^{-1} e_j, \qquad j \in \mathbb{N}.$$

Quadrature points

$\boxed{\text{solve}}$

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Quadrature points

solve-then-discretise

Adaptive computation of $z \mapsto (A - zI)^{-1}$

$v = \sum_{j=1}^{M} \langle v, e_j \rangle e_j$

$\mathcal{P}_n: l^2(\mathbb{N}) \longrightarrow \mathbb{C}^n$
$\mathcal{P}_n^*: \mathbb{C}^n \longrightarrow l^2(\mathbb{N})$

$\mathcal{P}_n =$ orthog-projection onto span$\{e_1, \ldots, e_n\}$, $n \geq M$

$T_n(z) = \mathcal{P}_n (A - zI) \mathcal{P}_n^* \in \mathbb{C}^{n \times n}$

$L_n(z) = \mathcal{P}_n (A - zI)^* (A - zI) \mathcal{P}_n^* \in \mathbb{C}^{n \times n}$

$r_n = L_n(z)^{-1} T_n(z)^* \mathcal{P}_n v \in \mathbb{C}^n$

$\min_{y \in \mathbb{C}^n} \|(A - zI)\mathcal{P}_n^* y - v\|$
Infinite-dimensional least-squares!

Theorem: $\|\mathcal{P}_n^* r_n - (A - zI)^{-1} v\|$

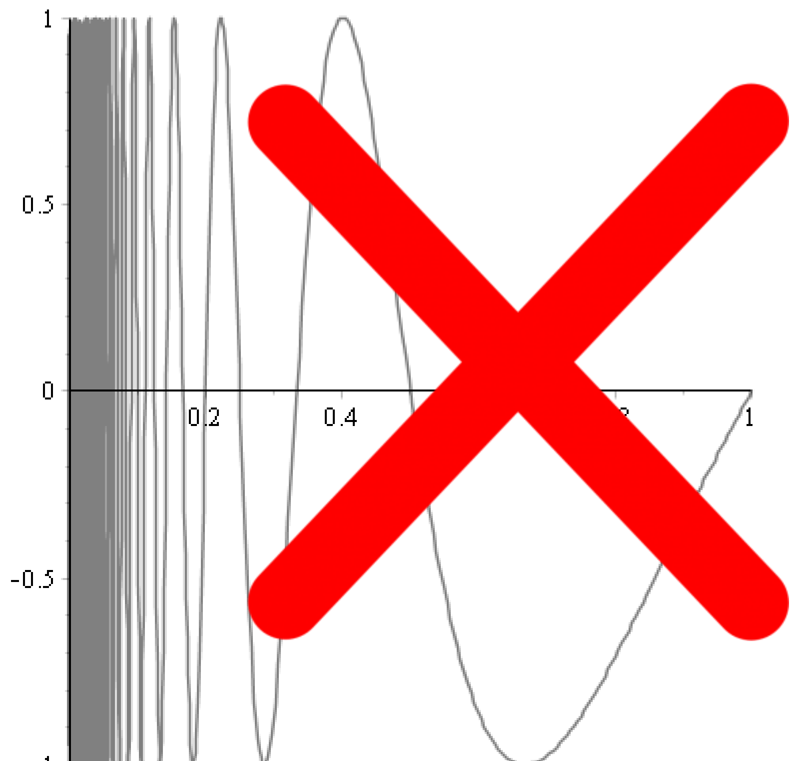
$$\leq \underbrace{\|(A - zI)^{-1}\|}_{\text{Bounded by Hille-Yosida}} \underbrace{\sqrt{r_n^* L_n(z) r_n - 2\mathrm{Re}\big((\mathcal{P}_n v)^* T_n(z) r_n\big) + \|v\|^2}}_{\text{Converges to zero and explicit! Adaptively increase } n \text{ to make small.}}$$

Example: differential operators on $L^2(\mathbb{R}^d)$

$$\frac{\partial u}{\partial t} = Au, \qquad [Av](x) = \sum_{k \in \mathbb{Z}^d_{\geq 0}, |k| \leq N} c_k(x)\, [\partial^k v](x)$$

Assume: $\{c_k\}$ poly bounded, locally bounded total variation.

Input: $(\{c_k\}, u_0, t, \varepsilon)$, coeffs. $\{c_k\}$, $u_0 \in L^2(\mathbb{R}^d)$, $t > 0$, $\varepsilon > 0$.



Wild oscillations only at infinity.

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Can access (or approximate with error control):

- Pointwise evals $c_k(q), u_0(q)\ \forall q \in \mathbb{Q}^d$.
- Poly growth bound on $c_k(x)$ as $\|x\| \to \infty$.
- Bounds on $\left\| c_k|_{[-n,n]^d} \right\|_{\mathrm{TV}}$, $\left\| u_0|_{[-n,n]^d} \right\|_{\mathrm{TV}}$, $\|u_0\|_{L^2(\mathbb{R}^d\setminus[-n,n]^d)}$

Much more general than Schwinger's problem!

Theorem: $\exists$ **universal** algorithm $\Gamma_{L^2(\mathbb{R}^d)}$ using above input such that

$$\left\| \Gamma_{L^2(\mathbb{R}^d)}(\{c_k\}, u_0, t, \varepsilon) - u(t) \right\|_{L^2(\mathbb{R}^d)} \leq \varepsilon.$$

How?

- Apply algorithm $\Gamma_{l^2(\mathbb{N})}$.

$\boxed{\text{solve-then-discretise}}$

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- Apply algorithm $\Gamma_{l^2(\mathbb{N})}$.
- Tensorised Hermite basis (orthonormal)

$$\psi_m(x) = N_m e^{-\frac{x^2}{2}} H_m(x), \qquad H_m(x) = (-1)^m e^{x^2} \frac{\mathrm{d}^m}{\mathrm{d}x^m} e^{-x^2}$$

solve-then-discretise

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- Compute inner products

$$\langle A\psi_k, \psi_j \rangle = \int_{\mathbb{R}^d} [A\psi_k](x)\overline{\psi_j(x)}\,\mathrm{d}x \longrightarrow \int_{|x_i|\le r} [A\psi_k](x)\overline{\psi_j(x)}\,\mathrm{d}x$$

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TRUNCATION

$$\boxed{\text{solve-then-discretise}}$$

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TRUNCATION

+ quasi-Monte Carlo numerical integration.

$\boxed{\text{solve-then-discretise}}$

How?

Other bases, quad rules possible!
(provided we have error control)

- Apply algorithm $\Gamma_{l^2(\mathbb{N})}$.
- Tensorised Hermite basis (orthonormal)

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solve-then-discretise

Two parts

- General strongly continuous semigroups.

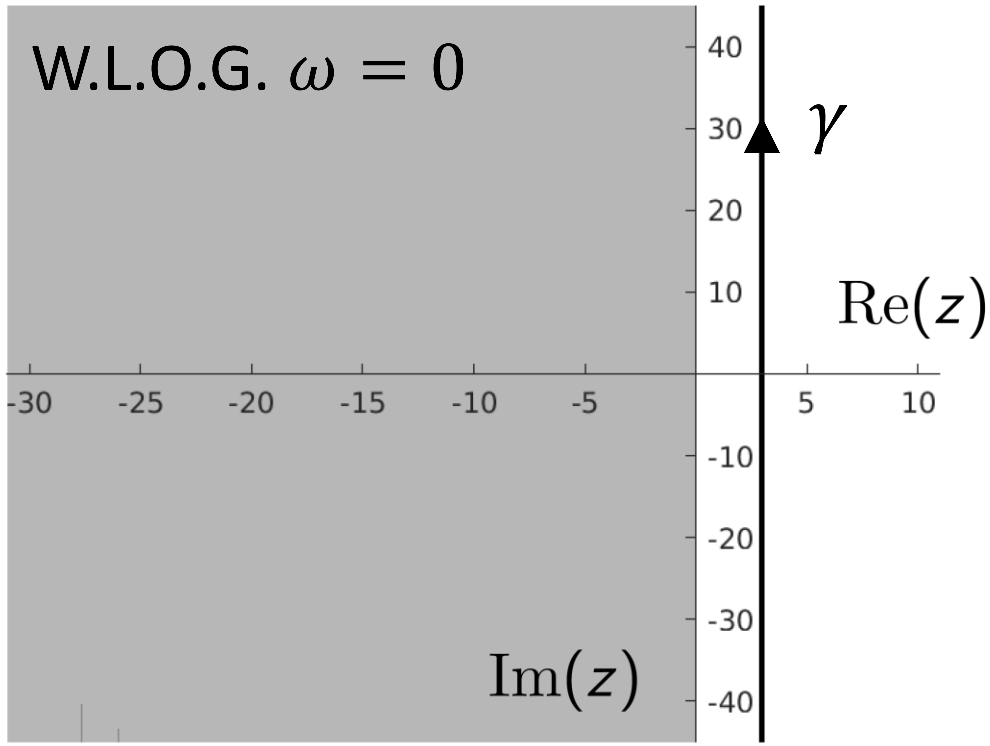
  E.g., Schrödinger equations, wave equations.

- Analytic semigroups and inverse Laplace transforms.

  E.g., diffusion equations.

solve-then-discretise

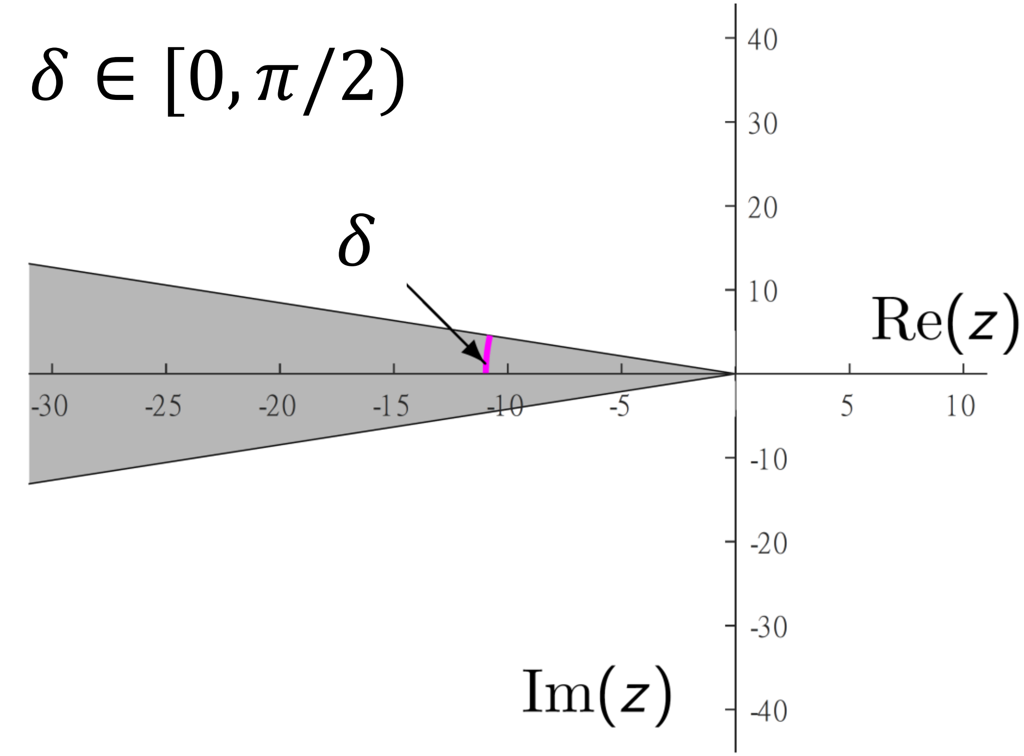
Analytic semigroups, inverse Laplace transforms



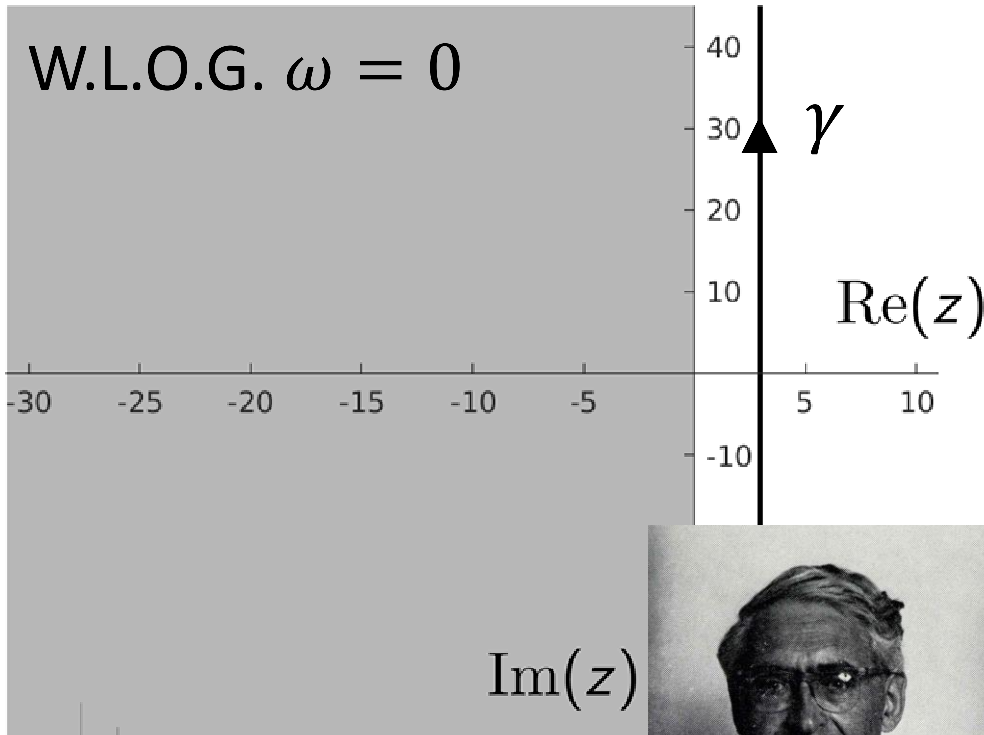
$\mathrm{Sp}(A)$

in a sector

$\Rightarrow$



Analytic semigroups, inverse Laplace transforms

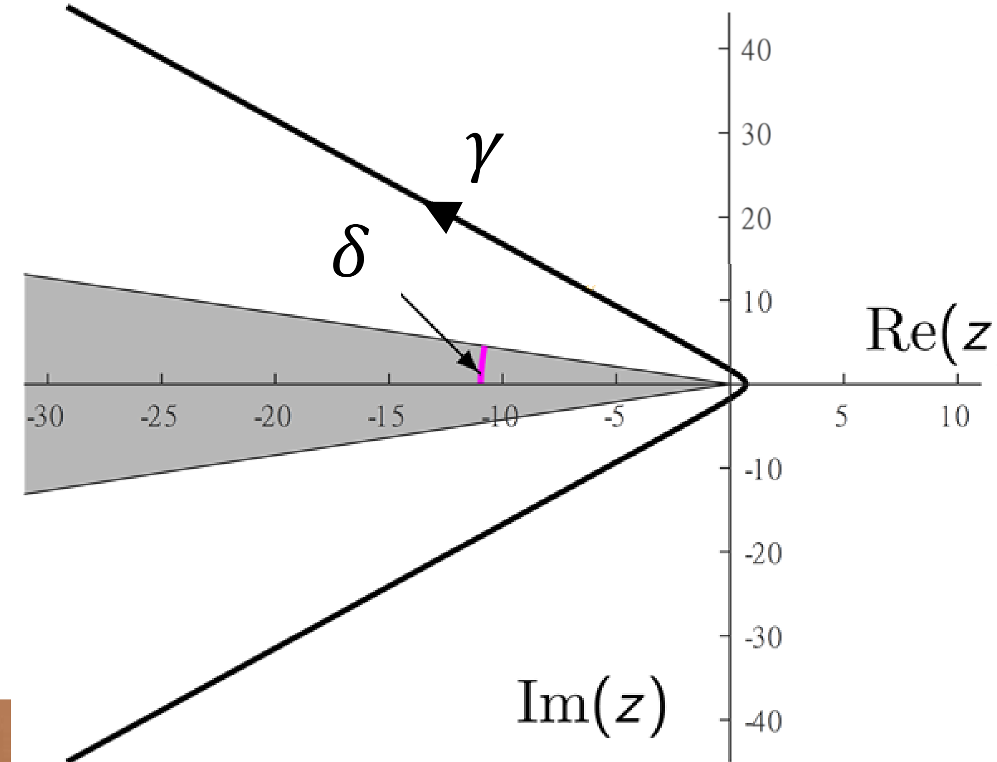


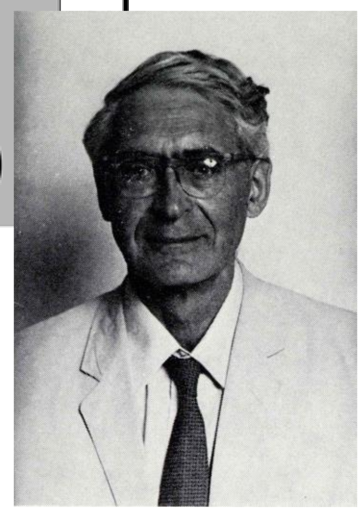
$\mathrm{Sp}(A)$

in a sector

$\Rightarrow$

Deform contour!





Alan Talbot

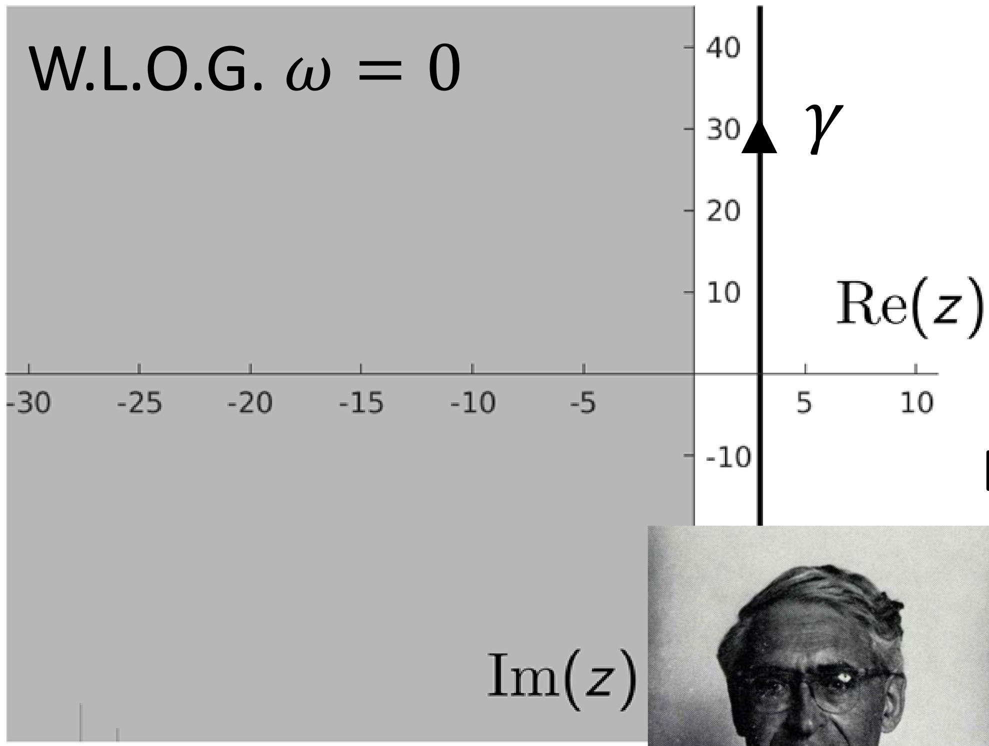
John C. Butcher

$$u(t) = \left[\frac{-1}{2\pi i}\int_\gamma e^{zt}\,(A - zI)^{-1}\mathrm{d}z\right] u_0$$

Exponential decay!

- Green, *"The Calculation of the Time-Responses of Linear Systems,"* **PhD thesis, Imperial College London**, 1955.
- Talbot, *"The accurate numerical inversion of Laplace transforms,"* **IMA J. Appl. Math.**, 1979.
- Butcher, *"On the numerical inversion of Laplace and Mellin transforms,"* **Proc. Conf. Data Processing and Aut. Comp. Mach.**, 1957.

Analytic semigroups, inverse Laplace transforms



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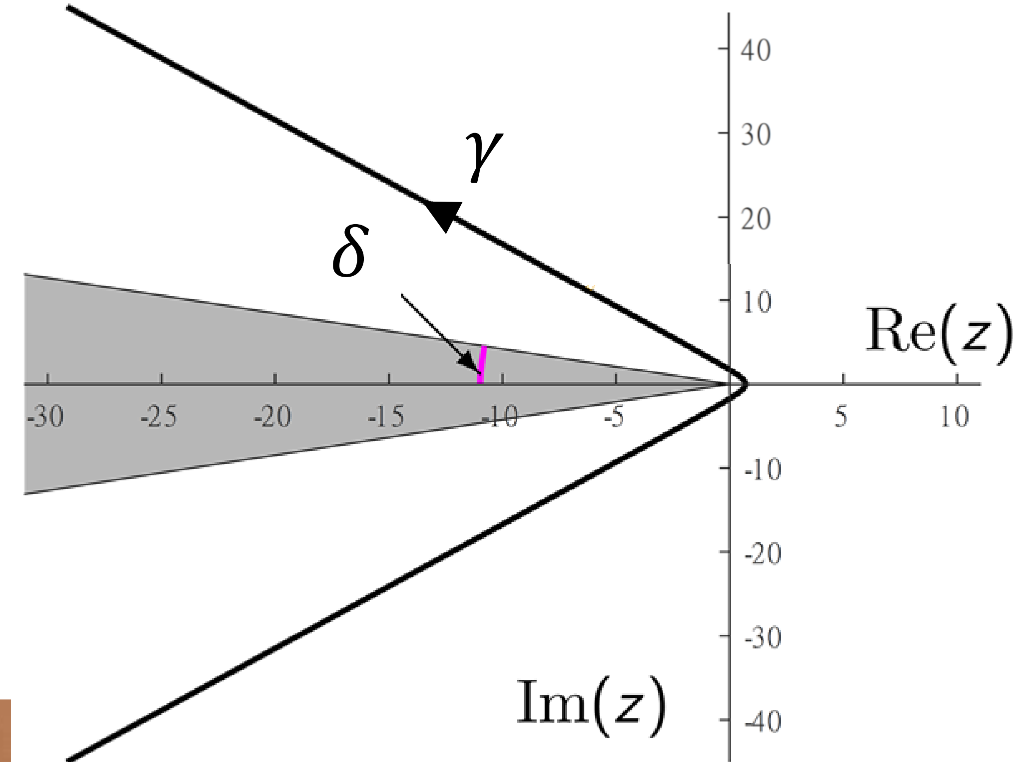
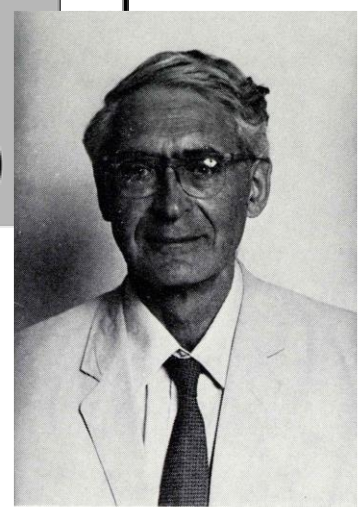


Choice of contour?



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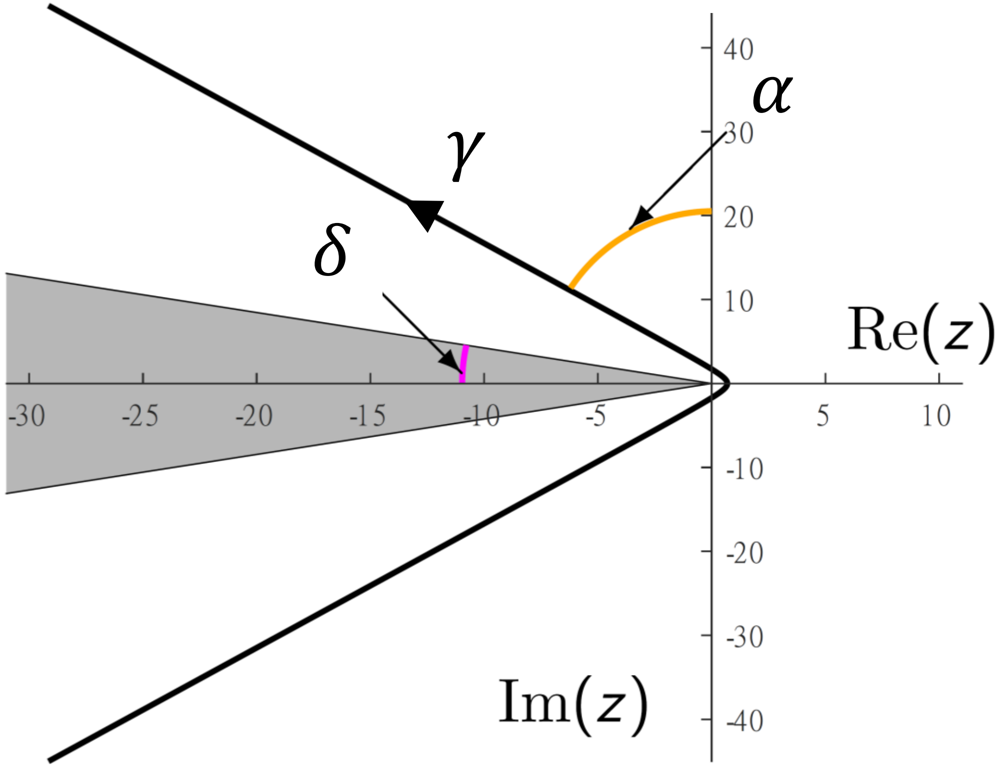
Analytic semigroups, inverse Laplace transforms

Maria Lopez-Fernandez

César Palencia



$$\gamma(s) = \mu(1 + \sin(is - \alpha)) \quad (s \in \mathbb{R})$$

$$\mu > 0, \qquad 0 < \alpha < \frac{\pi}{2} - \delta$$

- Lopez-Fernandez, Palencia, *"On the numerical inversion of the Laplace transform of certain holomorphic mappings,"* **Appl. Numer. Math.**, 2004.

Analytic semigroups, inverse Laplace transforms

Maria Lopez-Fernandez

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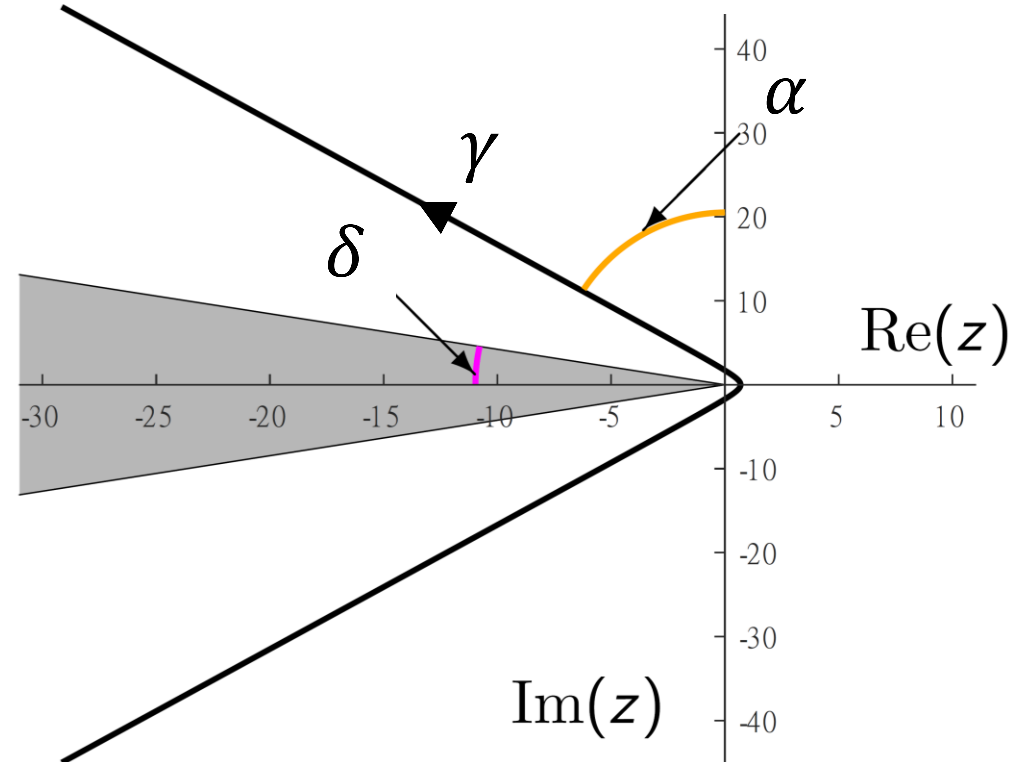


$$\gamma(s) = \mu(1 + \sin(is - \alpha)) \quad (s \in \mathbb{R})$$

$$\mu > 0, \qquad 0 < \alpha < \frac{\pi}{2} - \delta$$

$$u(t) \approx \frac{-h}{2\pi i} \sum_{j=-N}^{N} e^{\gamma(jh)t} \gamma'(jh)(A - \gamma(jh)I)^{-1} u_0$$

Trapezoidal rule!

Computed in parallel, reused for different t.

Nick Trefethen

Andre Weideman

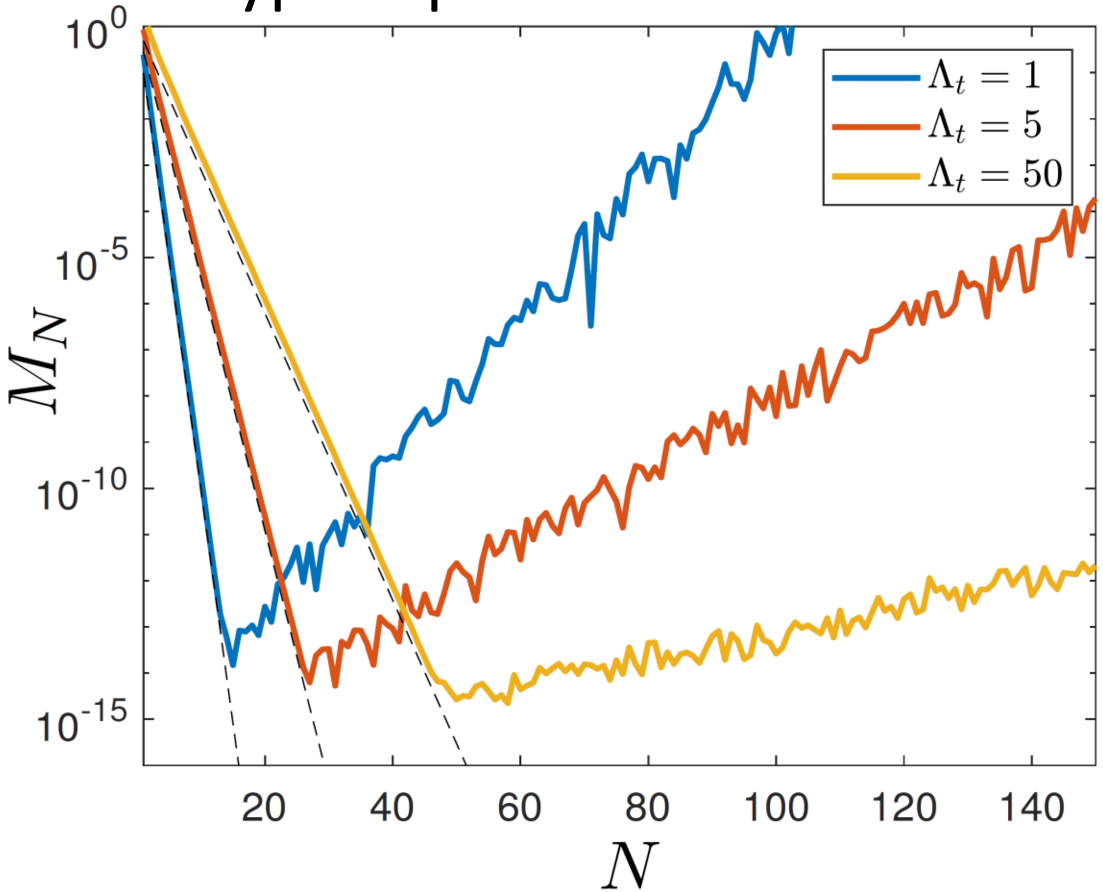
- Lopez-Fernandez, Palencia, *"On the numerical inversion of the Laplace transform of certain holomorphic mappings,"* **Appl. Numer. Math.**, 2004.
- Weideman, Trefethen, *"Parabolic and hyperbolic contours for computing the Bromwich integral,"* **Math. Comp.**, 2007.
- Trefethen, Weideman, *"The exponentially convergent trapezoidal rule,"* **SIAM Rev.**, 2014.

Exponential convergence… but instability

$$1 = \frac{1}{2\pi i}\int_{\gamma} \frac{e^{zt}}{z}\,\mathrm{d}z \approx \frac{h}{2\pi i}\sum_{j=-N}^{N} \frac{e^{\gamma(jh)t}}{\gamma(jh)}\gamma'(jh)$$

M_N = max error over $t \in [t_0, t_1], \Lambda_t = t_1/t_0$

Typical parameter choices



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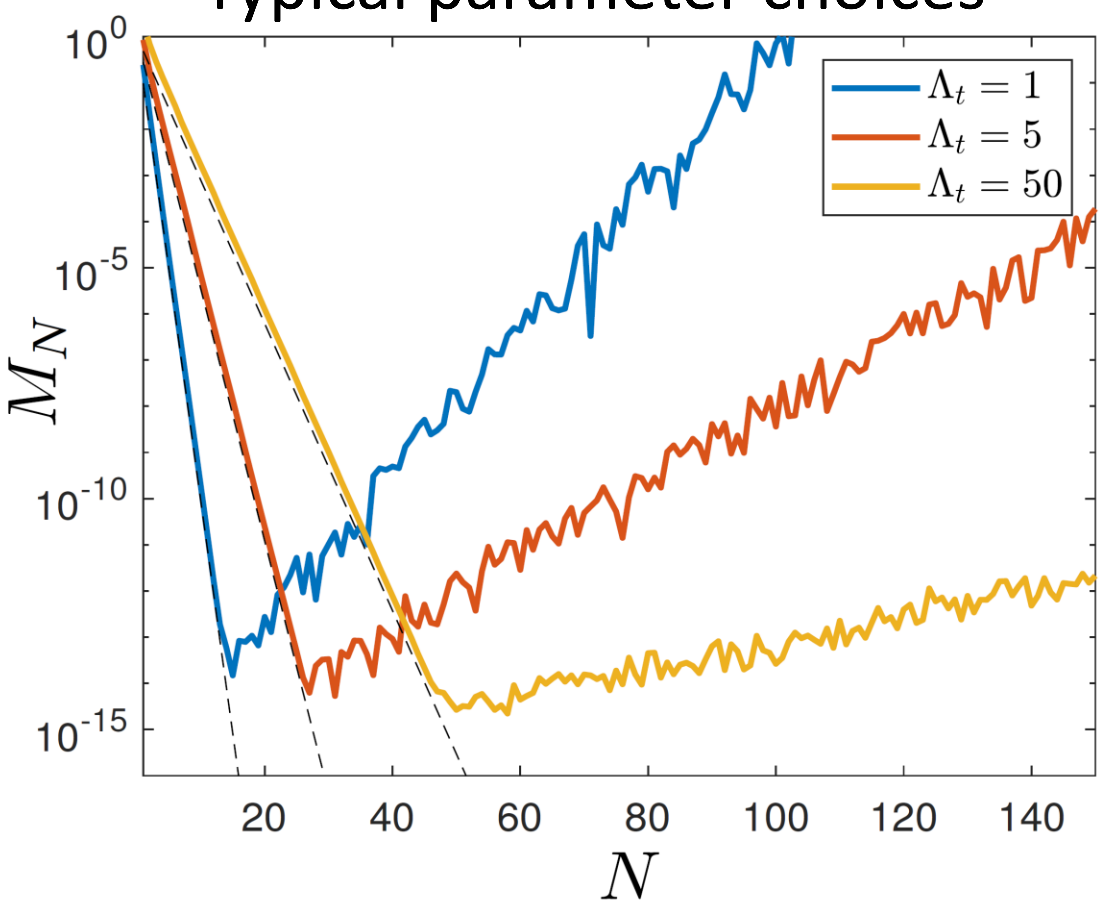

$$\lim_{N\to\infty} \max \mathrm{Re}(\gamma(jh)) = \infty \implies$$ **instability!**

Exponential convergence… but instability

$$1 = \frac{1}{2\pi i}\int_{\gamma} \frac{e^{zt}}{z}\,\mathrm{d}z \approx \frac{h}{2\pi i}\sum_{j=-N}^{N} \frac{e^{\gamma(jh)t}}{\gamma(jh)}\gamma'(jh)$$

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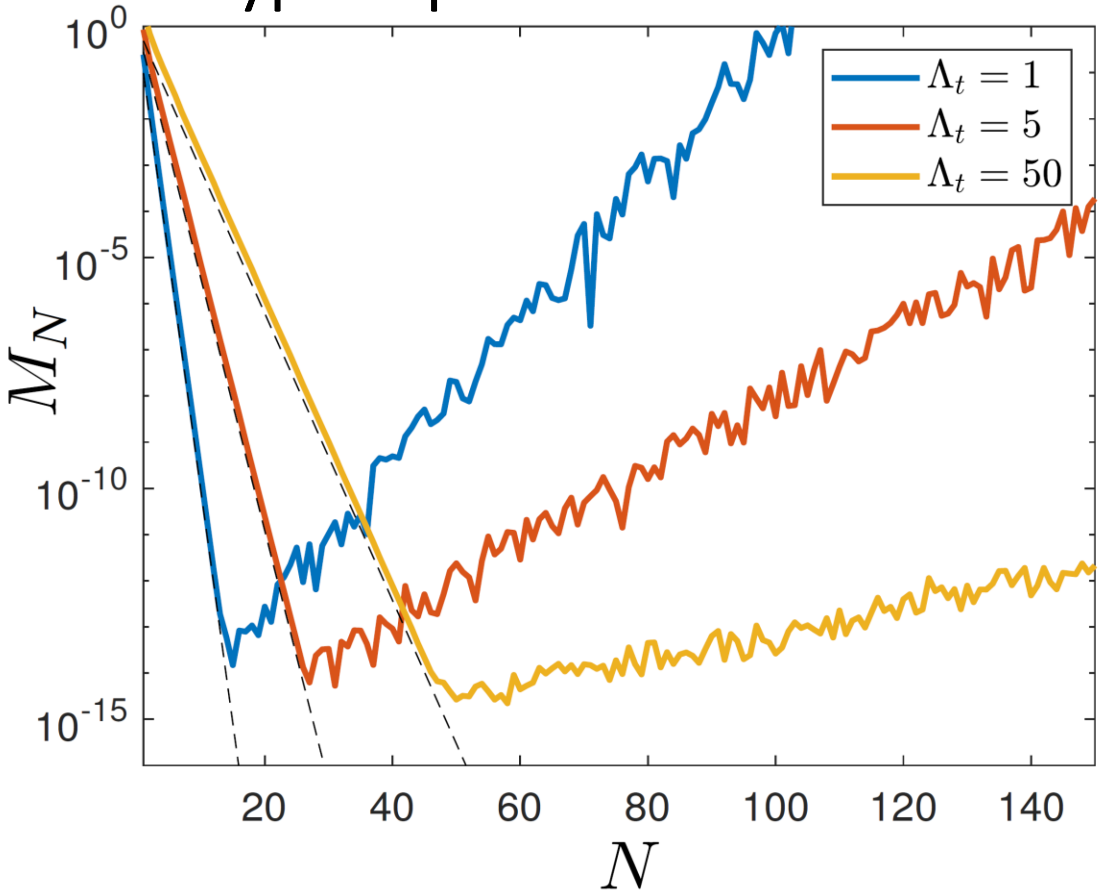
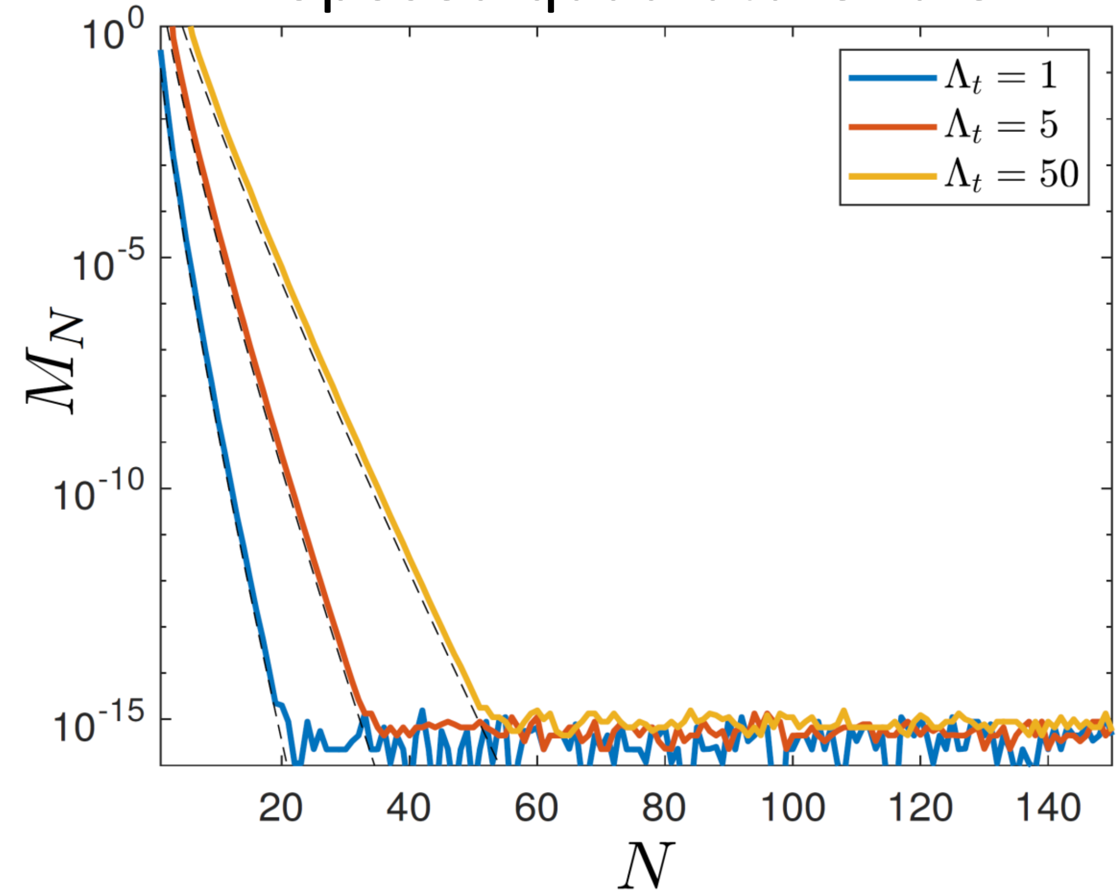
Typical parameter choices



Proposed quadrature rule…



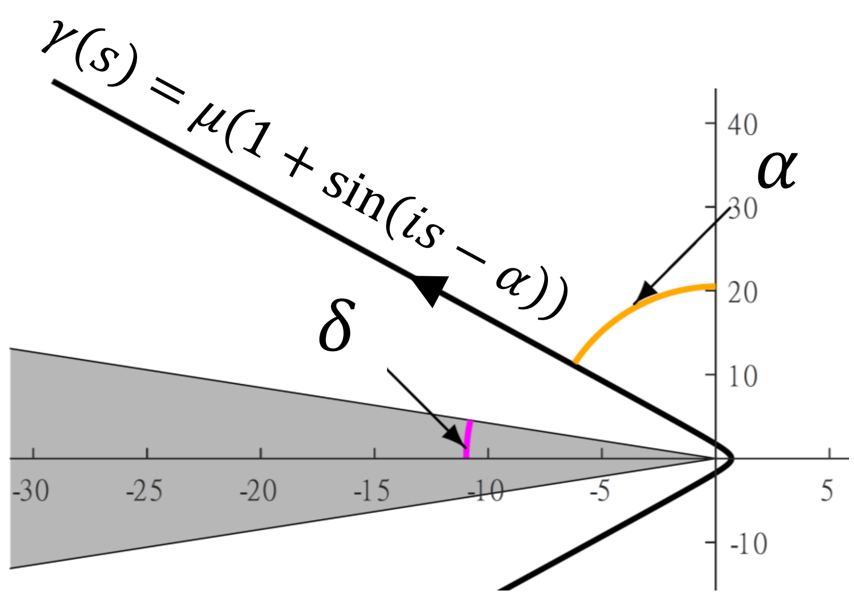
Enforcing stability

$$u_N(t) = \frac{-h}{2\pi i} \sum_{j=-N}^{N} e^{\gamma(jh)t} \gamma'(jh)(A - \gamma(jh)I)^{-1} u_0$$

$$t \in [t_0, t_1], \qquad \Lambda_t = t_1/t_0$$

- Enforce $\max \mathrm{Re}(\gamma(jh))t_1 \leq \beta$ (= 3)
- Avoid γ approaching $\mathrm{Sp}(A)$ as $N \longrightarrow \infty$

(truncation size needed for $(A - zI)^{-1}$ blows up as $z \to \mathrm{Sp}(A)$)



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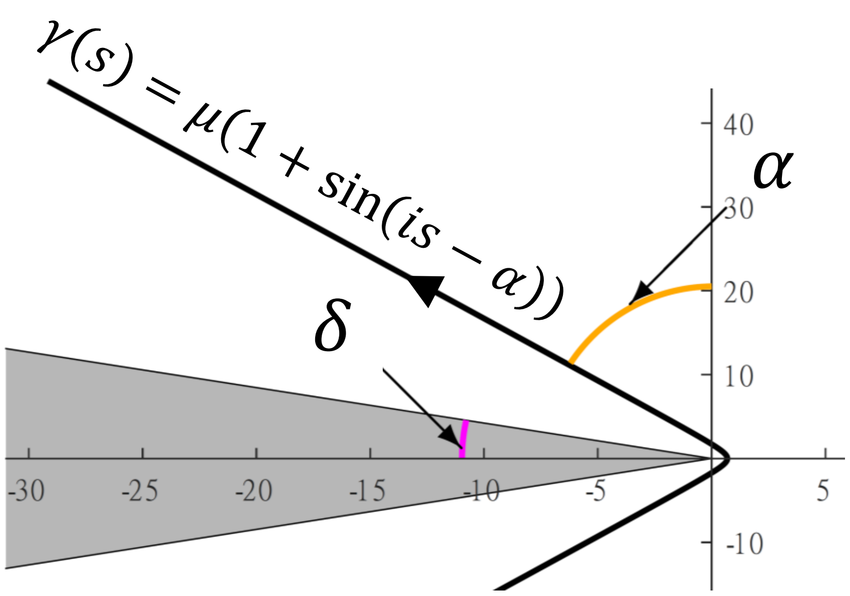
$$\underbrace{E_1 = \mathcal{O}(e^{-2\pi(\pi/2-\alpha-\delta)/h}), E_2 = \mathcal{O}(e^{\mu t_1 - 2\pi\alpha/h})}_{h \text{ error}}, \underbrace{E_3 = \mathcal{O}(e^{\mu t_0(1-\sin(\alpha)\cosh(hN))})}_{\text{Truncation of sum error } (N)}$$



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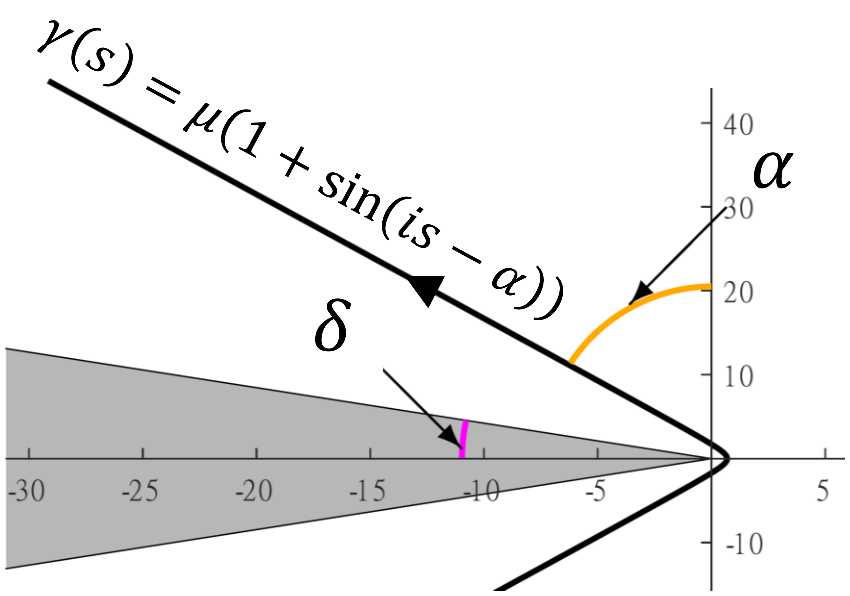


$$h = \frac{1}{N} W\left(\Lambda_t N \frac{\pi(\pi-2\delta)}{\beta \sin((\pi-2\delta)/4)}\left(1 - \sin\left(\frac{\pi-2\delta}{4}\right)\right)\right)$$

$$\mu = \frac{\beta/t_1}{1-\sin((\pi-2\delta)/4)}$$

$$\alpha = \frac{h\mu t_1 + \pi^2 - 2\pi\delta}{4\pi}$$

Enforcing stability

$$u_N(t) = \frac{-h}{2\pi i} \sum_{j=-N}^{N} e^{\gamma(jh)t} \gamma'(jh)(A - \gamma(jh)I)^{-1} u_0$$

$$t \in [t_0, t_1], \qquad \Lambda_t = t_1/t_0$$

Computed with error $\leq \eta$

- Enforce $\max \mathrm{Re}(\gamma(jh))t_1 \leq \beta$ (= 3)
- Avoid γ approaching $\mathrm{Sp}(A)$ as $N \longrightarrow \infty$

(truncation size needed for $(A - zI)^{-1}$ blows up as $z \rightarrow \mathrm{Sp}(A)$)

Theorem: Suppose each $(A - \gamma(jh)I)^{-1}u_0$ computed with error $\leq \eta$.
$\exists$ explicit constants $C_1, C_2, C_3 > 0$ such that

$$\|u_N(t) - u(t)\| \leq C_1\eta + \underbrace{C_2 \exp(-C_3(\pi - 2\delta)N/\log(\Lambda_t N))}_{\text{Quadrature error}}.$$

Resolvent error

solve-then-discretise

Example: beam equations

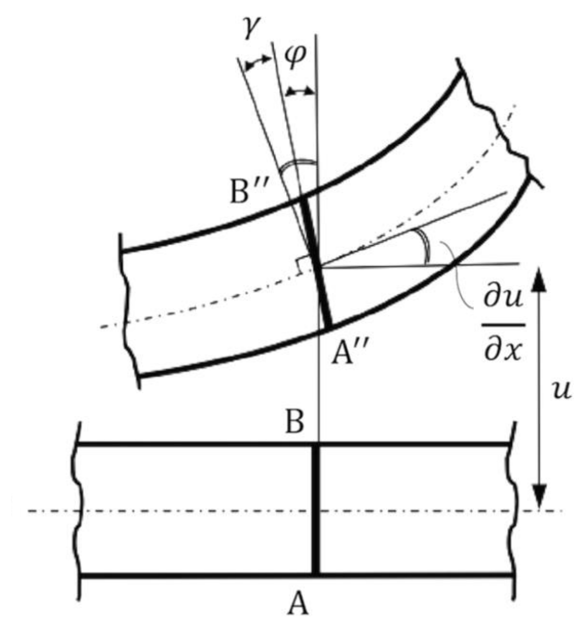
$$\rho(x)\frac{\partial^2 u}{\partial t^2}+\frac{\partial^2}{\partial x^2}\left[a(x)\frac{\partial^2}{\partial x^2}+b(x)\mathcal{D}_t^{\tau}\frac{\partial^2}{\partial x^2}\right]u(x,t)=f(x,t),\qquad 0<\tau<2.$$

density   flexural rigidity   viscoelastic damping   transverse displacement   forcing

$$[\mathcal{D}_t^{\tau} g\,](t)=\frac{1}{\Gamma(\lceil\tau\rceil-\tau)}\int_0^t (t-s)^{\lceil\tau\rceil-\tau-1}g^{(\lceil\tau\rceil)}(s)\,\mathrm{d}s$$

$$u(\pm 1,t)=u_x(\pm 1,t)=0$$

$$(u,u_t)\in\mathcal{H}=H_0^2([-1,1])\times L^2([-1,1])$$



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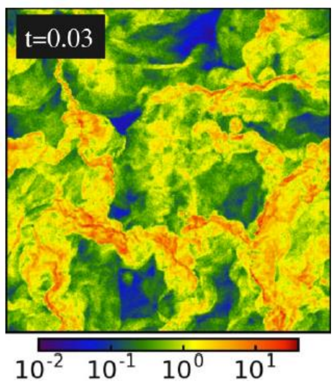
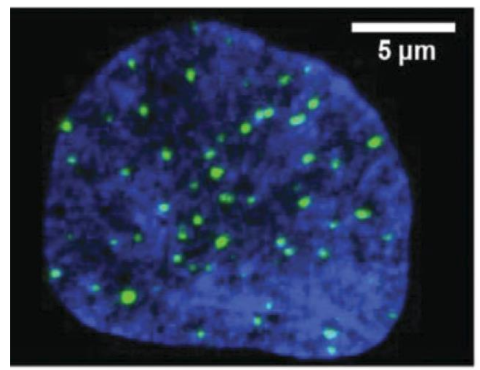
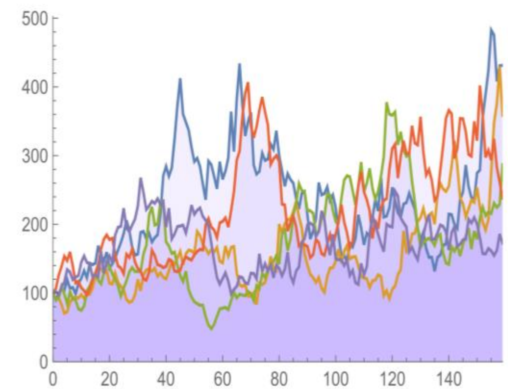


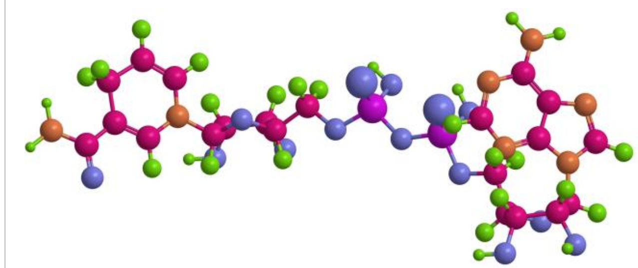
Anomalous transport



Cell biology and chemistry



Finance

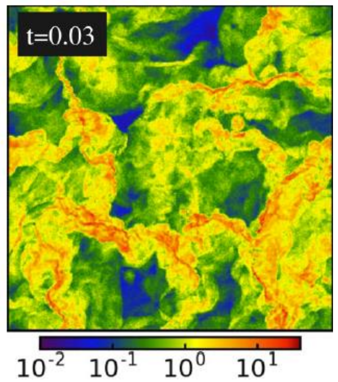


Polymer structures

- Karniadakis, Hesthaven, Podlubny, *"Special Issue on Fractional PDEs: Theory, Numerics, and Applications,"* **J. Comput. Phys.**, 2015.

Example: beam equations

$$\rho(x)\frac{\partial^2 u}{\partial t^2} + \frac{\partial^2}{\partial x^2}\left[a(x)\frac{\partial^2}{\partial x^2} + b(x)\mathcal{D}_t^{\tau}\frac{\partial^2}{\partial x^2}\right]u(x,t) = f(x,t), \qquad 0 < \tau < 2.$$



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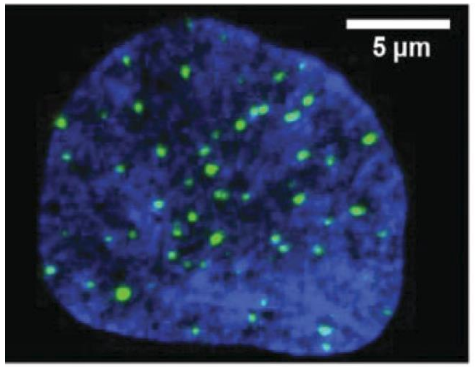

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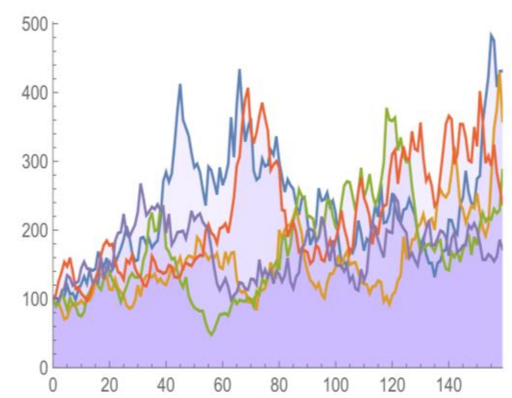

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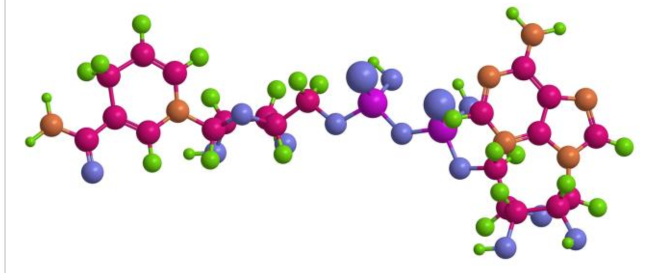

Polymer structures

CHALLENGES

- Non-local time derivative.
- Large memory consumption.
- Singularities as $t \downarrow 0$.

Very expensive for discretise-then-solve e.g., time-stepping & finite elements.

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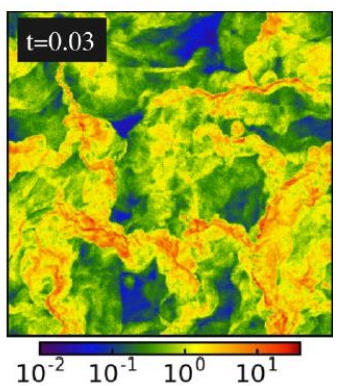

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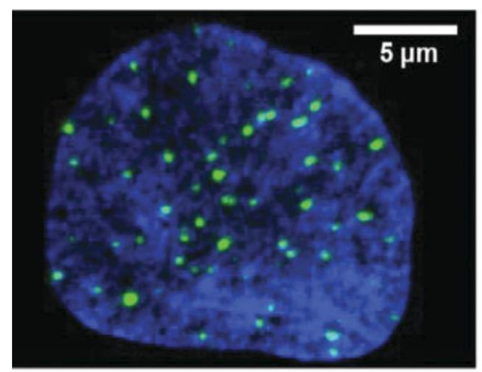
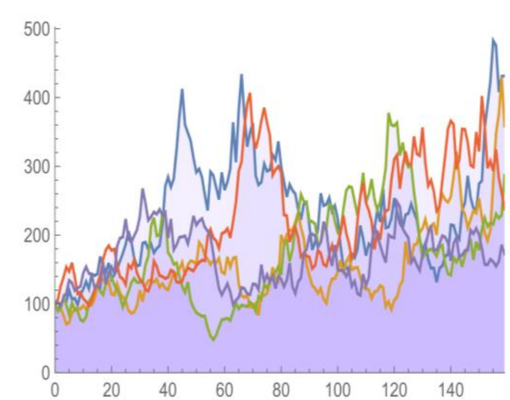


Cell biology and chemistry



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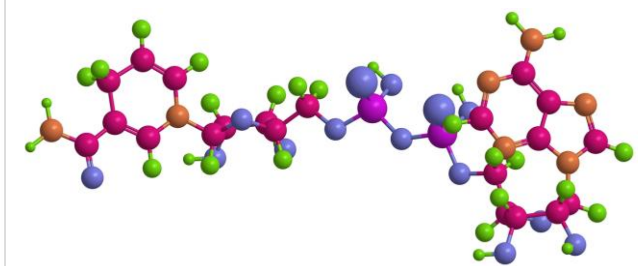


Polymer structures

CHALLENGES

- Non-local time derivative.
- Large memory consumption.
- Singularities as $t \downarrow 0$.

Very expensive for discretise-then-solve e.g., time-stepping & finite elements.

Solution: $\boxed{\text{solve-then-discretise}}$

Example: beam equations

$$\rho(x)\frac{\partial^2 u}{\partial t^2}+\frac{\partial^2}{\partial x^2}\left[a(x)\frac{\partial^2}{\partial x^2}+b(x)\mathcal{D}_t^\tau\frac{\partial^2}{\partial x^2}\right]u(x,t)=f(x,t),\qquad 0<\tau<2.$$

$$T(z)=z^2+\frac{1}{\rho(x)}\frac{\partial^2}{\partial x^2}\left[a(x)\frac{\partial^2}{\partial x^2}+z^\tau b(x)\frac{\partial^2}{\partial x^2}\right]$$

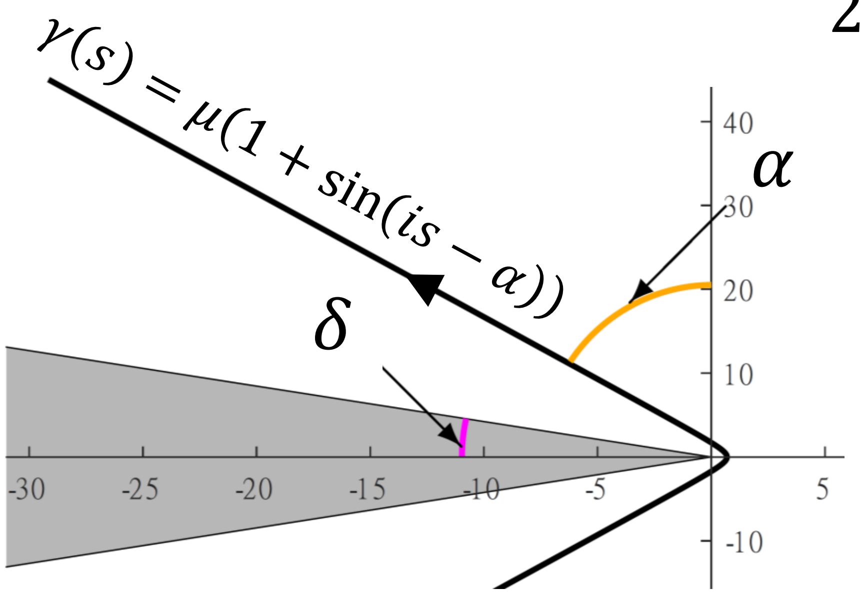
Replaces $A-zI$.

$$g(x,z)=\frac{\hat{f}(x,z)}{\rho(x)}+zu(x,0)+\frac{\partial u}{\partial t}(x,0)+\frac{1}{\rho(x)}\frac{\partial^2}{\partial x^2}b(x)\frac{\partial^2}{\partial x^2}\sum_{k=1}^{\lceil\tau\rceil}z^{\tau-k}\frac{\partial^{k-1}u}{\partial t^{k-1}}(x,0)$$

Laplace domain

$$u(t)=\frac{1}{2\pi i}\int_\gamma e^{zt}\,T(z)^{-1}g(x,z)\mathrm{d}z$$

Solve $T(z)^{-1}g(x,z)$ adaptively.



Complex spectrum.

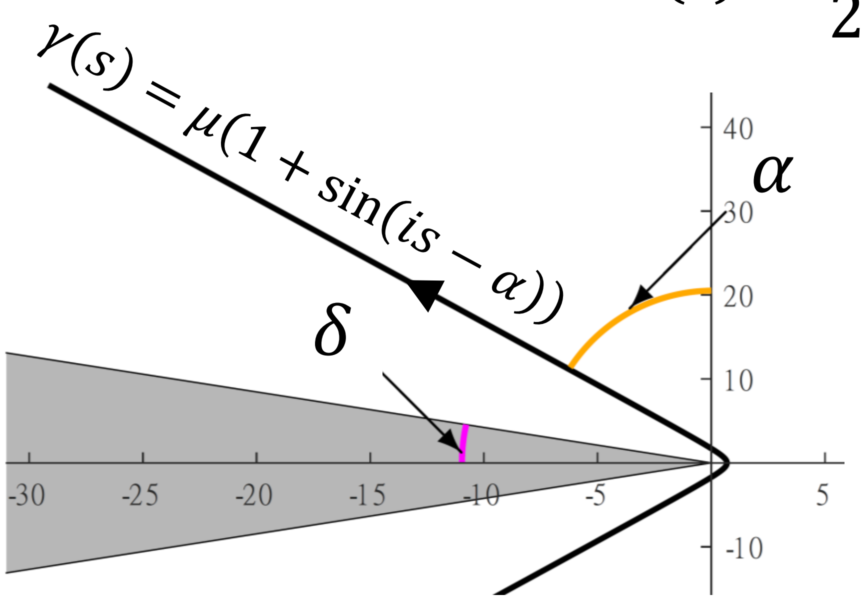
Non-empty continuous spectrum.

Example: beam equations

$$\rho(x)\frac{\partial^2 u}{\partial t^2}+\frac{\partial^2}{\partial x^2}\left[a(x)\frac{\partial^2}{\partial x^2}+b(x)\mathcal{D}_t^\tau\frac{\partial^2}{\partial x^2}\right]u(x,t)=f(x,t),\qquad 0<\tau<2.$$

$$\left.\begin{aligned}
&T(z)=z^2+\frac{1}{\rho(x)}\frac{\partial^2}{\partial x^2}\left[a(x)\frac{\partial^2}{\partial x^2}+z^\tau b(x)\frac{\partial^2}{\partial x^2}\right]\quad\longleftarrow\ \text{Replaces } A-zI.\\
&g(x,z)=\frac{\hat{f}(x,z)}{\rho(x)}+zu(x,0)+\frac{\partial u}{\partial t}(x,0)+\frac{1}{\rho(x)}\frac{\partial^2}{\partial x^2}b(x)\frac{\partial^2}{\partial x^2}\sum_{k=1}^{\lceil\tau\rceil}z^{\tau-k}\frac{\partial^{k-1}u}{\partial t^{k-1}}(x,0)
\end{aligned}\right\}\ \textit{Laplace domain}$$

$$u(t)=\frac{1}{2\pi i}\int_\gamma e^{zt}\,T(z)^{-1}g(x,z)\mathrm{d}z$$



Solve $T(z)^{-1}g(x,z)$ adaptively.

MUCH easier in infinite dimensions!

$$\boxed{\begin{gathered}\|T(z)^{-1}\|\leq\frac{1}{\mathrm{dist}\big(z,\mathcal{N}(T(z))\big)},\\ \mathcal{N}(T(z))=\{\langle T(z)v,v\rangle : v\in\mathcal{D}(T(z)),\|v\|=1\}\end{gathered}}$$

Example: beam equations

$$\rho(x)\frac{\partial^2 u}{\partial t^2} + \frac{\partial^2}{\partial x^2}\left[a(x)\frac{\partial^2}{\partial x^2} + b(x)\mathcal{D}_t^\tau \frac{\partial^2}{\partial x^2}\right]u(x,t) = f(x,t), \qquad 0 < \tau < 2.$$

$$T(z) = z^2 + \frac{1}{\rho(x)}\frac{\partial^2}{\partial x^2}\left[a(x)\frac{\partial^2}{\partial x^2} + z^\tau b(x)\frac{\partial^2}{\partial x^2}\right]$$

Replaces $A - zI$.

$$g(x,z) = \frac{\hat{f}(x,z)}{\rho(x)} + zu(x,0) + \frac{\partial u}{\partial t}(x,0) + \frac{1}{\rho(x)}\frac{\partial^2}{\partial x^2}b(x)\frac{\partial^2}{\partial x^2}\sum_{k=1}^{\lceil\tau\rceil} z^{\tau-k}\frac{\partial^{k-1}u}{\partial t^{k-1}}(x,0)$$

Laplace domain

$$u(t) = \frac{1}{2\pi i}\int_\gamma e^{zt}\, T(z)^{-1} g(x,z)\mathrm{d}z$$

Solve $T(z)^{-1}g(x,z)$ adaptively.

MUCH easier in infinite dimensions!

- **No time-stepping, low memory.**
- **Avoid singularities as $t \downarrow 0$.**
- **Parallelizable, reuse comp. over t.**
- **Exponential convergence.**

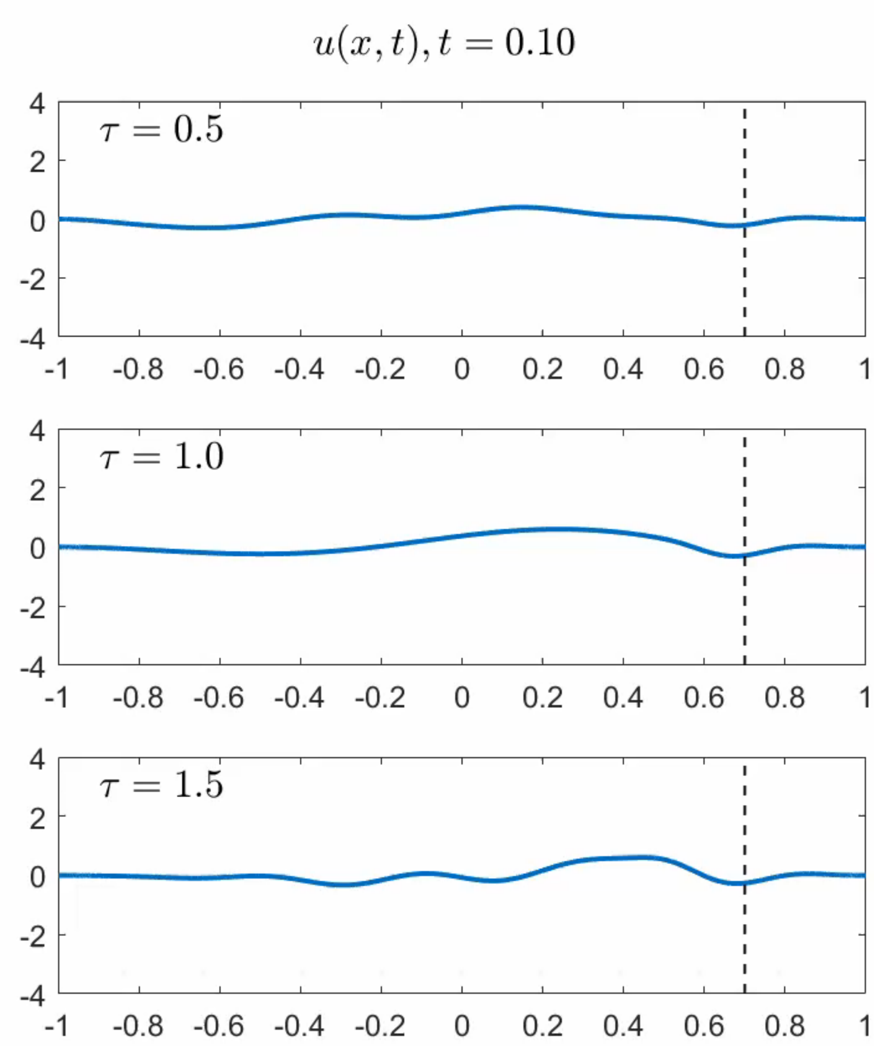
$$\boxed{\begin{gathered}\|T(z)^{-1}\| \leq \frac{1}{\mathrm{dist}\left(z, \mathcal{N}\left(T(z)\right)\right)}, \\ \mathcal{N}(T(z)) = \left\{\langle T(z)v, v\rangle : v \in \mathcal{D}\left(T(z)\right), \|v\| = 1\right\}\end{gathered}}$$

NB: Solve $T(z)^{-1}g(x,z)$ using ultraspherical spectral method (Olver, Townsend, SIREV 2013)

Example: beam equations

$$u(x,0) = \sin(5\pi x)(1-x^2)^2$$
$$u_t(x,0) = x$$

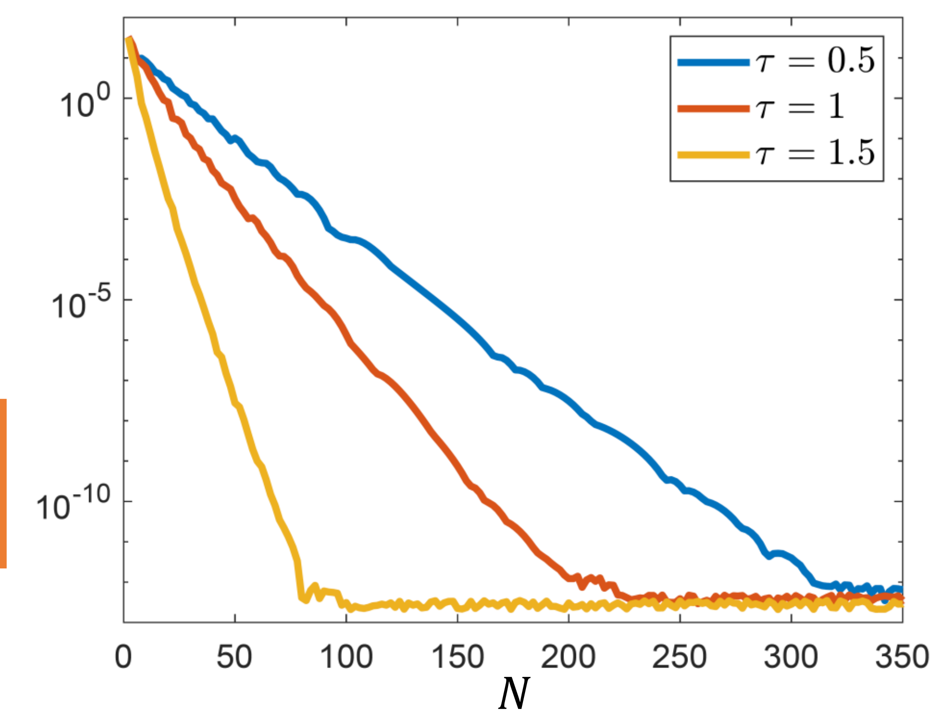
$$\rho(x)\frac{\partial^2 u}{\partial t^2} + \frac{\partial^2}{\partial x^2}\left[a(x)\frac{\partial^2}{\partial x^2} + b(x)\mathcal{D}_t^{\tau}\frac{\partial^2}{\partial x^2}\right]u(x,t) = f(x,t), \qquad 0<\tau<2.$$



$$a(x) = 1 + x^3/2, \qquad b(x) = \tanh\big(10(x-0.7)\big) + 1.01$$
$$\rho(x) = 1 + x/2, \qquad f(x,t) = 10\cos(20t)\sin(\pi x)$$

$$E_N = \max_{t\in[0.1,10]} \|u(\cdot,t) - u_N(\cdot,t)\|_{H^2} + \left\|\frac{\partial u}{\partial t}(\cdot,t) - \frac{\partial u_N}{\partial t}(\cdot,t)\right\|_{L^2}$$

$E_N \leq 10^{-10}$
in $\approx \mathcal{O}(1)$ second!



Conclusion

$$\frac{\mathrm{d}u}{\mathrm{d}t} = Au, \qquad u(0) = u_0 \in \mathcal{H}$$

$\boxed{\text{solve-then-discretise}}$ $\Longrightarrow$ **convergence, error control.**

- Regularised contour method for general strongly continuous semigroups.
  E.g., PDEs on unbounded domain $L^2(\mathbb{R}^d)$.

  Adaptive truncation.

- Optimised stable quadrature for analytic semigroups.
  Extends to inverse Laplace transform, e.g., time-fractional PDEs.

  Rapid convergence, high accuracy, low memory.

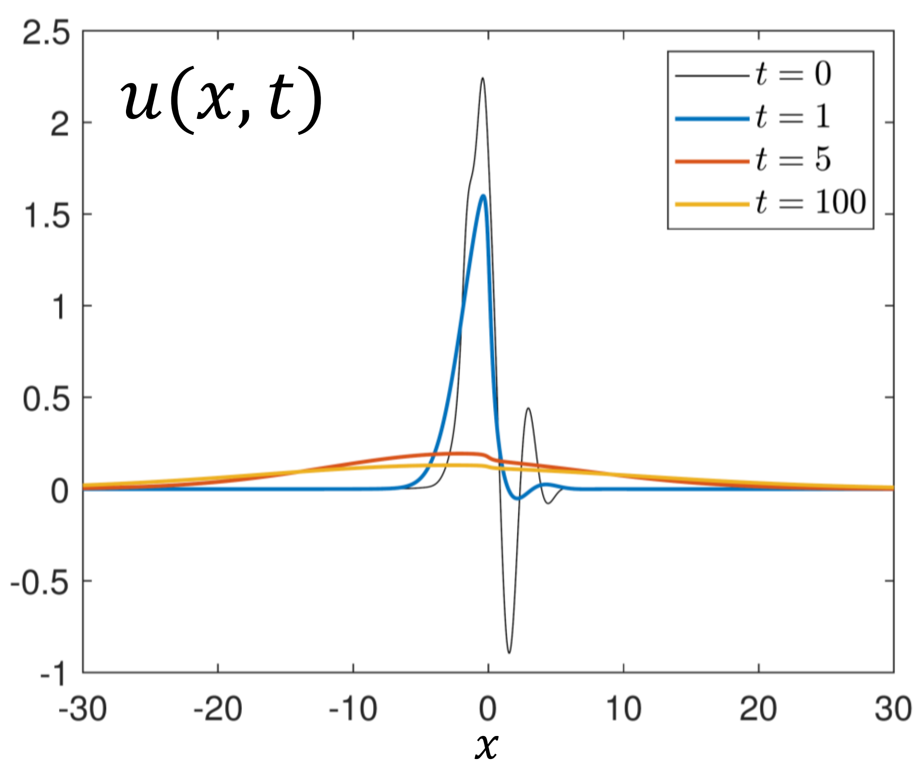
- Rigorous, practical & flexible:
  - Choice of contour and quadrature.
  - Only need to solve linear systems with error control.

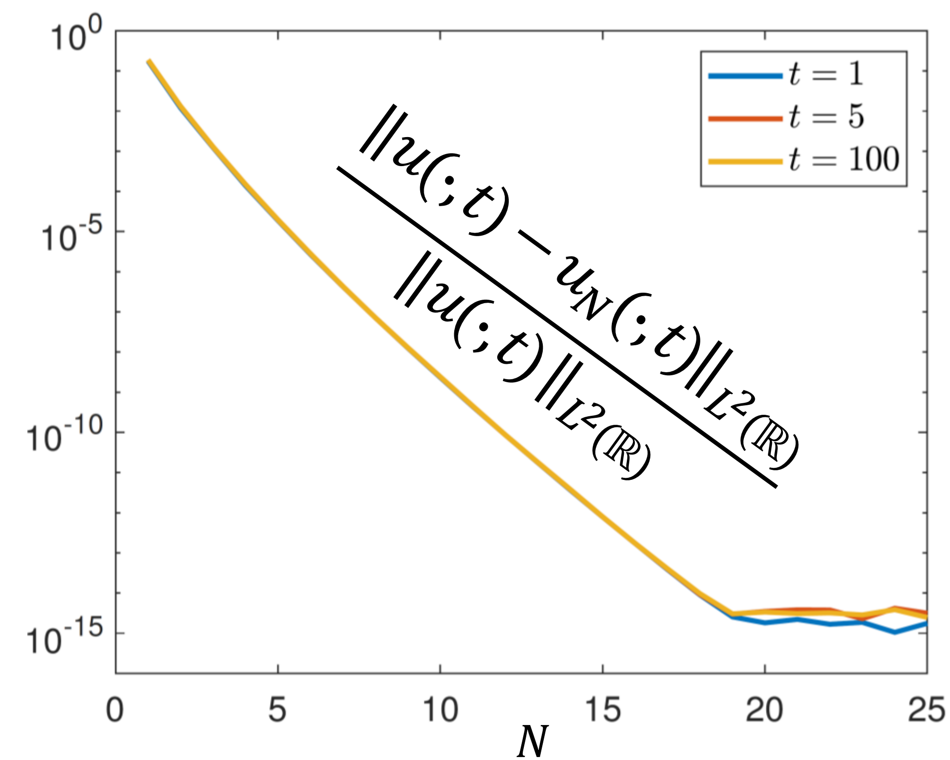
Example: diffusion equation on $\mathbb{R}$

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left[\left(1.1 - \frac{1}{1+x^2}\right)\frac{\partial}{\partial x}\right]u, \qquad u_0(x) = e^{-\frac{(x-1)^2}{5}}\cos(2x) + \frac{2}{1+(x+1)^4}.$$

$$\phi_n(x) = \frac{1}{\sqrt{5\pi}}\frac{(1+ix/5)^n}{(1-ix/5)^{n+1}}$$

Basis: Malmquist-Takenaka functions
Iserles, Webb, *"Fast Computation of Orthogonal Systems with a Skew-Symmetric Differentiation Matrix,"* **CPAM** 2021.





References

[1] Colbrook, Matthew J. "Computing semigroups with error control." *SIAM Journal on Numerical Analysis* 60.1 (2022): 396-422.

[2] Colbrook, Matthew J., and Lorna J. Ayton. "A contour method for time-fractional PDEs and an application to fractional viscoelastic beam equations." *Journal of Computational Physics* 454 (2022): 110995.