Computing semigroups and solutions of time-fractional PDEs with error control

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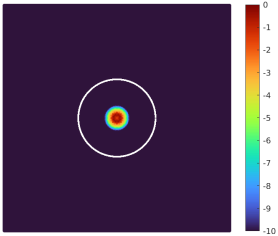
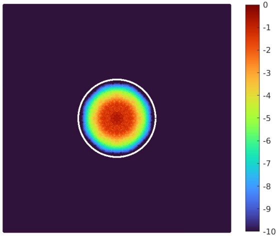
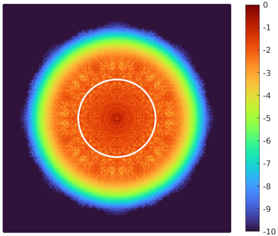
M. Colbrook, "*Computing semigroups with error control*", SIAM Journal on Numerical Analysis, to appear.
M. Colbrook and L. Ayton, "*A contour method for time-fractional PDEs*", Journal of Computational Physics, under revision.







The finite-dimensional case

$$\frac{du}{dt} = \mathbb{A}u, \quad \mathbb{A} \in \mathbb{C}^{n\times n}, \quad u(0) = u_0 \in \mathbb{C}^n \quad \Rightarrow \quad u(t) = \exp(t\mathbb{A})u_0 = \sum_{j=0}^{\infty} \frac{t^j}{j!}\mathbb{A}^j u_0.$$

E.g., if $\mathbb{A} = PDP^{-1}$, $D = \mathrm{diag}(d_1, ..., d_n)$ diagonal, then

$$u(t) = P \begin{pmatrix} e^{d_1 t} & & & \\ & e^{d_2 t} & & \\ & & \ddots & \\ & & & e^{d_n t} \end{pmatrix} P^{-1} u_0.$$

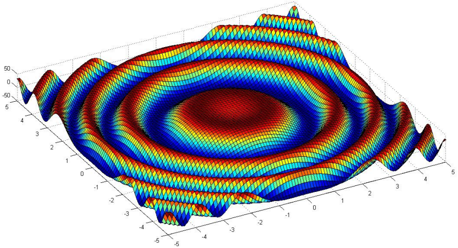
(Usually much better ways to compute this, but that's a different story...)

· C. Moler, C. Van Loan, "*Nineteen dubious ways to compute the exponential of a matrix, twenty-five years later*," SIAM review, 2003.
· N. Higham, "*The scaling and squaring method for the matrix exponential revisited*," SIAM Journal on Matrix Analysis and Applications, 2005.
· A. Frommer and B. Hashemi, "*Computing enclosures for the matrix exponential*," SIAM Journal on Matrix Analysis and Applications, 2020.

The infinite-dimensional case

Linear operator A on an infinite-dimensional Hilbert space $\mathcal{H}$,

$$\frac{du}{dt} = Au, \quad u(0) = u_0 \in \mathcal{H}.$$



Common examples:

- Time-dependent PDEs.
- Infinite discrete systems.

GOAL: Compute the solution $u(t)$ at time $t > 0$. Ideally with error control.

Some common techniques

- **Domain truncation and absorbing boundary conditions:** B. Engquist and A. Majda, "*Absorbing boundary conditions for numerical simulation of waves,*" PNAS, 1977.
- **Rational approximations:** M. Crouzeix, S. Larsson, S. Piskarev and V. Thomé, "*The stability of rational approximations of analytic semigroups,*" BIT, 1993.
- **Splitting methods:** R. McLachlan and G. R. Quispel, "*Splitting methods,*" Acta Numerica, 2002.
- **Exponential integrators:** M. Hochbruck and A. Ostermann, "*Exponential integrators,*" Acta Numerica, 2010.
- **Krylov methods:** J. Liesen and Z. Strakos, "*Krylov subspace methods,*" OUP, 2013.
- **Galerkin methods:** C. Lasser and C. Lubich, "*Computing quantum dynamics in the semiclassical regime,*" Acta Numerica, 2020.
- **Contour methods (in this talk):** A. Talbot, "*The accurate numerical inversion of Laplace transforms,*" IMA Journal of Applied Mathematics, 1979.
  N. Guglielmi, M. López-Fernández and M. Manucci, "*Pseudospectral roaming contour integral methods for convection-diffusion equations,*" Journal of Scientific Computing, 2021.

Each area has hundreds of papers and many great mathematicians who have written them!

Philosophy of the new approach

Previous approaches: A is discretised to $\mathbb{A} \in \mathbb{C}^{n\times n}$ and we use some sort of finite-dimensional solver – "**truncate-then-solve**"

Typical difficulties:

- Can be very difficult to bound the error when we go from A to $\mathbb{A}$.
- Sometimes $\mathbb{A}$ does not respect key properties of the system.
- Sometimes $\mathbb{A}$ is more complicated to study (e.g., where are its eigenvalues?).
- PDEs on unbounded domains - two truncations: the physical domain, then the operator restricted to this domain. How do we rigorously deal with domain truncation?

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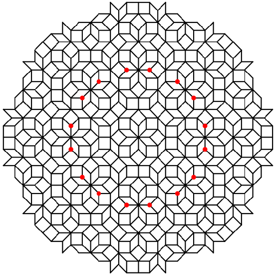
Example: discrete Laplacian



Finite portion of the aperiodic infinite Ammann–Beenker tile - red dots correspond to u_0.

Very interesting transport properties but notoriously difficult to compute. Graph Laplacian:

$$[\Delta_{\mathrm{AB}}\psi]_i = \sum_{i\sim j} (\psi_j - \psi_i), \quad \{\psi_j\}_{j\in\mathbb{N}} \in \ell^2(\mathbb{N}).$$

Schrödinger equation and wave equation:

$$iu_t = -\Delta_{\mathrm{AB}} u \quad \text{and} \quad u_{tt} = \Delta_{\mathrm{AB}} u.$$

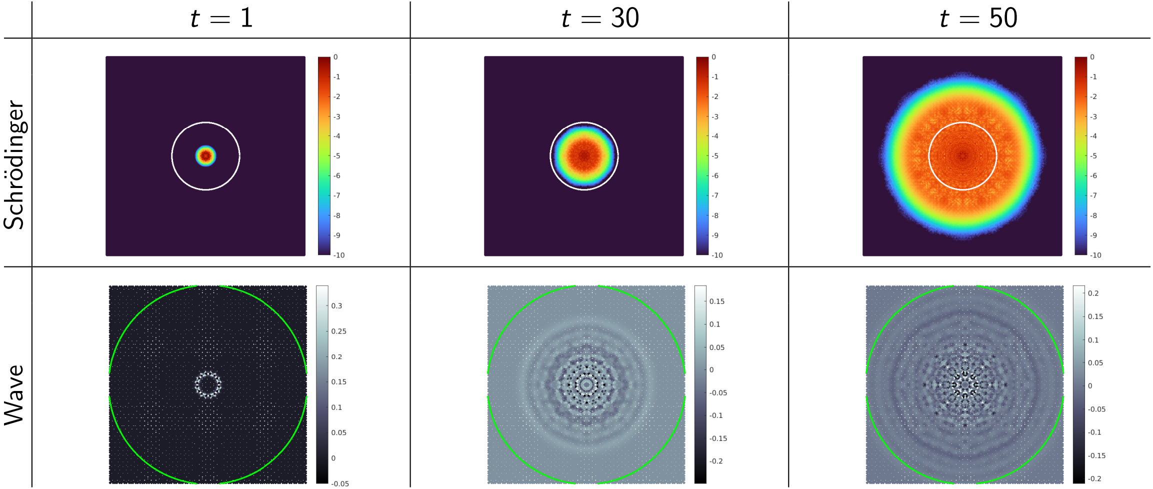
Quasicrystals

Quasicrystal: Aperiodic material with long-range order.

- Discovered by Dan Shechtman in 1982 (awarded Nobel prize in Chemistry 2011).
- Luca Bindi and Paul Steinhardt discovered icosahedrite, first natural quasicrystal (awarded 2018 Aspen Institute Prize for scientific collaboration between Italy and US).
- Many exotic physical properties and beginning to be used in
  - heat insulation
  - LEDs, solar absorbers, and energy coatings
  - reinforcing materials, e.g., low-friction gears
  - bone repair (hardness, low friction, corrosion resistance)...
- E.g., what's the analogy of periodic physics for aperiodic systems?

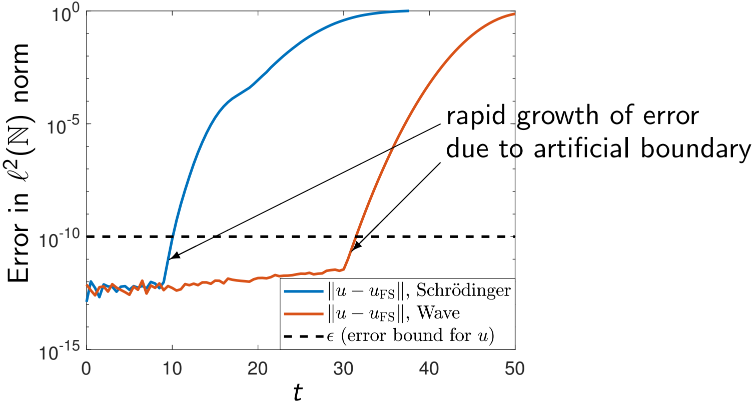
· D. Johnstone, M. Colbrook, A. Nielsen, P. Öhberg, C. Duncan, "*Bulk localised transport states in infinite and finite quasicrystals via magnetic aperiodicity*," arXiv preprint.

Computed solutions with guaranteed accuracy $\epsilon = 10^{-10}$



Top row: `log10`$(|u(t)|)$ for Schrödinger equation. Bottom row: $u(t)$ for wave equation.

$u_{\mathrm{FS}} =$ solution by direct diagonalisation of 10001×10001 truncation.



As t increases, we need more vertices (basis vectors) to capture the solution.
The method of this talk allows this to be done rigorously and adaptively.

When is our equation well-posed?

$$\frac{du}{dt} = Au, \quad u(0) = u_0 \in \mathcal{H}. \tag{1}$$

Eq. (1) well-posed $\Leftrightarrow$ A generates a strongly continuous semigroup $(u(t) = \exp(tA)u_0)$

Spectrum: $\mathrm{Sp}(A) = \{z : A - zI \text{ not invertible}\}$

Theorem (Hille–Yosida Theorem)

A generates a strongly continuous semigroup if and only if A is densely defined and there exists $\omega \in \mathbb{R}$, $M > 0$ such that

$$\textit{if } \mathrm{Re}(z) > \omega, \textit{ then } z \notin \mathrm{Sp}(A) \textit{ and } \|(A - zI)^{-n}\| \leq \frac{M}{(\mathrm{Re}(z) - \omega)^n}, \quad \forall n \in \mathbb{N}.$$

Two open foundations problems

Q.1: *Computing semigroups with error control: Does there exist an algorithm with input:*

- *a generator A of a strongly continuous semigroup on $\mathcal{H}$,*
- *a time $t > 0$,*
- *an arbitrary initial condition $u_0 \in \mathcal{H}$,*
- *an error tolerance $\epsilon > 0$,*

that computes an approximation of $\exp(tA)u_0$ to accuracy ϵ in $\mathcal{H}$?

Q.2: *For $\mathcal{H} = L^2(\mathbb{R}^d)$ is there a large class of partial differential operators A on the unbounded domain $\mathbb{R}^d$ where the answer to Q.1 is yes?*

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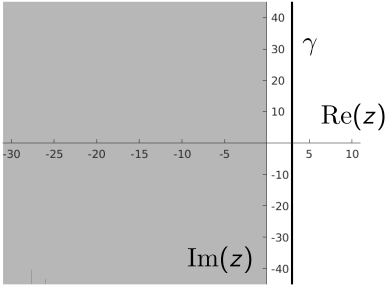
We will provide resolutions to both problems!

We will also extend the techniques to other scenarios such as time-fractional PDEs!

A first attempt

$$\frac{du}{dt} = Au, \quad u(0) = u_0 \in \mathcal{H}.$$

Take Laplace transform (denoted $\hat{\cdot}$) $\Rightarrow$ $\hat{u}(z) = \int_0^\infty e^{-zt} u(t) dt = -(A - zI)^{-1} u_0.$



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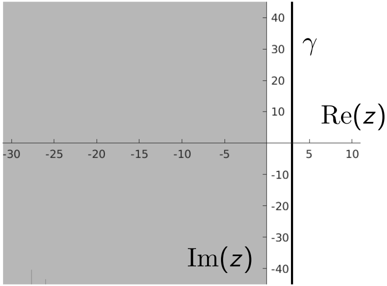

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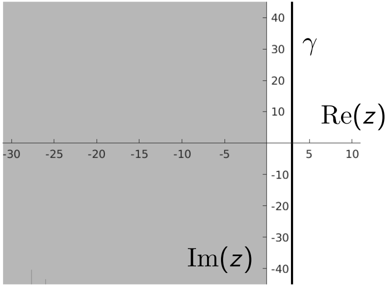

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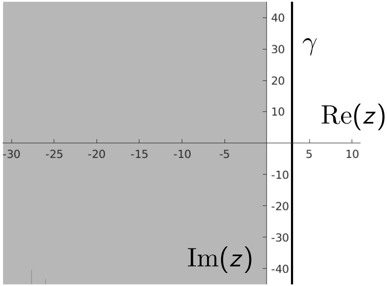

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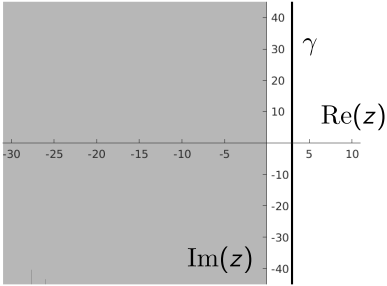

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Problems:

- Integrand does not decay!
- How do we compute $(A - zI)^{-1}$?
- How do we bound error of approximating the integral?

Q.1: $\mathcal{H} = \ell^2(\mathbb{N})$ with inner product $\langle \cdot, \cdot \rangle$

Input ($\Omega_{\ell^2(\mathbb{N})}$): (A, u_0, t) s.t. A generates strongly continuous semigroup, $u_0 \in \ell^2(\mathbb{N})$, $t > 0$.

Allow access to:

- Arbitrary precision approximations of:

  $$\text{(Matrix evaluations)} \quad \langle Ae_k, e_j \rangle, \quad \langle Ae_k, Ae_j \rangle, \quad \forall j, k \in \mathbb{N},$$

  $$\text{(Coefficient evaluations)} \quad \langle u_0, u_0 \rangle, \quad \langle u_0, e_j \rangle, \quad \forall j \in \mathbb{N}.$$

- Constants M, ω satisfying conditions in Hille–Yosida Theorem.

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Theorem 1 (Strongly continuous semigroups on $\ell^2(\mathbb{N})$ computed with error control)

There exists a universal algorithm $\Gamma_{\ell^2(\mathbb{N})}$ using the above, such that

$$\|\Gamma_{\ell^2(\mathbb{N})}(A, u_0, t, \epsilon) - \exp(tA)u_0\|_{\ell^2(\mathbb{N})} \leq \epsilon, \quad \forall \epsilon > 0 \text{ and } (A, u_0, t) \in \Omega_{\ell^2(\mathbb{N})}.$$

- Regularisation (a standard trick from functional analysis):

$$\exp(tA)u_0 = (A - (\omega+2)I)^2 \left[\frac{-1}{2\pi i} \int_{\omega+1-i\infty}^{\omega+1+i\infty} \underbrace{\frac{e^{zt}(A - zI)^{-1}}{(z-(\omega+2))^2}}_{\text{now decays}} \, dz \right] u_0 .$$

Idea of proof

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- A few reductions (using Hille–Yosida theorem) to approximating the operator

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- Truncation + quadrature for decaying integrand.
- Apply $(A-zI)^{-1}$ using least-squares and adaptive truncations by controlling residuals.

Q.2: $\mathcal{H} = L^2(\mathbb{R}^d)$

$$[Au](x) = \sum_{k \in \mathbb{Z}^d_{\geq 0}, |k| \leq N} a_k(x) \partial^k u(x).$$

Input (Ω_{PDE}): (A, u_0, t) such that A generates a strongly continuous semigroup on $L^2(\mathbb{R}^d)$, $u_0 \in L^2(\mathbb{R}^d)$ and $t > 0$

Allow access to:

- Arbitrary precision pointwise evaluations $a_k(q), u_0(q), q \in \mathbb{Q}^d$.
- Bounds on growth rate and 'oscillations' of coefficients.
- Sequence $c_n \to 0$ with $\| u_0|_{[-n,n]^d} - u_0 \|_{L^2(\mathbb{R}^d)} \leq c_n$.
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Theorem 2 (PDE semigroups on $L^2(\mathbb{R}^d)$ computed with error control)

There exists a universal algorithm Γ_{PDE} using the above, such that

$$\|\Gamma_{\mathrm{PDE}}(A, u_0, t, \epsilon) - \exp(tA)u_0\|_{L^2(\mathbb{R}^d)} \leq \epsilon, \quad \forall \epsilon > 0 \text{ and } (A, u_0, t) \in \Omega_{\mathrm{PDE}}$$

Idea of proof

- Reduce to Q.1 using (tensor product) Hermite basis

$$\psi_m(x) = (2^m m!\sqrt{\pi})^{-1/2} e^{-x^2/2} H_m(x), \quad H_m(x) = (-1)^m e^{x^2} \frac{d^m}{dx^m} e^{-x^2}.$$

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- Compute inner products (with error control)

$$\langle Ae_k, Ae_j \rangle = \int_{\mathbb{R}^d} (A\psi_{m(k)}) \overline{(A\psi_{m(j)})} dx, \quad \langle Ae_k, e_j \rangle = \int_{\mathbb{R}^d} (A\psi_{m(k)}) \psi_{m(j)} dx,$$

using quasi-Monte Carlo numerical integration.

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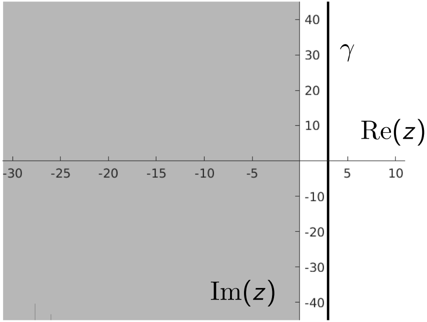
  using quasi-Monte Carlo numerical integration.
- Similar techniques deal with u_0.

Analytic semigroups



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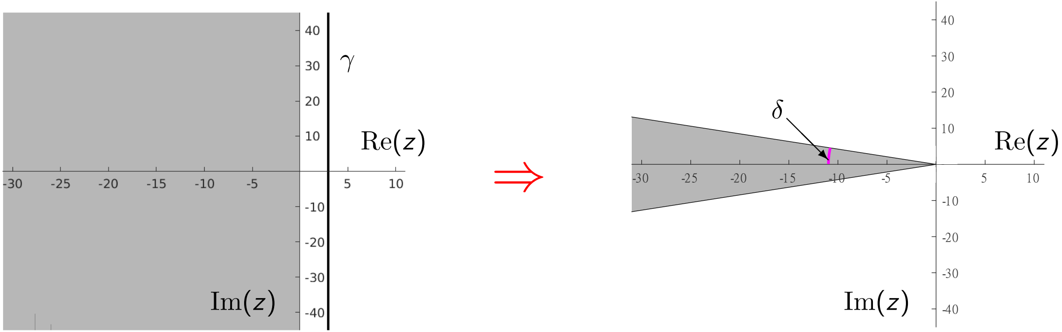

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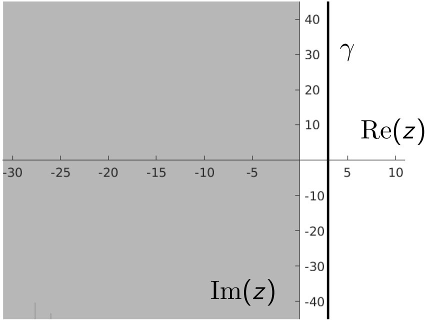
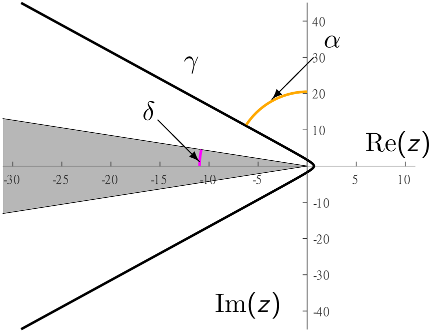


$\Rightarrow$



$$\exp(tA)u_0 = \left[\frac{-1}{2\pi i}\int_\gamma e^{zt}(A - zI)^{-1}\,dz\right] u_0$$

$$\gamma(s) = \mu(1 + \sin(is - \alpha)), \quad \mu > 0, \quad 0 < \alpha < \frac{\pi}{2} - \delta \quad (s \in \mathbb{R}).$$

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· J. Weideman, L.N. Trefethen, "*Parabolic and hyperbolic contours for computing the Bromwich integral*," Mathematics of Computation, 2007.

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Leads to 'optimal' h, μ and α as functions of N, Λ_t and δ.

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Leads to 'optimal' h, μ and α as functions of N, Λ_t and δ.

Problem: Numerical instability since $\max(\mathrm{Re}(z_j)) \to \infty$ as $N \to \infty$.

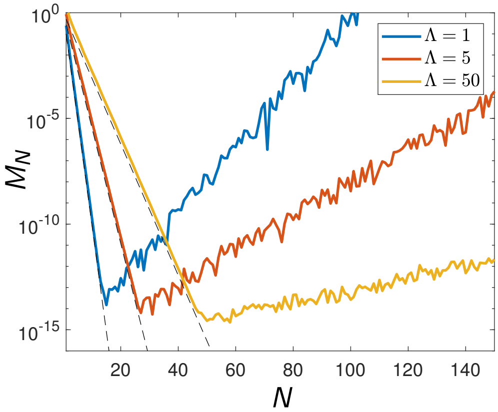
· J. Weideman, L.N. Trefethen, "*Parabolic and hyperbolic contours for computing the Bromwich integral*," Mathematics of Computation, 2007.

Instability (even in scalar case)

$$1 = \frac{1}{2\pi i}\int_\gamma \frac{e^{zt}}{z}dz.$$

$$M_N = \text{ max error for } t \in [t_0, t_1].$$

Previous parameter choices



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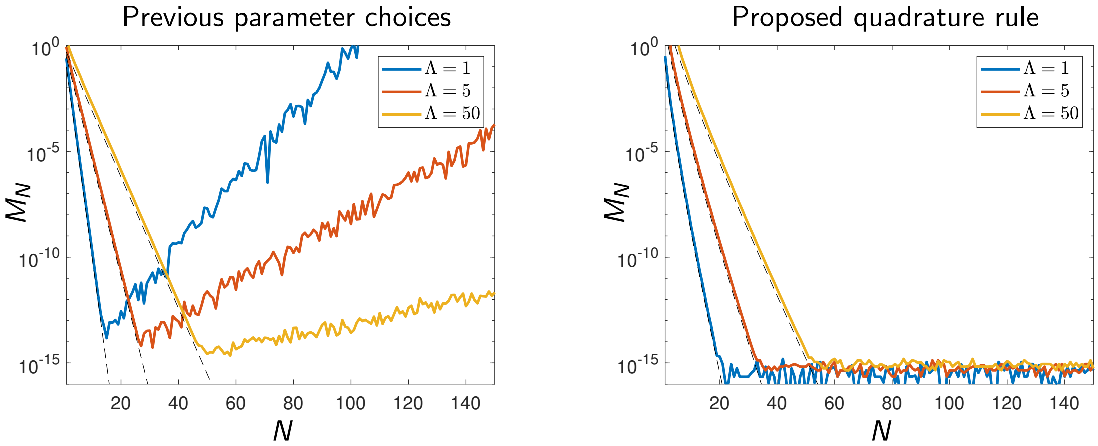

Enforcing stability

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Idea: Enforce $\max(\mathrm{Re}(z_j))t_1 \leq \beta$ as $N \to \infty$ for stability.

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$$h = \frac{1}{N}W\Big(\Lambda_t N \frac{\pi(\pi - 2\delta)}{\beta \sin\left(\frac{\pi-2\delta}{4}\right)}\Big(1 - \sin\left(\frac{\pi - 2\delta}{4}\right)\Big)\Big), \quad \mu = \frac{\beta/t_1}{1 - \sin((\pi - 2\delta)/4)}, \quad \alpha = \frac{h\mu t_1 + \pi^2 - 2\pi\delta}{4\pi}.$$

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Algorithm: Stable and rapidly convergent algorithm for analytic semigroups.

Input: A (generator of an analytic semigroup with angle $\delta \in [0, \pi/2)$), $u_0 \in \mathcal{H}$, $0 < t_0 \le t_1 < \infty$, $\beta > 0$, $N \in \mathbb{N}$ and $\eta > 0$.

1: Let γ be defined as above with α, μ and h given by above, where $\Lambda_t = t_1/t_0$.
2: Set $z_j = \gamma(jh)$ and $w_j = \frac{h}{2\pi i}\gamma'(jh)$.
3: Solve $(A - z_j I)R_j = -u_0$ for $-N \le j \le N$ to an accuracy η.

Output: $u_N(t) = \sum_{j=-N}^{N} e^{z_j t} w_j R_j$ for $t \in [t_0, t_1]$.

Theorem 3 (Stable & rapidly convergent algorithm for analytic semigroups)

Explicit constant C such that for any $t_0 \leq t \leq t_1$,

$$\|\exp(tA)u_0 - u_N(t)\|_{\mathcal{H}} \leq \underbrace{\left(2\mu e^{\frac{\beta}{1-\sin(\alpha)}}\pi^{-1}\int_0^\infty e^{x-\mu t \sin(\alpha)\cosh(x)}dx\right)\eta}_{\textit{numerical error due to inexact resolvent}}$$

$$+ \underbrace{Ce^{\frac{\beta}{1-\sin(\alpha)}} \cdot \exp\left(-\frac{N\pi(\pi-2\delta)/2}{\log(\Lambda_t \frac{\sin(\pi/4-\delta/2)^{-1}-1}{\beta} N\pi(\pi-2\delta))}\right)}_{\textit{quadrature error}}$$

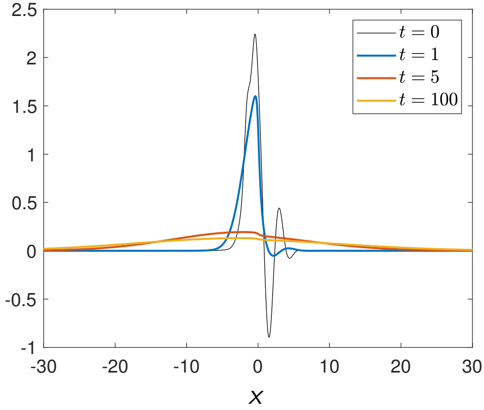
$$= \mathcal{O}(\eta) + \mathcal{O}(\exp(-cN/\log(N))).$$

Example on $L^2(\mathbb{R})$ demonstrating convergence

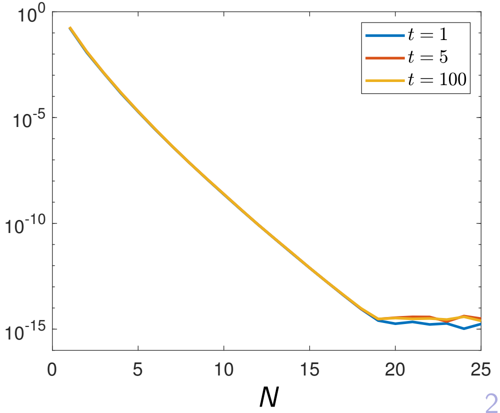
$$u_t = [(1.1 - 1/(1+x^2))u_x]_x, \quad u_0(x) = e^{-\frac{(x-1)^2}{5}}\cos(2x) + 2[1+(x+1)^4]^{-1}.$$

$$\textbf{Basis: } \phi_n(x) = \pi^{-1/2}(1+ix)^n(1-ix)^{-(n+1)}, \quad n \in \mathbb{Z}.$$

Solutions ($\epsilon = 10^{-12}$)



Relative errors



What about fractional derivatives?

$$[\mathcal{D}_t^\nu g](t) = \begin{cases} \dfrac{1}{\Gamma(n-\nu)} \displaystyle\int_0^t (t-\tau)^{n-\nu-1} g^{(n)}(\tau) d\tau, & \text{if } n-1 < \nu < n, \\ g^{(n)}(t), & \text{if } \nu = n. \end{cases}$$

Time-fractional equation: $\sum_{j=1}^M \mathcal{D}_t^{\nu_j} A_j u = f(t)$ for $t \geq 0, \quad n_j - 1 < \nu_j \leq n_j.$

Applications: Solid mechanics, biology, electrochemistry, finance, signal processing, anomalous diffusion, statistics, astrophysics, etc. (Explosion of interest over last $\approx$ 15 years.)

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- Non-local time derivative.
- Hard to get high accuracy.
- Large memory consumption.
- Singularities as $t \downarrow 0$.

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Contour method in this talk:

- Global approximation.
- Exponential convergence and linear complexity.
- No time-stepping needed, parallelisable, reuse computations at different times.
- Avoids singularities (looks straight ahead to $t > 0$).

$$\sum_{j=1}^{M} \mathcal{D}_t^{\nu_j} A_j u = f(t) \text{ for } t \geq 0, \quad n_j - 1 < \nu_j \leq n_j.$$

Operator: $T(z) = \sum_{j=1}^{M} z^{\nu_j} A_j, \qquad T(z) : \mathcal{D}(T) \subset \mathcal{H} \to \mathcal{H}.$

Known function: $K(z) = \hat{f}(z) + \sum_{j=1}^{M} A_j \sum_{k=1}^{n_j} z^{\nu_j - k} u^{(k-1)}(0), \qquad K : \mathbb{C} \to \mathcal{H}.$

Aside on causality: Can replace $\hat{f}(z)$ by $\int_0^t e^{-zs} f(s) ds$ and approximate via quadrature.

$$T(z)\hat{u}(z) = K(z) \text{ (posed in } \mathcal{H}) \Rightarrow u(t) = \frac{1}{2\pi i} \int_\gamma e^{zt} \left[T(z)^{-1} K(z) \right] dz$$

Method: Apply the above stable and exponentially convergent quadrature rule.

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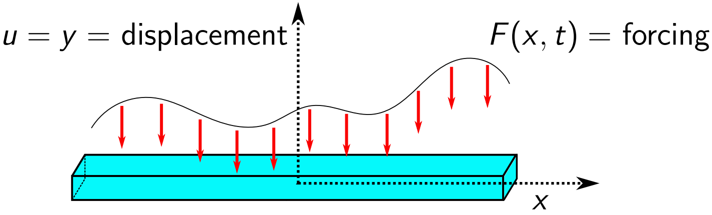
Challenges:

- Must analyse generalised spectrum $\mathrm{Sp}(T) = \{z \in \mathbb{C} : T(z) \text{ is not invertible}\}$.
  NB: Often easier for infinite-dimensional operator as opposed to discretisation:

$$\|T(z)^{-1}\| \leq [\mathrm{dist}(0, \mathcal{N}(T(z)))]^{-1}, \quad \mathcal{N}(T(z)) := \{\langle T(z)v, v\rangle : v \in \mathcal{D}(T(z)), \|v\| = 1\}.$$

- For high accuracy, need generalised spectrum contained in sector to deform contour.

Fractional beam equations



Stress-strain relation: $\underbrace{\sigma(x,t)}_{\text{stress}} = E_0(x)\underbrace{\epsilon(x,t)}_{\text{strain}} + E_1(x)\mathcal{D}_t^{\nu}\underbrace{\epsilon(x,t)}_{\text{strain}}.$

$$\frac{\partial^2 y}{\partial t^2} + \frac{1}{\rho(x)}\frac{\partial^2}{\partial x^2}\left[a(x)\frac{\partial^2 y}{\partial x^2} + b(x)\mathcal{D}_t^{\nu}\frac{\partial^2 y}{\partial x^2}\right] = \frac{F(x,t)}{\rho(x)}, \quad x \in [-1,1], \quad a(x) > 0.$$

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

Fractional beam equations

Modern materials (e.g., embedded polymers, biomaterials) have exotic structural properties.
Elastic and viscous properties captured experimentally

$\Updownarrow$ Numerical validation (100s of papers)

Models used to fit stress-strain relationships.
Time-fractional derivatives popular (accurate with few parameters).

Problem: Numerical methods typically suffer from (1) limited accuracy and high computational cost, or (2) restricted to the constant beam parameters that allow semi-analytical results.

Fast and accurate numerical method crucial for interaction between theory and experiments!

Quasi-linearisation of $[T(z)]y = z^2 y + \frac{1}{\rho(x)} \frac{\partial^2}{\partial x^2}\left[a(x)\frac{\partial^2 y}{\partial x^2} + z^\nu b(x)\frac{\partial^2 y}{\partial x^2}\right]$

$\mathcal{H}^2_{\mathrm{BC1}}$, $\mathcal{H}^2_{\mathrm{BC2}}$: Sobolev subspaces of $H^2(-1,1)$ capturing BCs.

$$\mathcal{H} = \mathcal{H}^2_{\mathrm{BC1}} \times L^2_\rho(-1,1), \quad \langle (u_0,u_1),(v_0,v_1)\rangle_{\mathcal{H}} = \int_{-1}^1 a(x)u_0''(x)\overline{v_0''(x)}dx + \int_{-1}^1 \rho(x)u_1(x)\overline{v_1(x)}dx.$$

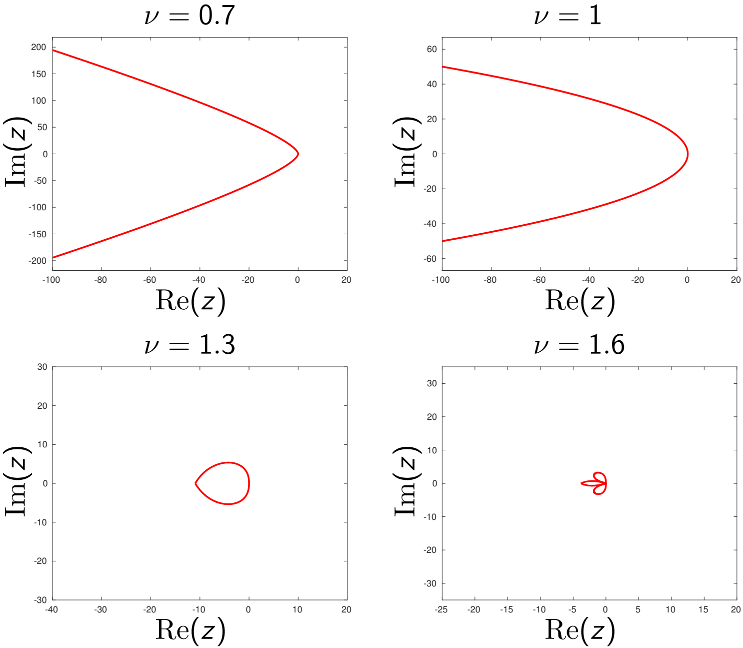
Linearise quadratic term:

$$[\mathcal{A}(z)]\left(u_0,u_1\right) = z\left(u_0,u_1\right) + \left(-u_1, \tfrac{1}{\rho}(au_0'' + z^{\nu-1}bu_1'')''\right),$$

$$\mathcal{D}(\mathcal{A}(z)) = \left\{(u_0,u_1) \in \mathcal{H}^2_{\mathrm{BC1}} \times \mathcal{H}^2_{\mathrm{BC1}} : au_0'' + z^{\nu-1}bu_1'' \in \mathcal{H}^2_{\mathrm{BC2}}\right\}.$$

$$[\mathcal{A}(z)]^{-1}\left(0,v\right) = \left([T(z)]^{-1}v, z[T(z)]^{-1}v\right), \quad \forall v \in L^2_\rho(-1,1).$$

Key point: Generalised spectrum of $\mathcal{A}(z)$ much easier to study.



ν = 0.7
ν = 1
ν = 1.3
ν = 1.6
Im(z)
Re(z)
200
150
100
50
0
-50
-100
-150
-200
-100
-80
-60
-40
-20
20
60
40
-60
30
10
-10
-30
-25
-15
-5
5
15

Computing $T(z)^{-1}$ and computational cost

Solve the ODEs using sparse spectral methods (expanded in n Chebyshev polynomials).

- Computation of $T(z)^{-1}$ converges exponentially in n with $\mathcal{O}(n)$ complexity.
- Quadrature error bounded by $\mathcal{O}(\exp(-cN/\log(N)))$ for N quadrature points.
- Solutions of ODEs computed in parallel and reused for different times $t \in [t_0, t_1]$.
- Avoids the large memory consumption/computation time of time stepping methods.
- Solution computed with explicit error control (10^{-8} in what follows).

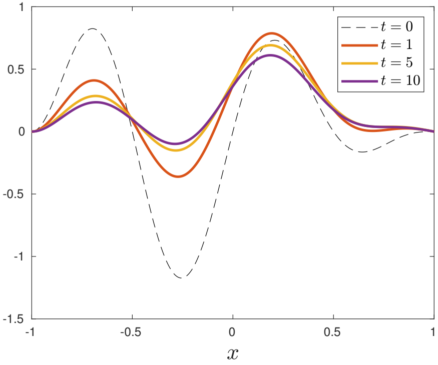
· S. Olver, A. Townsend, "*A fast and well-conditioned spectral method*," SIAM Review, 2013.

Toy example

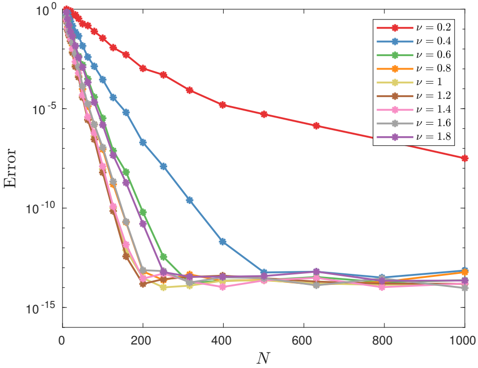
$$a = \cosh(x), \quad b = \sin(\pi x) + 2, \quad \rho = \tanh(x) + 2, \quad F(x,t) = \cos(20t)\sin(\pi x),$$

$$y(x,0) = \sin(2\pi x)(1-x^2)(1-x), \quad \frac{\partial y}{\partial t}(x,0) = 0.$$

$\nu = 0.4$



Max error over $t \in [1, 10]$

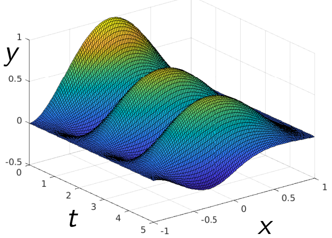


Physical example

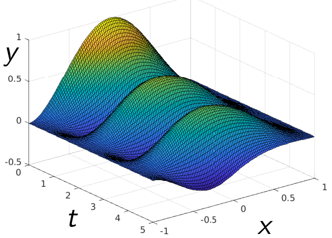
$$a = 1, \quad b = 1.01 + \tanh(10x) \text{ (weakly damped for } x < 0\text{, strongly damped for } x > 0\text{)},$$

$$\rho = 1, \quad F(x,t) = \cos(\pi t)(24 - \pi^2(1 - x^2)^2), \quad y(x,0) = (1 - x^2)^2, \quad \frac{\partial y}{\partial t}(x,0) = 0.$$

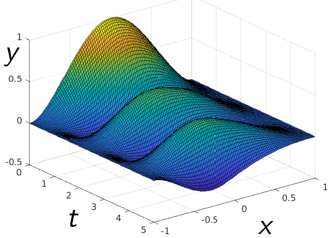
$\nu = 0.5$



$\nu = 0.7$

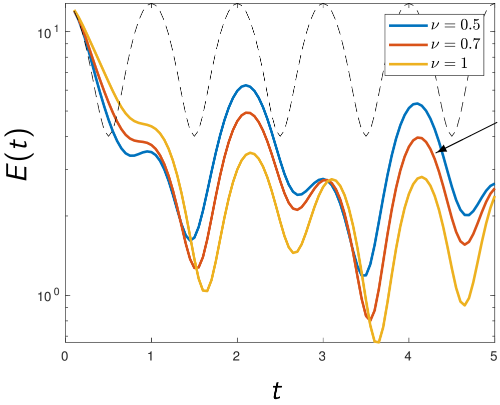


$\nu = 1$



Physical example

Energy (computed with error control): $E(t) = \dfrac{1}{2}\displaystyle\int_{-1}^{1} a(x)|y_{xx}(x,t)|^2 + \rho(x)|y_t(x,t)|^2 dx.$



oscillates due to forcing

Wider framework

How: Deal with operators directly, instead of previous 'truncate-then-solve'.
(e.g., adaptive truncations to compute the resolvent with error control)

$\Rightarrow$ Compute many properties for the first time.

Framework: Classify problems in a computational hierarchy measuring intrinsic difficulty.

$\Rightarrow$ Algorithms realise boundaries of what computers can achieve.

Other recent examples:

- Computing spectra $\mathrm{Sp}(A)$ of operators.
- Computing spectral measures of operators.
- Koopman operators (cf. Koopmania)
- Optimisation and neural networks (finite-dimensional problems!).

· Colbrook, "*The Foundations of Infinite-Dimensional Spectral Computations*," PhD diss., 2020.
· Colbrook, Roman, Hansen, "*How to compute spectra with error control*" Physical Review Letters, 2019.
· Colbrook, "*Computing spectral measures and spectral types*" Communications in Mathematical Physics, 2021.
· Colbrook, Horning, Townsend, "*Computing spectral measures of self-adjoint operators*" SIAM Review, 2021.
· Colbrook, Townsend, "*Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems*" arXiv, out this morning!
· Colbrook, Antun, Hansen "*Can stable and accurate neural networks be computed?*," PNAS, to appear.

Conclusion

Key points:

- **Q.1:** Semigroups can be computed with error control via a universal algorithm.
- **Q.2:** Extends to PDEs (e.g., on unbounded domain $L^2(\mathbb{R}^d)$).
- New <u>stable</u> and rapidly convergent quadrature rule for analytic semigroups.
- Extends to time-fractional PDEs via Laplace transform (need to bound gen. spectrum).
- Methods are part of a wider framework (e.g., deals with inf-dim operators directly).

Future work:

- Non-autonomous cases and non-linear cases (e.g., splitting).
- Other time-fractional PDEs can now be tackled. E.g., 2D fractional beam equations.

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A question for Mattia and Nicola: What if $\|(A - zI)^{-1}\|$ can't be studied analytically? Can we combine with roaming methods and new infinite-dimensional methods for computing pseudospectra with error control?

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For papers and code: http://www.damtp.cam.ac.uk/user/mjc249/home.html