Computing semigroups with error control

And a framework for infinite-dimensional computations

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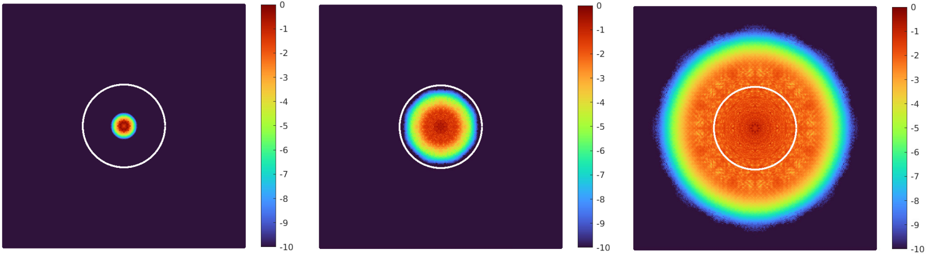
Papers:

M.J. Colbrook, "Computing semigroups with error control"

M.J. Colbrook and L.J. Ayton, "A contour method for time-fractional PDEs"



The finite-dimensional case

Solve for $u : \underbrace{[0,\infty)}_{\text{'time'}} \to \mathbb{C}^n$ s.t.

$$\frac{du}{dt} = \mathbb{A}u, \quad \mathbb{A} \in \mathbb{C}^{n\times n}, \quad u(0) = u_0 \in \mathbb{C}^n.$$

$$u(t) = \exp(t\mathbb{A})u_0 = \sum_{j=0}^{\infty} \frac{t^j}{j!}\mathbb{A}^j u_0.$$

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 another story...)

The infinite-dimensional case

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

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

GOAL: Compute the solution at time t.

Philosophy of the approach

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

Domain truncation and absorbing boundary conditions (e.g. when A represents a differential operator on an unbounded domain), Galerkin methods, Krylov methods, rational approximations, Runge–Kutta methods, series expansions, splitting methods, exponential integrators, ...

Typical difficulties:

- Often very difficult to bound the error when we go from A to $\mathbb{A}$.
- Sometimes $\mathbb{A}$ is more complicated to study (e.g. where are it's eigenvalues?).
- Sometimes $\mathbb{A}$ does not respect key properties of the system.
- For PDEs on unbounded domains, there are two truncations: the physical domain and then the operator restricted to this domain.

PHILOSPHY OF THIS TALK: Solve-then-discretise.

Open **Foundations** Questions

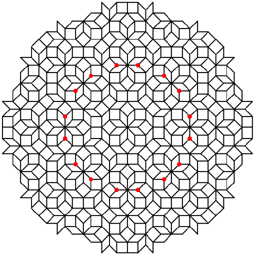
Q.1: *Can we compute semigroups with error control? I.e., does there exist an algorithm that given a generator A of a strongly continuous semigroup on $\mathcal{H}$, time $t > 0$, arbitrary $u_0 \in \mathcal{H}$ and error tolerance $\epsilon > 0$, computes an approximation of $\exp(tA)u_0$ to accuracy ϵ in $\mathcal{H}$?*

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

We'll provide resolutions to these two problems!

NB: Q2 has recently been solved in the positive for Schrödinger operators using weighted Sobolev bounds on the initial condition for rigorous domain truncation [Becker & Hansen, 2020]. We'll aim to go much broader.

Example



Aperiodic (no repeating pattern) infinite Ammann–Beenker (AB) tiling. Such structures have very interesting transport properties but notoriously difficult to compute. Graph Laplacian:

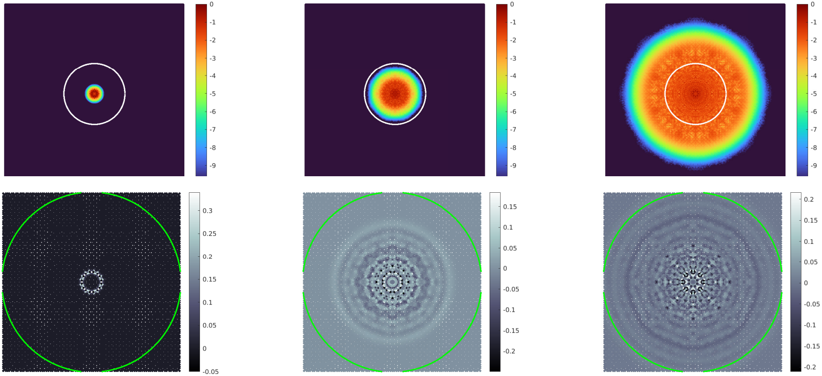
$$[\Delta_{\mathrm{AB}}\psi]_i = \sum_{i\sim j} (\psi_j - \psi_i)\,, \quad \{\psi_j\}_{j\in\mathbb{N}} \in l^2(\mathbb{N}).$$

Schrödinger equation and wave equation:

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

Example

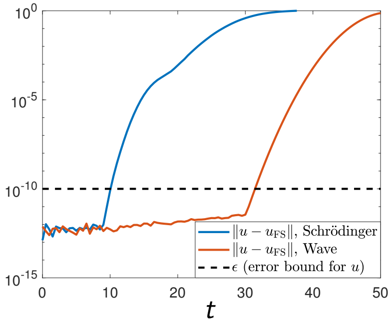
Solutions computed with **guaranteed accuracy** $\epsilon = 10^{-10}$.



Top row: `log10`$(|u(t)|)$ computed for the Schrödinger equation at times $t = 1$ (left), $t = 10$ (middle) and $t = 50$ (right). Bottom row: $u(t)$ computed for the wave equation at times $t = 1$ (left), $t = 30$ (middle) and $t = 50$ (right).

Example

u_{FS}: solution by direct diagonalisation of 10001×10001 truncation.



Small difference for small t, then grows quickly due to boundary effects.
As t increases, need more vertices (basis vectors) to capture the solution - method of this talk allows this to be done rigorously and adaptively.

Strongly continuous semigroup

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

Definition

Strongly cts semigroup is a map $S : [0, \infty) \to \underbrace{\mathcal{L}(\mathcal{H})}_{\text{bounded operators on } \mathcal{H}}$ *s.t.*

(1) $S(0) = I$

(2) $S(s + t) = S(s)S(t), \quad \forall s, t \geq 0$

(3) $\lim_{t \downarrow 0} S(t)v = v$ *for all* $v \in \mathcal{H}$.

The infinitesimal generator A *of* S *is defined via* $Ax = \lim_{t\downarrow 0} \frac{1}{t}(S(t) - I)x$, *where* $\mathcal{D}(A)$ *is all* $x \in X$ *such that the limit exists, write* $S(t) = \exp(tA)$.

Why we care: A generates C_0-semigroup $\Leftrightarrow$ (1) well-posed

Hille–Yosida Theorem

$$\mathrm{Sp}(A) = \{z : A - zI \text{ not invertible}\}, \quad \rho(A) := \mathbb{C}\backslash\mathrm{Sp}(A)$$

$$R(z, A) = (A - zI)^{-1} \text{ for } z \in \rho(A)$$

Theorem

A closed operator A generates a C_0-semigroup if and only if A is densely defined and there exists $\omega \in \mathbb{R}$, $M > 0$ with

(1) $\{\lambda \in \mathbb{R} : \lambda > \omega\} \subset \rho(A)$.

(2) *For all $\lambda > \omega$ and $n \in \mathbb{N}$, $(\lambda - \omega)^n \|R(\lambda, A)^n\| \leq M$.*

Under these conditions, $\|\exp(tA)\| \leq M \exp(\omega t)$ and if $\mathrm{Re}(\lambda) > \omega$ then $\lambda \in \rho(A)$ with

$$\|R(\lambda, A)^n\| \leq \frac{M}{(\mathrm{Re}(\lambda) - \omega)^n}, \quad \forall n \in \mathbb{N}.$$

$$\exp(tA)u_0 = \left[\frac{-1}{2\pi i}\int_{\sigma - i\infty}^{\sigma + i\infty} \underbrace{e^{zt}(A - zI)^{-1}}_{\text{no decay?!}}\, dz\right] u_0, \quad \text{for } \sigma > \omega,$$

Case 1: $\mathcal{H} = l^2(\mathbb{N})$

$\mathrm{span}\{e_n : n \in \mathbb{N}\}$ forms a core of A and $A^* \Rightarrow$ matrix $A_{j,k} = \langle Ae_k, e_j \rangle$.

Ω_{C_0}: (A, u_0, t) s.t. A generates C_0-semigroup, $u_0 \in l^2(\mathbb{N})$ and $t > 0$.

Allow access to:

- Matrix evaluations $\{f^{(1)}_{j,k,m}, f^{(2)}_{j,k,m} : j, k, m \in \mathbb{N}\}$ such that
$$|f^{(1)}_{j,k,m}(A) - \langle Ae_k, e_j \rangle| \leq 2^{-m}, \quad |f^{(2)}_{j,k,m}(A) - \langle Ae_k, Ae_j \rangle| \leq 2^{-m}.$$
- Coefficient/norm evaluations $\{f_{j,m} : j \in \mathbb{N} \cup \{0\}, m \in \mathbb{N}\}$ such that
$$|f_{0,m}(u_0) - \langle u_0, u_0 \rangle| \leq 2^{-m}, \quad |f_{j,m}(u_0) - \langle u_0, e_j \rangle| \leq 2^{-m}.$$
- Constants M, ω satisfying conditions in Hille–Yosida Theorem.

Theorem 1 (C_0-semigroups on $l^2(\mathbb{N})$ computed with error control)

There exists a universal algorithm Γ using the above, s.t.

$$\|\Gamma(A, u_0, t, \epsilon) - \exp(tA)u_0\| \leq \epsilon, \quad \forall \epsilon > 0, (A, u_0, t) \in \Omega_{C_0}.$$

Idea of proof

- Regularisation:

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

- Use well-posedness to reduce to $u_0 = e_k$ for some $k \in \mathbb{N}$ and

$$\exp(tA)e_k = (A-(\omega+2)I) \left[\frac{-1}{2\pi i} \int_{\omega+1-i\infty}^{\omega+1+i\infty} \frac{e^{zt}R(z,A)}{(z-(\omega+2))^2} dz \right] (A-(\omega+2)I)e_k.$$

- Final reduction to

$$\left[\frac{1}{2\pi i} \int_{\omega+1-i\infty}^{\omega+1+i\infty} \frac{\exp(zt)R(z,A)}{(z-(\omega+2))^2} dz \right] e_l.$$

- Truncation + quadrature for decaying integrand.

At each step, use adaptive computation of $R(z,A)$ with **error control**.

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

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

$$\mathcal{A}_r = \{f \in \mathrm{Meas}([-r,r]^d) : \|f\|_\infty + \mathrm{TV}_{[-r,r]^d}(f) < \infty\}.$$

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

(1) Smooth, compactly supported functions form a core of A and A^*.

(2) At most polynomial growth: There exists $C_k > 0$ and $B_k \in \mathbb{N}$ s.t. almost everywhere on $\mathbb{R}^d$, $|a_k(x)| \leq C_k(1 + |x|^{2B_k})$.

(3) Locally bounded total variation: $\forall r > 0$, $u_0|_{[-r,r]^d}, a_k|_{[-r,r]^d} \in \mathcal{A}_r$.

NB: Very mild assumptions.
e.g. discontinuous coefficients with arbitrary wild oscillations at infinity

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

Allow access to:

(a) Pointwise coefficient evaluations: $\{S_{k,q,m}\}$ s.t.

$$|S_{k,q,m}(A) - a_k(q)| \leq 2^{-m}, \quad \forall q \in \mathbb{Q}^d.$$

(b) Pointwise initial condition evaluations: $\{S_{q,m}\}$ s.t.

$$|S_{q,m}(u_0) - u_0(q)| \leq 2^{-m}, \quad \forall q \in \mathbb{Q}^d.$$

(c) Bounds on growth and total variation: $\{C_k, B_k\}$ s.t. $|a_k(x)| \leq C_k(1 + |x|^{2B_k})$ and positive sequences $\{b_n\}_{n\in\mathbb{N}}$ and $\{c_n\}_{n\in\mathbb{N}}$ s.t.

$$\max_{|k|\leq N} \|a_k\|_{\mathcal{A}_n} \leq b_n, \quad \|u_0\|_{\mathcal{A}_n} \leq c_n.$$

(d) Decay of initial condition: A positive sequence $\{d_n\}_{n\in\mathbb{N}}$,

$$\|u_0|_{[-n,n]^d} - u_0\|_{L^2(\mathbb{R}^d)} \leq d_n, \quad \lim_{n\to\infty} d_n = 0,$$

(e) Constants M, ω satisfying conditions in Hille–Yosida Theorem.

Theorem 2 (PDO C_0-semigroups on $L^2(\mathbb{R}^d)$ computed with error control)

There exists a universal algorithm Γ using the above, s.t.

$$\|\Gamma(A, u_0, t, \epsilon) - \exp(tA)u_0\| \leq \epsilon, \quad \forall \epsilon > 0, (A, u_0, t) \in \Omega_{\mathrm{PDE}}$$

Idea of proof

- Reduce to Case 1 using (tensor product) basis

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

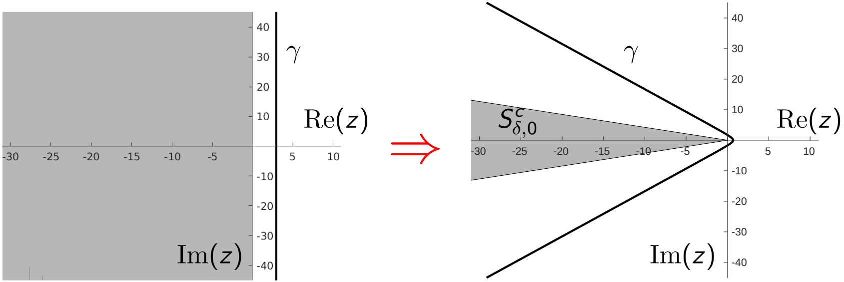
- Compute inner products (with error control)

$$\langle \hat{A}e_k, \hat{A}e_j \rangle = \int_{\mathbb{R}^d} (A\psi_{m(k)}) \overline{(A\psi_{m(j)})} dx$$
$$\langle \hat{A}e_k, e_j \rangle = \int_{\mathbb{R}^d} (A\psi_{m(k)}) \psi_{m(j)} dx, \quad \langle \hat{u}_0, e_j \rangle = \int_{\mathbb{R}^d} u_0 \psi_{m(i)} dx,$$

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

NB: Choice of Hermite functions simply convenient in the proof (allows a very large class of coefficients to be treated). Other bases and domains clearly work if relevant integrals can be computed with error control.

Case 3: Analytic semigroups



$$S_{\delta,\sigma} := \{z \in \mathbb{C} : \arg(z - \sigma) < \pi - \delta\}.$$

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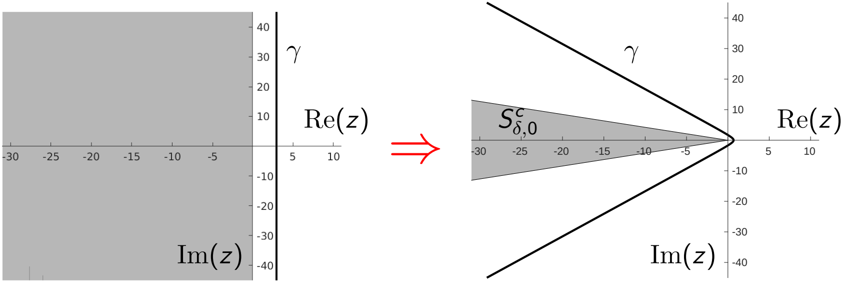

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$$\gamma(s) = \sigma + \mu(1 + \sin(is - \alpha)), \quad \mu > 0, \quad 0 < \alpha < \frac{\pi}{2} - \delta.$$

$$\exp(tA)u_0 \approx \underbrace{\frac{-h}{2\pi i} \sum_{j=-N}^{N} e^{z_j t} R(z_j, A)\gamma'(jh)}_{\text{truncated Trapezoidal rule}}, \quad z_j = \gamma(jh).$$

Case 3: Analytic semigroups

Compute $\exp(tA)$ for $t \in [t_0, t_1]$ where $0 < t_0 \le t_1$, $\Lambda = t_1/t_0$.
Using [Weideman & Trefethen 2007], three error terms:

$$\underbrace{\mathcal{O}\left(e^{\sigma t_1 - 2\pi\left(\frac{\pi}{2}-\alpha-\delta\right)/h}\right) + \mathcal{O}\left(e^{\sigma t_1 + \mu t_1 - 2\pi\frac{\alpha}{h}}\right)}_{\text{discretisation error of the integral}} + \underbrace{\mathcal{O}\left(e^{\sigma t_1 + \mu t_0 (1 - \sin(\alpha)\cosh(hN))}\right)}_{\text{truncation error of sum}}.$$

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Problem: numerical instability as $N \to \infty$

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Problem: numerical instability as $N \to \infty$

Idea: enforce $\gamma(0)t_1 - \sigma t_1 = \mu t_1(1-\sin(\alpha)) \leq \beta$ for stability as $N \to \infty$.

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

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

$$\alpha = (h\mu t_1 + \pi^2 - 2\pi\delta)/(4\pi).$$

Case 3: Analytic semigroups

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

Suppose we use the above quadrature rule and compute each $R(z_j, A)u_0$ to an accuracy η. Let $u_N(t)$ denote the output for $N \in \mathbb{N}$. Then there exists a constant C s.t. for any $t_0 \leq t \leq t_1$,

$$\underbrace{e^{-\sigma t}\left\|\exp(tA)u_0 - u_N(t)\right\|}_{\textit{error with intrinsic stability factor}} \leq \left(2\mu e^{\frac{\beta}{1-\sin(\alpha)}}\pi^{-1}\int_0^\infty e^{x-\mu t\sin(\alpha)\cosh(x)}dx\right)\eta$$

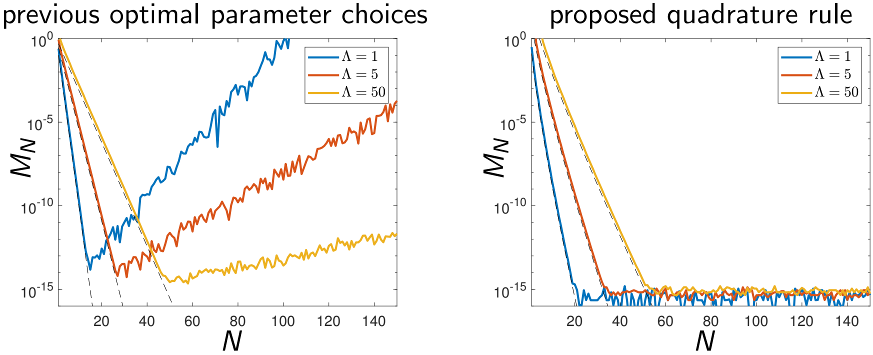
$$+ Ce^{\frac{\beta}{1-\sin(\alpha)}} \cdot \exp\left(-\frac{N\pi(\pi-2\delta)/2}{\log(\Lambda\frac{\sin(\pi/4-\delta/2)^{-1}-1}{\beta}N\pi(\pi-2\delta))}\right)$$

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

Numerical example showing stability

$$e^{-\lambda t} = \frac{1}{2\pi i}\int_\gamma \frac{e^{zt}}{z-\lambda}\,dz, \quad \lambda \geq 0.$$

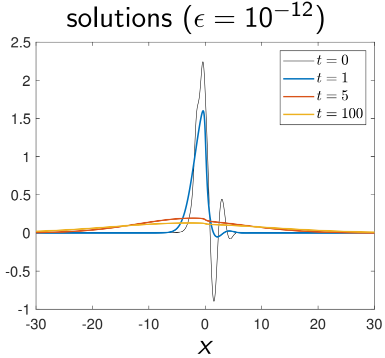
$$M_N = \text{ max error for } t \in [t_0, t_1].$$

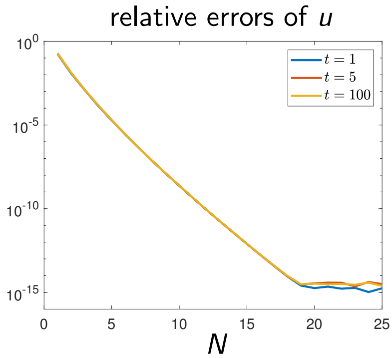


Numerical example on $L^2(\mathbb{R})$ demonstrating convergence

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

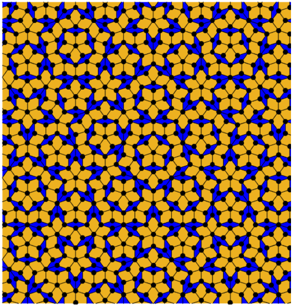
Basis: $\phi_n(x) = \pi^{-1/2}(1+ix)^n(1-ix)^{-(n+1)}, \quad n \in \mathbb{Z}.$





Application: Bulk Localised States

Quasicrystals: aperiodic structures with long-range order.

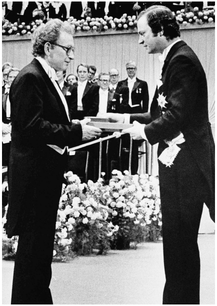


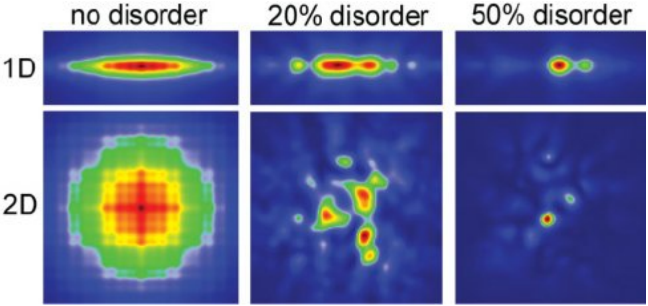
Left: D. Shechtman, **Nobel Prize in Chem. 2011** for discovering quasicrystals.
Right: Penrose tile, canonical model used in physics.

Vertex model: site at each vertex and bonds along edges of tiles.

Application: Bulk Localised States

Periodic systems have extended states (not localised), but add disorder...





Left: P. Anderson, **Nobel Prize in Phys. 1977** for discovering Anderson localisation. Right: Examples in 1D and 2D photonic lattices.

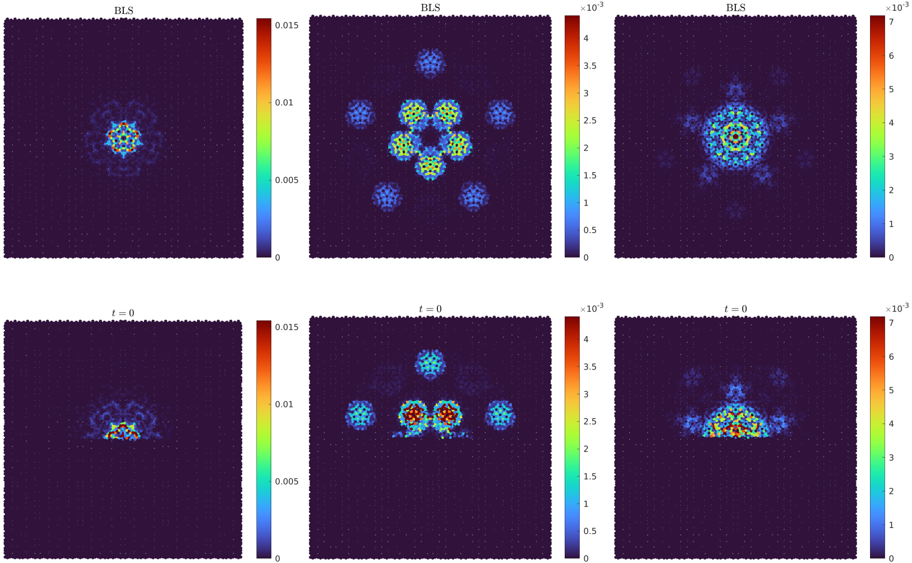
What happens in aperiodic systems? Do we need disorder?

Application: Bulk Localised States

- **Bulk Localised States (BLSs):** New states for magnetic quasicrystals
  - localised
  - "in-gap" (confirmed via comp. of inf-dim (topological) Chern numbers)
  - support transport
- **Cause (also confirmed with toy models):** Interplay of magnetic field with incommensurate areas of building blocks of quasicrystal.
- Not due to an internal edge, impurity or defect in the system.

$\rightsquigarrow$ NEW EXCITING PHYSICS!

Transport: **Error control** allows us to be **certain** of this phenomenon.



Extension: high-order Cauchy problems

$$u^{(N)} + A_{N-1}u^{(N-1)} + \cdots + A_0 u = 0 \text{ for } t \geq 0,$$
$$u^{(j)}(0) = u_j \text{ for } j = 0, ..., N-1.$$

$$\mathcal{A} = \begin{pmatrix} 0 & I & & \\ & 0 & I & \\ & & \ddots & \ddots \\ -A_0 & -A_1 & \cdots & -A_N \end{pmatrix}, \quad \mathcal{U} = \begin{pmatrix} u \\ u^{(1)} \\ \vdots \\ u^{(N-1)} \end{pmatrix}.$$

$$\Downarrow$$

$$\frac{d\mathcal{U}}{dt} = \mathcal{A}\mathcal{U} \text{ for } t \geq 0.$$

Extension: time-fractional PDEs via Laplace transform

$$\sum_{j=1}^{M} {}^{\mathcal{I}_j}\mathcal{D}_t^{\nu_j} A_j q = f(t) \text{ for } t \geq 0,$$

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

$$\underbrace{\left[\sum_{j=1}^{M} z^{\nu_j} A_j\right]}_{T(z)} \hat{q}(z) = \underbrace{\hat{f}(z) + \sum_{\mathcal{I}_j = \mathrm{C} \text{ or } \nu_j = n_j} A_j \sum_{k=1}^{n_j} z^{\nu_j - k} q^{(k-1)}(0)}_{K(z)}.$$

$$q(t) = \frac{1}{2\pi i} \int_{\omega - i\infty}^{\omega + i\infty} e^{zt} \underbrace{\left[T(z)^{-1} K(z)\right]}_{\hat{q}(z) \in \mathcal{H}} dz,$$

Extension: time-fractional PDEs via Laplace transform

Challenges:

- Analysis of (generalised) spectrum of $T(z)$. MUCH easier to figure out for infinite-dimensional operator as opposed to truncation.
- No natural generalisation of Hille–Yosida.
- For high accuracy, need generalised spectrum to lie in LHP. (Think of this as problem not being too stiff.)

Advantages of contour approach:

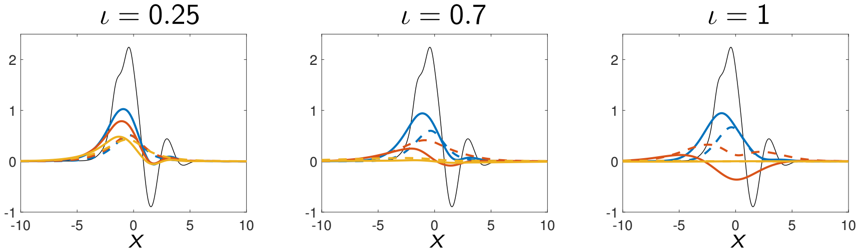
- Avoid the large memory consumption/computation time of time stepping methods applied to time-fractional PDEs.
- High accuracy over large time intervals.
- Resolvents for quadrature rule computed in parallel and reused for different times.
- For suitable generalised spectra, quadrature converges rapidly (and stably) as before.

Example: complex perturbed fractional diffusion equation

$$\mathrm{Sp}(A) \subset \overline{\mathcal{N}(A)} \cup \overline{\mathcal{N}(A^*)}, \quad \mathcal{N}(A) := \{\langle Ax, x\rangle : x \in \mathcal{D}(A), \|x\| = 1\}.$$

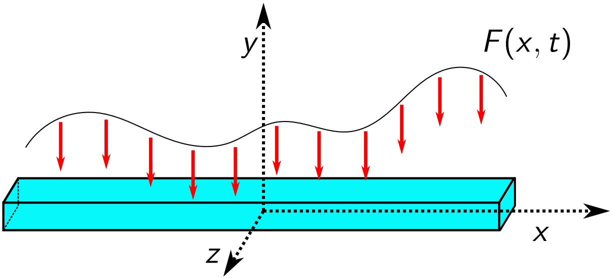
$$\|R(z, A)\| \leq [\mathrm{dist}(z, \overline{\mathcal{N}(A)})]^{-1} \;\; \forall z \notin \overline{\mathcal{N}(A)} \cup \overline{\mathcal{N}(A^*)}.$$

$$D_t^{\iota} u = u_{xx} + iu/(1 + x^2), \quad 0 < \iota \leq 1.$$



Solutions ($\epsilon = 10^{-12}$) for various ι at $t = 1$ (blue), $t = 5$ (red) and $t = 50$ (yellow). The real parts are shown as solid lines, and the imaginary parts as dashed lines (u_0 shown in black).

Fractional beam equations



Viscoelastic constituent equation (stress-strain relation):

$$\underbrace{\sigma(x,z,t)}_{\text{stress}} = E_0(x)\,\underbrace{\epsilon(x,z,t)}_{\text{axial strain}} + E_1(x)\,{}^{\mathcal{I}}\mathcal{D}_t^{\nu}\,\epsilon(x,z,t).$$

Leads to (y = transverse displacement)

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

Quasi-linearisation of $T(z)$

$\mathcal{H}^2_{\mathrm{BC1}}$ and $\mathcal{H}^2_{\mathrm{BC2}}$ suitable Sobolev spaces capturing BCs.
Consider the product space $\mathcal{H}^2_{\mathrm{BC1}} \times L^2_{\tilde{\rho}}(-1,1)$ equipped with

$$\langle (u_0,u_1),(v_0,v_1)\rangle = \int_{-1}^{1} a(x)u_0''(x)\overline{v_0''(x)}dx + \int_{-1}^{1} \tilde{\rho}(x)u_1(x)\overline{v_1(x)}dx.$$

For $z \in \mathbb{C}\backslash\mathbb{R}_{\leq 0}$, consider the following operator

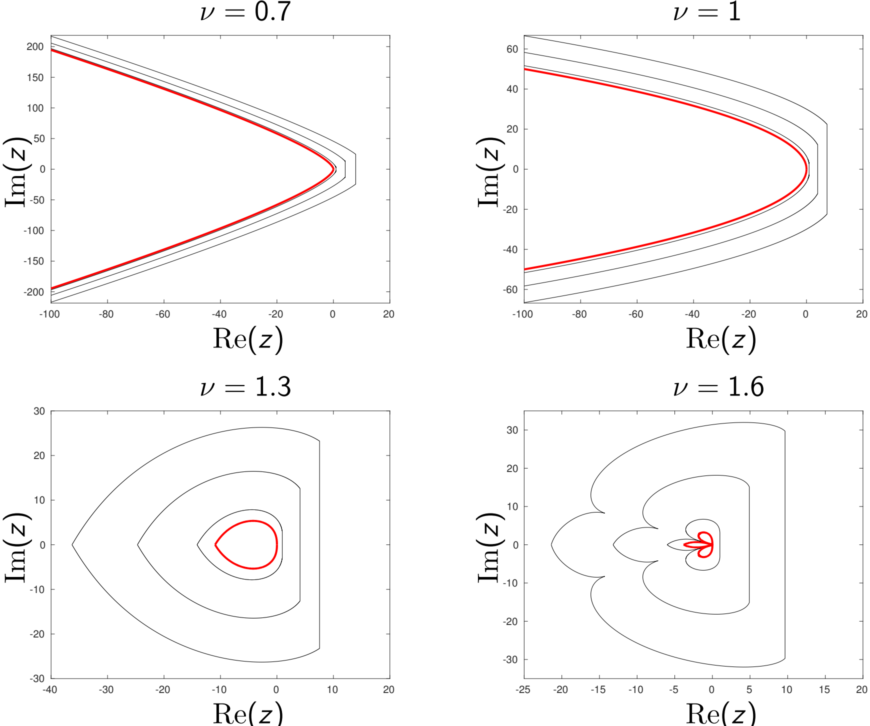
$$[\mathcal{A}(z)]\left(u_0,u_1\right) = z\left(u_0,u_1\right) + \left(-u_1, \tfrac{1}{\tilde{\rho}}(au_0'' + z^{\nu-1}bu_1'')''\right),$$

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

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

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

$\Rightarrow$ can compute solutions with error control as before



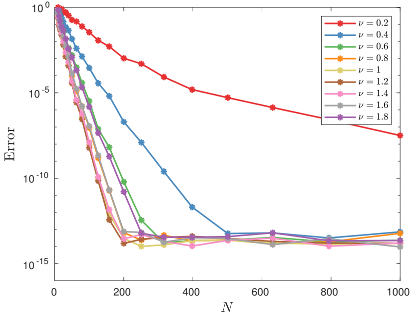
$\nu = 0.7$
$\nu = 1$
$\nu = 1.3$
$\nu = 1.6$
Im(z)
Re(z)

Example

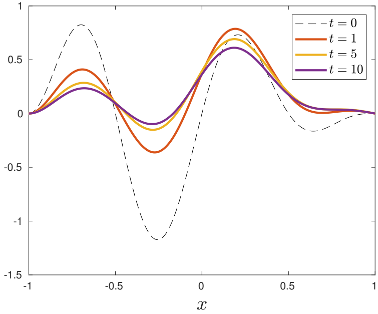
$$a = \cosh(x), \quad b = \sin(\pi x)+2, \quad \tilde{\rho} = \tanh(x)+2, \quad F(x,t) = \cos(20t)\sin(\pi x),$$

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

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



$\nu = 0.4$



Recall **Foundations** Questions

Q.1: *Can we compute semigroups with error control? I.e., does there exist an algorithm that given a generator A of a strongly continuous semigroup on $\mathcal{H}$, time $t > 0$, arbitrary $u_0 \in \mathcal{H}$ and error tolerance $\epsilon > 0$, computes an approximation of $\exp(tA)u_0$ to accuracy ϵ in $\mathcal{H}$?*

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YES! ✓

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

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YES! ✓

Moreover, results and techniques carry over to a wide class of time-fractional PDEs.

Wider Framework

How: Deal with operators directly, instead of previous ‘truncate-then-solve’

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

Framework: Classify problems in a computational hierarchy measuring their intrinsic difficulty and the optimality of algorithms.

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

Other recent examples:

- Computing spectra.
- Computing spectral measures.
- Optimisation and neural networks.

Conclusion

Key points:

- Semigroups can be computed with error control via a universal algorithm.
- Extends to PDEs (e.g. unbounded domains).
- New stable quadrature rule for analytic semigroups.
- Results carry over to time-fractional PDEs via Laplace transform (but need to bound generalised spectrum).
- Methods are part of a wider framework that deals with operators directly in an infinite-dimensional manner.

Future work:

- Nonlinear cases (e.g. splitting).
- Non-autonomous cases.
- Efficient methods with error control for Schrödinger semigroups.
- Whole host of time-fractional PDEs can now be tackled.

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

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