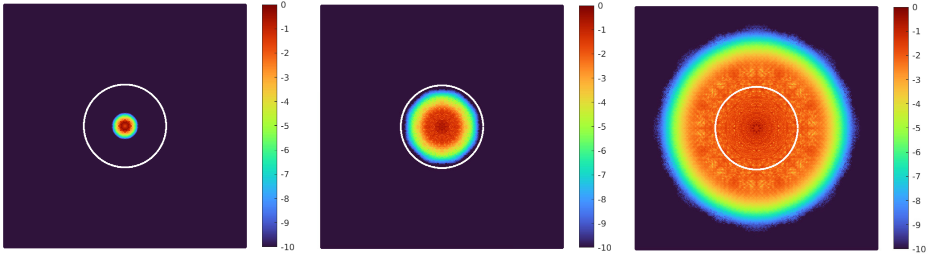
# Computing semigroups with error control

**Matthew J. Colbrook** **University of Cambridge**

**Papers:**
M.J. Colbrook, "Computing semigroups with error control"
M.J. Colbrook and L.J. Ayton, "A contour method for time-fractional PDEs"
(extension of current talk to time-fractional PDEs)



# The infinite-dimensional problem

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

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

$\boxed{\textbf{GOAL: } \text{Rigorously compute the solution at time } t.}$

# 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**"

**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 its 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

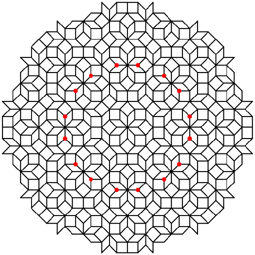
**Q.1:** *Can we compute semigroups with error control? I.e., does there exist an algorithm that given a generator $A$ of a strongly continuous semigroup on $\mathcal{H}$, time $t > 0$, arbitrary $u_0 \in \mathcal{H}$ and error tolerance $\epsilon > 0$, computes an approximation of $\exp(tA)u_0$ to accuracy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

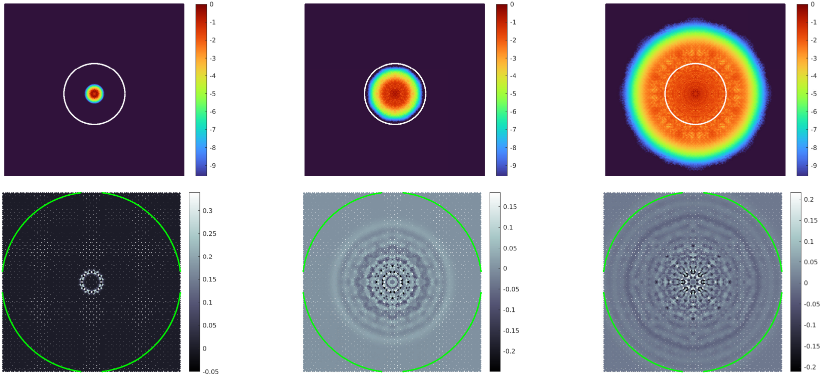
$$[\Delta_{\mathrm{AB}}\psi]_i = \sum_{i\sim j} (\psi_j - \psi_i)\,, \quad \{\psi_j\}_{j\in\mathbb{N}} \in l^2(\mathbb{N}).$$

Schrödinger equation and wave equation:

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

# Example

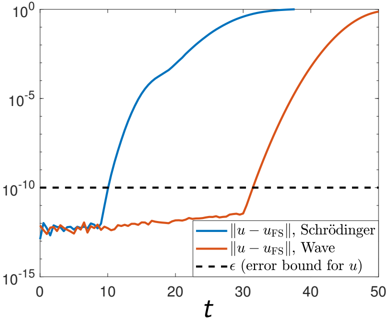
Solutions computed with **guaranteed accuracy** $\epsilon = 10^{-10}$.




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

$u_{\mathrm{FS}}$: solution by direct diagonalisation of $10001 \times 10001$ 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 $A_{j,k} = \langle Ae_k, e_j \rangle$.

$\Omega_{C_0}$: $(A, u_0, t)$ 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 $M, \omega$ 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 $\Gamma$ 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: PDEs on $L^2(\mathbb{R}^d)$

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

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

$\Omega_{\mathrm{PDE}}$ 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 $\mathbb{R}^d$, $|a_k(x)| \leq C_k(1 + |x|^{2B_k})$.

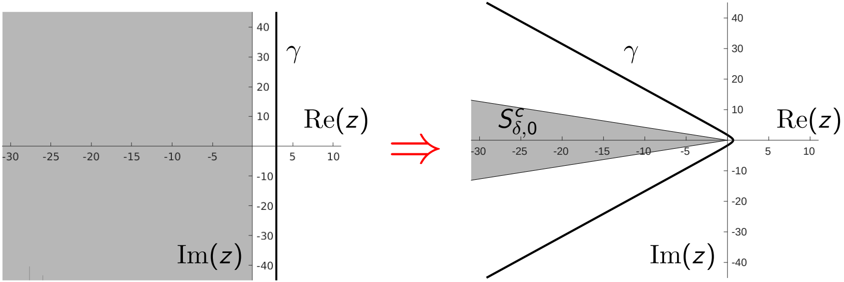
(3) Locally bounded total variation: $\forall r > 0$, $u_0|_{[-r,r]^d}, a_k|_{[-r,r]^d} \in \mathcal{A}_r$.

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

*There exists a universal algorithm $\Gamma$ using pointwise evaluations of coefficients and $u_0$, s.t.*

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

# Case 3: Analytic semigroups




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

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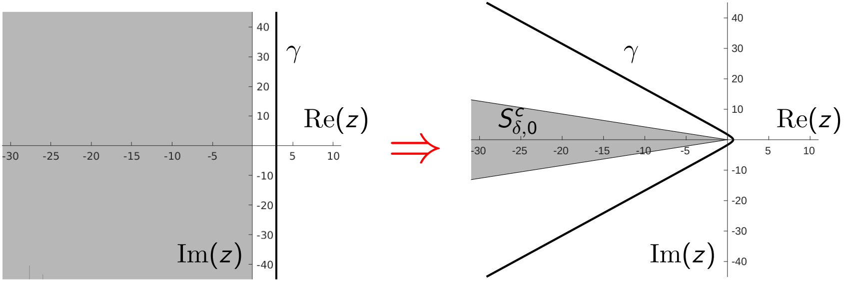


$$S_{\delta,\sigma} := \{z \in \mathbb{C} : \arg(z-\sigma) < \pi - \delta\}.$$

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

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

# Case 3: Analytic semigroups

Compute $\exp(tA)$ for $t \in [t_0, t_1]$ where $0 < t_0 \leq t_1$, $\Lambda = t_1/t_0$.
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 $N \to \infty$.

Compute each $R(z_j, A)u_0$ to an accuracy $\eta$, optimal parameters now give

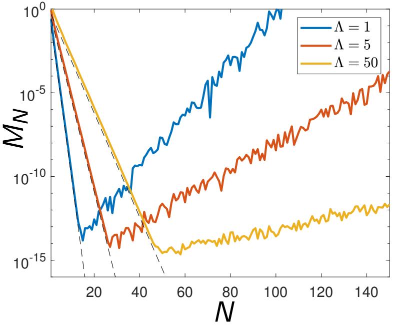
$$\underbrace{e^{-\sigma t}\left\|\exp(tA)u_0 - u_N(t)\right\|}_{\text{error with intrinsic stability factor}} = \mathcal{O}(\eta) + \mathcal{O}(\exp(-cN/\log(N))).$$

# Numerical example showing stability

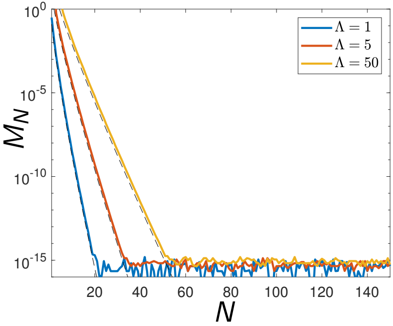
$$e^{-\lambda t} = \frac{1}{2\pi i}\int_\gamma \frac{e^{zt}}{z-\lambda}dz, \quad \lambda \geq 0.$$

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

previous optimal parameter choices




proposed quadrature rule

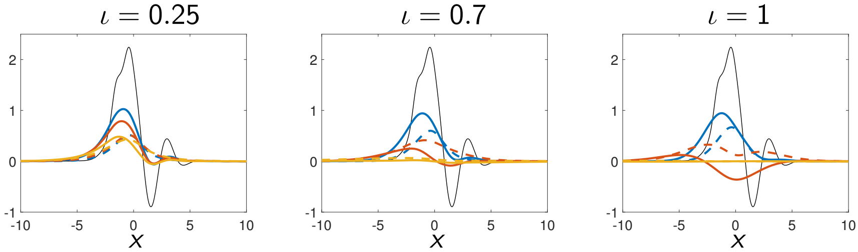


# Example: complex perturbed fractional diffusion equation

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

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

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




Solutions ($\epsilon = 10^{-12}$) for various $\iota$ 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).

# 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 transforms.

**Future work:**

- Nonlinear cases (e.g. splitting).
- Non-autonomous cases.
- Efficient methods with error control for Schrödinger semigroups.

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

# References


- Main paper:
  M.J. Colbrook. "Computing semigroups with error control." *preprint*.
- Extension to time-fractional:
  M.J. Colbrook, L.J. Ayton. "A contour method for time-fractional PDEs." *preprint*.
- Application in physics:
  D. Johnstone, M.J. Colbrook, A.E. Nielsen, P. Ohberg, C.W. Duncan. "Bulk Localised Transport States in Infinite and Finite Quasicrystals via Magnetic Aperiodicity." *preprint*.
- Adaptive method of computing resolvent with error control:
  M.J. Colbrook. "Computing spectral measures and spectral types." *Communications in Mathematical Physics* (2021).
- S. Becker, A. Hansen. "Computing solutions of Schrödinger equations on unbounded domains." *preprint* (2020).
- J.A.C. Weideman, L.N. Trefethen. "Parabolic and hyperbolic contours for computing the Bromwich integral." *Math. Comp.* (2007).