

Structure-Preserving Numerical Methods for the Lindblad Master Equation

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In collaboration with

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The Lindblad Master Equation

$\mathcal{H}$: separable complex Hilbert space,

$\rho \in \mathcal{T}_1(\mathcal{H})$: density operator, $\rho \geq 0$, $\text{Tr}(\rho) = 1$,

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Under reasonable assumptions, the Cauchy problem (L) is well-posed (uniqueness of the weak solution) and the semigroup $(e^{t\mathcal{L}})_{t \geq 0}$ is well-defined and a **quantum channel** (completely positive, trace-preserving map).

Single mode: $\mathcal{H} = \ell^2(\mathbb{N})$

Fock basis $\{|n\rangle\}_{n \geq 0}$, orthonormal.

Ladder operators

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

with $a|0\rangle = 0$ and $[a, a^\dagger] = \text{Id}$.

Number operator

$$\hat{n} = \frac{1}{2}(-\Delta_q + q^2 - 1) = a^\dagger a, \quad \hat{n}|n\rangle = n|n\rangle$$

Position / momentum

$$\mathbf{q} = \frac{a+a^\dagger}{\sqrt{2}}, \quad \mathbf{p} = \frac{a-a^\dagger}{i\sqrt{2}} = -i\partial_q$$

Quantum channels (CPTP maps)

A map $\Phi: \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$ is a *quantum channel* if it is:

- **Completely positive (CP):**
 $(\text{Id} \otimes \Phi)(\rho) \geq 0$ for all $\rho \geq 0$;
- **Trace-preserving (TP):**
 $\text{Tr}(\Phi(\rho)) = \text{Tr}(\rho)$.

Kraus decomposition (finite dim.): Φ is CPTP iff

$$\Phi(\rho) = \sum_k K_k \rho K_k^\dagger, \quad \sum_k K_k^\dagger K_k = \text{Id}.$$

Contraction: $\|\Phi(\rho - \sigma)\|_1 \leq \|\rho - \sigma\|_1$.

$$L_1 = \sqrt{\kappa_2} (a^2 - \alpha^2)$$

$$L_2 = \sqrt{\kappa_1 (1 + n_{\text{th}})} a$$

$$L_3 = \sqrt{\kappa_1 n_{\text{th}}} a^\dagger$$

$$\kappa_2 = 1$$

two-photon rate

$$\kappa_1 = 10^{-2}$$

single-photon loss

$$n_{\text{th}} = 0.1$$

thermal photons

$$\alpha^2 = 4$$

target amplitude

$$\rho_0 = |0\rangle\langle 0|$$

vacuum initial state

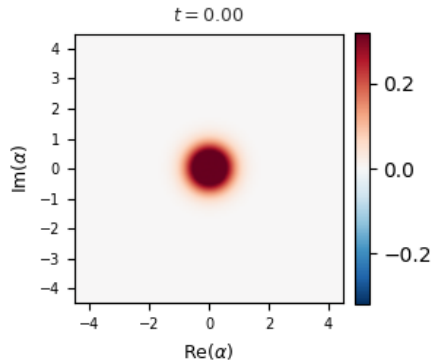
Motivating Example — Simulation

```
import dynamiqs as dq
jax.config.update("jax_enable_x64", True)
N = 30 # Fock truncation

a = dq.destroy(N)
I = dq.eye(N)

L1 = sqrt(kappa_2) * (a @ a - alpha2 * I)
L2 = sqrt(kappa_1 * (1 + n_th)) * a
L3 = sqrt(kappa_1 * n_th) * dq.dag(a)

result = dq.mesolve(
    0, [L1, L2, L3], dq.fock_dm(N, 0), jnp.
        linspace(0, 2.0, 200),
    method=dq.method.Tsit5(atol=1e-6, rtol=1e-6))
```



Reference Lindblad equation

$$\frac{d}{dt}\rho = \mathcal{L}(\rho), \quad \rho(0) = \rho_0$$

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↓ Space discretisation (P_N , Fock truncation)

Space-truncated ODE (Galerkin / Fock truncation)

$$\frac{d}{dt}\rho_N = \mathcal{L}_N(\rho_N), \quad \rho_N(0) = P_N\rho_0P_N$$

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↓ Time discretisation (step size Δt or atol and rtol for adaptive methods)

Time-discrete scheme

$$\rho_N^{n+1} = \Phi_{\Delta t}(\rho_N^n)$$

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Time-discrete scheme

$$\rho_N^{n+1} = \Phi_{\Delta t}(\rho_N^n)$$

↓ Finite-precision arithmetic (e.g. 32-bit or 64-bit floating-point)

Floating-point computation

$$\tilde{\rho}_N^{n+1} = \mathfrak{fl}(\Phi_{\Delta t}(\tilde{\rho}_N^n))$$

Numerical Complexity

Cost of the basic operations, Hilbert space dimension N

Lindbladian evaluation $\mathcal{L}_N(\rho)$

$$\mathcal{L}_N(\rho) = -i[H_N, \rho] + \sum_{k=1}^K \mathcal{D}[L_k^{(N)}](\rho)$$

$\mathcal{L}_N$ acts on $N \times N$ matrices. With $K = O(1)$ dissipators, each term costs $O(N^3)$:

$$\text{cost} = O(N^3)$$

Inversion of $\mathcal{L}_N$

$\mathcal{L}_N$ is a linear map on $\mathbb{C}^{N \times N}$, i.e. an $N^2 \times N^2$ matrix. Dense inversion costs:

$$\text{cost} = O(N^6)$$

(e.g. for steady-state or implicit schemes) — very expensive!

Operator-level routines (SVD, Cholesky, inversion, squareroot, ...)

Operations on a single $N \times N$ matrix:

$$\text{cost} = O(N^3)$$

Comparable to one Lindbladian evaluation — cheap relative to inversion.

Introduction

I · Space Discretisation

- a) Galerkin discretisation
- b) A priori estimates
- c) A posteriori estimates

II · Time Discretisation

- a) A CFL condition and stiffness
- b) Structure-preserving schemes
- c) Time and space error separation

III · Fast Steady State Computation



Space Discretisation

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Galerkin Discretisation

I · Space Discretisation · a) Galerkin discretisation

Original problem

$$\frac{d}{dt}\rho(t) = \mathcal{L}(\rho(t)), \quad \rho(0) = \rho_0$$

Fock-space truncation

$$P_N = \sum_{n=0}^N |n\rangle\langle n| \quad \text{projector onto } \mathcal{H}_N = \text{span}\{|0\rangle, \dots, |N\rangle\} \subset \mathcal{H}$$

$$H_N = P_N H P_N, \quad L_k^{(N)} = P_N L_k P_N$$

$$\mathcal{L}_N(\rho) = -i[H_N, \rho] + \sum_k \mathcal{D}[L_k^{(N)}](\rho)$$

$$\frac{d}{dt}\rho_N(t) = \mathcal{L}_N(\rho_N(t)), \quad \rho_N(0) = P_N \rho_0 P_N$$

Properties of the truncation

- Linear approximation: $\mathcal{H}_N$ is a Hilbert subspace of $\mathcal{H}$
- Structure-preserving: $\mathcal{L}_N$ is a Lindbladian acting on $\mathcal{T}_1(\mathcal{H}_N) \subset \mathcal{T}_1(\mathcal{H})$

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- $\rho_N(t) = e^{t\mathcal{L}_N}(P_N\rho_0P_N) \neq P_Ne^{t\mathcal{L}}(\rho_0)P_N$
- $L_N^\dagger L_N \neq P_N L^\dagger L P_N$ in general, thus $\mathcal{L}_N(P_N \cdot P_N) \neq P_N \mathcal{L}(P_N \cdot P_N) P_N$

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Two questions

- **A priori:** does $\rho_N(t) \rightarrow \rho(t)$, and at what rate?
- **A posteriori:** given $(\rho_N(s))_{s \leq t}$, can we bound $\|\rho(t) - \rho_N(t)\|_1$ to get a certificate?

A Priori Estimates

I · Space Discretisation · b) A priori estimates

Convergence $\rho_N(t) \rightarrow \rho(t)$ is **not guaranteed without further assumptions.**

Not every symmetric $P(a, a^\dagger)$ is essentially self-adjoint on $\mathcal{H}_f = \text{span} \{|k\rangle\}_{k \geq 0}$.

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A funny example (S. Ashhab, F. Fischer, D. Lonigro, D. Braak, and D. Burgarth)

$$H = i((a^\dagger)^3 - a^3)$$

For every $t > 0$: $e^{tH_{6N}}|0\rangle$ and $e^{tH_{6N+3}}|0\rangle$ both converge, but to **different limits**.

Consequence: convergence of the Galerkin scheme requires assumptions on H and the $(L_k)_k$.

Quantum Sobolev spaces:

$$\mathcal{H}^k = \mathcal{D}(\hat{n}^{k/2}) = \{\psi \in \mathcal{H} \mid \|\hat{n}^{k/2}\psi\| < \infty\}$$
$$\mathcal{W}^{k,1} = \{\rho \in \mathcal{T}_1(\mathcal{H}) \mid \|(1 + \hat{n})^{k/2}\rho(1 + \hat{n})^{k/2}\|_1 < \infty\}$$

A priori estimates (Fagnola–Chebotarev '90s; Gondolf, Möbus, Rouzé):

$$\frac{d}{dt} \text{Tr}(\rho_t \hat{n}^k) = \text{Tr}(\rho_t \mathcal{L}^*(\hat{n}^k))$$

What remains to be done: bound $\mathcal{L}^*(\hat{n}^k)$ in quadratic form sense.

Growth bound

$$\mathcal{L}^*(\hat{n}^k) \leq w_k (1 + \hat{n})^k$$

$$\Rightarrow \|\rho_t\|_{\mathcal{W}^{k,1}} \leq e^{w_k t} \|\rho_0\|_{\mathcal{W}^{k,1}}$$

Uniform (dissipative) bound

$$\mathcal{L}^*(\hat{n}^k) \leq c_k - \eta_k \hat{n}^k$$

$$\Rightarrow \|\rho_t\|_{\mathcal{W}^{k,1}} \leq \frac{c_k}{\eta_k} + \|\rho_0\|_{\mathcal{W}^{k,1}}$$

A Priori Convergence Theorem

I · Space Discretisation · b) A priori estimates

Theorem (R-Rouchon, 2025)

Assume: H, L_j polynomials of degrees p_H, p_j ; $\mathcal{L}^*(\hat{n}^k) \leq w_k (1 + \hat{n})^k$ for all $k \geq 0$. Set $d := \max(p_H, 2 \max_j p_j)$.

Then for all $k > d$:

$$\|\rho(t) - \rho_N(t)\|_1 \leq \frac{C_k t}{N^{(k-d)/2}} \|\rho\|_{L^\infty(0,t; \mathcal{W}^{k,1})}$$

Tools : Duhamel's formula, interpolation inequalities, and Markov inequality.

A Posteriori Estimates

Assume we have access to the Galerkin solution $\rho_N(t)$, and want to bound the error $\|\rho(t) - \rho_N(t)\|_1$.

Usually, quite subtle because the Galerkin space is not included in the domain of $\mathcal{L}$.

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Here trivial : $\xi_N = \rho - \rho_N$ satisfies $\dot{\xi}_N = \mathcal{L}(\rho) - \mathcal{L}_N(\rho_N) = \mathcal{L}(\xi_N) + (\mathcal{L} - \mathcal{L}_N)(\rho_N)$, so (Duhamel's formula)

$$\xi_N(t) = e^{t\mathcal{L}}\xi_N(0) + \int_0^t e^{(t-s)\mathcal{L}}(\mathcal{L} - \mathcal{L}_N)(\rho_N(s)) ds.$$

Hence,

$$\|\rho(t) - \rho_N(t)\|_1 \leq \|\rho_0 - P_N\rho_0P_N\|_1 + \int_0^t \|(\mathcal{L} - \mathcal{L}_N)(\rho_N(s))\|_1 ds.$$

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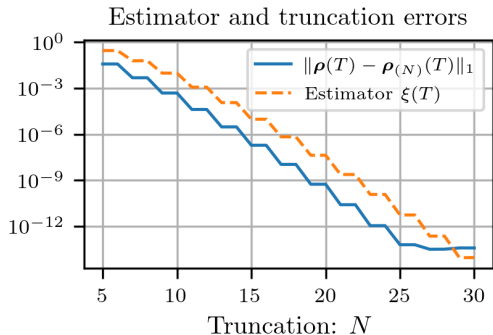
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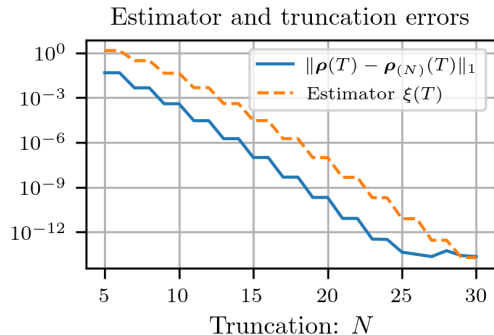
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As $\mathcal{L} - \mathcal{L}_N$ is explicitly computable (as an operator on $\mathcal{H}_{N+d}$), this gives a computable error bound.

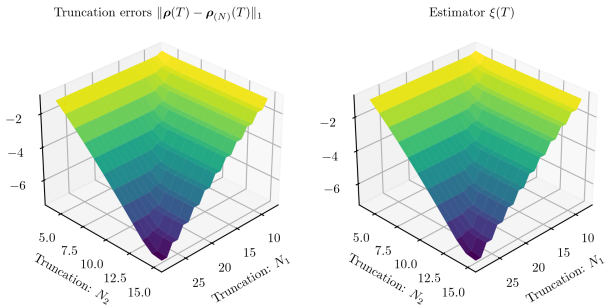


Cat-qubit: $\Gamma = a^2 - \alpha^2 \text{Id}$, $\alpha = 1$, $T = 1$



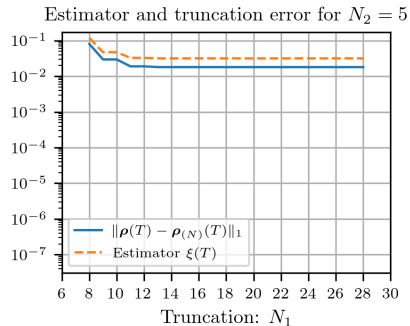
Squeezed cat: $\Gamma = (\cosh r a + \sinh r a^\dagger)^2 - \alpha^2 \text{Id}$,
 $r = 5/4$

Both: $\rho_0 = |0\rangle\langle 0|$, reference solution at $N = 40$. Staircase pattern: parity symmetry means only odd N contribute. Estimator $\xi(T)$ (dashed orange) is computed solely from ρ_N and provides a valid, tight upper bound on $\|\rho(T) - \rho_N(T)\|_1$.



Truncation error $\|\rho(T) - \rho_{(N)}(T)\|_1$ (left) and estimator $\xi(T)$ (right) as a function of (N_1, N_2) . Axes in log scale.

Cat-qubit with lossy buffer cavity: $\mathbf{H} = (a^2 - \alpha^2 \text{Id})\mathbf{b}^\dagger + \text{h.c.}$, $\alpha = 1$, $T = 1$. The estimator correctly identifies which truncation dimension limits accuracy.

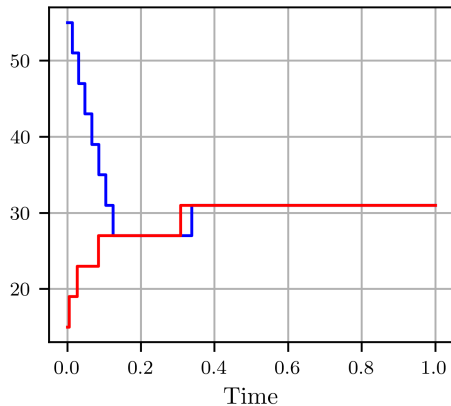


Slice at $N_2 = 5$: error saturates as N_1 grows.

Mode 2 is the bottleneck.

Running estimator $\dot{\xi} = \|(\mathcal{L} - \mathcal{L}_N)\rho_N\|_1$ steers automatic resizing of N — no manual truncation choice.

Density matrices' sizes along time

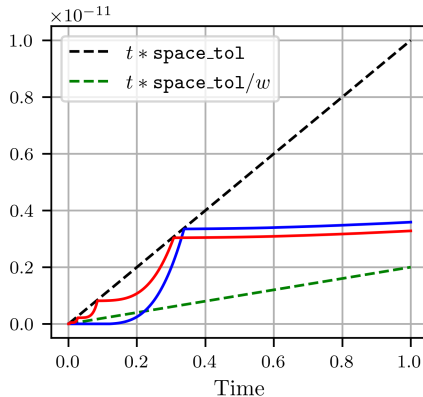


Truncation N over time

Cat-qubit, $\alpha = 1$, $\text{space_tol} = 10^{-11}$, $w = 5$. • Start $N = 15$: grows to $N = 31$. • Start $N = 55$: shrinks to $N = 31$.

Implemented in `dynamics_adaptive`.

Estimate on the truncation error along time



Estimator $\xi(t)$ vs. budget $t \cdot \text{space_tol}$



Time Discretisation

Introduction

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II · Time Discretisation

- a) A CFL condition and stiffness
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III · Fast Steady State Computation

Explicit RK (e.g. RK4): classic workhorse.

Adaptive RK (e.g. Tsit5, Dormand–Prince): embeds a pair of order- $p/p+1$ solutions to estimate the local error and tune Δt automatically.

Main drawbacks: simple, robust, super efficient, works in most cases.

A CFL Condition and Stiffness

II · Time Discretisation · a) A CFL condition and stiffness

Example: two-photon loss channel, $\dot{\rho} = \mathcal{D}[a^2](\rho)$, Galerkin truncation to $\mathcal{H}_N = \text{span}\{|0\rangle, \dots, |N\rangle\}$.

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The **first-order explicit Euler** scheme reads

$$\mathcal{E}_1^{\Delta t, N}(\rho) = \rho + \Delta t \left(a_N^2 \rho (a_N^\dagger)^2 - \frac{1}{2} (a_N^\dagger)^2 a_N^2 \rho - \frac{1}{2} \rho (a_N^\dagger)^2 a_N^2 \right).$$

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Focus on the **last diagonal coefficient** :

$$\langle N | \mathcal{E}_1^{\Delta t, N}(\rho) | N \rangle = (1 - \Delta t \cdot N(N-1)) \langle N | \rho | N \rangle.$$

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CFL condition

The scheme is **unstable** if $\Delta t \cdot N(N-1) > 2$, i.e. $\Delta t \lesssim 2/N^2$: increasing spatial resolution forces a quadratically smaller time step.

Structure-Preserving Schemes

II · Time Discretisation · b) Structure-preserving schemes

Explicit Euler ($H = 0$, $G = -\frac{1}{2} \sum_j L_j^\dagger L_j$): $\rho_{n+1} = \rho_n + \Delta t \left(G \rho_n + \rho_n G^\dagger + \sum_j L_j \rho_n L_j^\dagger \right).$

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CP scheme. Set $M_0 = \text{Id} + \Delta t G$, $M_j = \sqrt{\Delta t} L_j$. Adding and removing $(\Delta t)^2 G \rho G^\dagger$ in the Euler step gives $\mathcal{A}_{\Delta t}(\rho) := \sum_{j \geq 0} M_j \rho M_j^\dagger = \rho + \Delta t \mathcal{L}(\rho) + O(\Delta t^2)$, which is **CP** (Kraus form), but **not TP**.

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Lu-Cao: $\bar{\mathcal{A}}_{\Delta t}(\rho) = \mathcal{A}_{\Delta t}(\rho) / \text{Tr}(\mathcal{A}_{\Delta t}(\rho))$ is positive and trace-preserving but **non-linear**.

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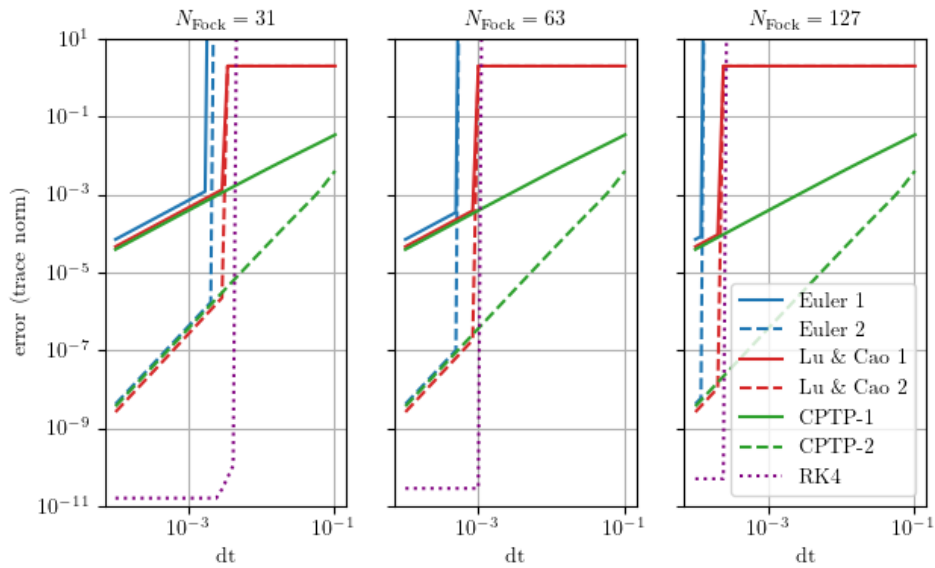
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Linear fix (Rouchon). $\mathcal{A}$ is TP $\iff \mathcal{A}^*(\text{Id}) = \text{Id}$. Compute:

$$\mathcal{A}_{\Delta t}^*(\text{Id}) = \sum_j M_j^\dagger M_j = \text{Id} + \frac{(\Delta t)^2}{4} \left(\sum_j L_j^\dagger L_j \right)^2 =: S_{\Delta t} \neq \text{Id}.$$

Replace $M_j \mapsto \tilde{M}_j = M_j S_{\Delta t}^{-1/2}$: $\sum_j \tilde{M}_j^\dagger \tilde{M}_j = S_{\Delta t}^{-1/2} S_{\Delta t} S_{\Delta t}^{-1/2} = \text{Id}$.

$\mathcal{F}_{\Delta t}(\rho) = \sum_j \tilde{M}_j \rho \tilde{M}_j^\dagger$ is **linear**, **CPTP**, stable for any $\Delta t > 0$, and first-order consistent.



Z-gate on dissipative cat-qubit ($\alpha^2 = 4$, $\kappa_1 = 0.01$, $\kappa_2 = 1$)

Time and Space Error Separation

Two independent sources of error: **spatial** ($N \rightarrow \infty$) and **temporal** ($\Delta t \rightarrow 0$). Can they be controlled separately?

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Inner limit: finite-dim time convergence (fixed N).

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Ongoing work with H. Hutin

Fully discrete quantitative bound:

$$\|\rho(t) - \Phi_{N, \Delta t}^{t/\Delta t}(P_N \rho_0 P_N)\|_1 \leq C(t, \rho_0)(\Delta t^p + N^{-r})?$$

For higher order Rouchon schemes and other renormalizations strategies (Cholesky, sparse approximation, etc.).



Fast Steady State Computation

Introduction

I · Space Discretisation

II · Time Discretisation

III · Fast Steady State Computation

Computing the Steady State

Context: In finite dimension, find $\rho_\infty \geq 0$, $\text{Tr}(\rho_\infty) = 1$ such that $\mathcal{L}(\rho_\infty) = 0$, assuming $\dim(\ker \mathcal{L}) = 1$.

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- **Time integration to $t \rightarrow \infty$:** simulate until convergence.
- **Solve the linear equation $\mathcal{L}(\rho) + \text{Tr}(\rho)\text{Id} = \text{Id}$,** Can be approached in several ways:
 - *Direct, dense:* LU or SVD on the full $N^2 \times N^2$ matrix — $O(N^6)$.
 - *Direct, sparse:* if operators are sparse (e.g. MUMPS).
 - *Iterative:* Krylov methods (GMRES, ...) — relies on a good preconditioner.

Inverting the No-Jump Dynamics

III · Fast Steady State Computation ·

Decompose the Lindbladian

$$\mathcal{L}(\rho) = \underbrace{\mathcal{L}_{\text{NJ}}(\rho)}_{\text{no-jump}} + \underbrace{\mathcal{K}(\rho)}_{\text{jumps}}, \quad \mathcal{L}_{\text{NJ}}(\rho) := G\rho + \rho G^\dagger, \quad \mathcal{K}(\rho) := \sum_j L_j \rho L_j^\dagger, \quad G := -iH - \frac{1}{2} \sum_j L_j^\dagger L_j$$

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Note that G is dissipative: $\text{sp}(G) \subset \{\lambda \in \mathbb{C} : \text{Re}(\lambda) \leq 0\}$.

- If there exists $\lambda \in \text{sp}(G)$ with $\text{Re}(\lambda) = 0$, then there exists ψ such that $H\psi = \lambda\psi$ and $L_j\psi = 0$, i.e. $\mathcal{L}(|\psi\rangle\langle\psi|) = 0$.
- Otherwise, G is Hurwitz and $\mathcal{L}_{\text{NJ}}$ is invertible. In this case, $\mathcal{L}_{\text{NJ}}^{-1}$ can be computed efficiently using the Bartels–Stewart algorithm (cost $O(N^3)$).

Steady State as Fixed Point of a CPTP Map

III · Fast Steady State Computation ·

Derive the fixed-point condition from $\mathcal{L}(\rho_\infty) = 0$

$$\mathcal{L}_{\text{NJ}}(\rho_\infty) + \mathcal{K}(\rho_\infty) = 0 \implies \rho_\infty = -\mathcal{L}_{\text{NJ}}^{-1}\mathcal{K}(\rho_\infty)$$

Natural fixed-point map: $\Psi := -\mathcal{L}_{\text{NJ}}^{-1}\mathcal{K}$.

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But $\Phi = -\mathcal{K}\mathcal{L}_{\text{NJ}}^{-1}$ is CPTP (see next slide).

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Algorithm (Beugnot–Gregory–R–Tilloy, ongoing work)

Key insight: Fixed points of Φ and Ψ are in one-to-one correspondence using $\mathcal{L}_{\text{NJ}}^{-1}$.

Algorithm: apply Arnoldi to Φ to find its fixed point ξ_∞ , then compute $\rho_\infty = -\mathcal{L}_{\text{NJ}}^{-1}(\xi_\infty)$.

G is Hurwitz $\Rightarrow \mathcal{L}_{\text{NJ}}^{-1}$ has an explicit integral formula

Step 1: integral formula for $\mathcal{L}_{\text{NJ}}^{-1}$. When G is Hurwitz, $GX + XG^\dagger = Y$ is solved by

$$\mathcal{L}_{\text{NJ}}^{-1}(Y) = - \int_0^\infty e^{tG} Y e^{tG^\dagger} dt.$$

$\Phi = -\mathcal{K}\mathcal{L}_{\text{NJ}}^{-1}$ is CPTP — Proof

III · Fast Steady State Computation ·

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$$\Phi(\xi) = -\mathcal{K}(\mathcal{L}_{\text{NJ}}^{-1}(\xi)) = \sum_j \int_0^\infty \underbrace{L_j e^{tG}}_{K_{j,t}} \xi \underbrace{(L_j e^{tG})^\dagger}_{K_{j,t}^\dagger} dt.$$

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Step 3: trace preservation. Using $\sum_j L_j^\dagger L_j = -(G + G^\dagger)$,

$$\sum_j \int_0^\infty K_{j,t}^\dagger K_{j,t} dt = - \int_0^\infty \frac{d}{dt} (e^{tG^\dagger} e^{tG}) dt = \left[-e^{tG^\dagger} e^{tG} \right]_0^\infty = \text{Id}.$$

Connection with a CPTP Time Integrator

III · Fast Steady State Computation ·

First-order exponential integrator [Chen–Borzì–Janković–Hartmann–Hervieux, SIAM 2026]

$$\begin{aligned}\rho_{n+1} &= e^{\delta t G} \rho_n e^{\delta t G^\dagger} + \sum_j \int_0^{\delta t} L_j e^{(\delta t-s)G} \rho_n e^{(\delta t-s)G^\dagger} L_j^\dagger ds \\ &= e^{\delta t G} \rho_n e^{\delta t G^\dagger} + \Phi(e^{\delta t G} \rho_n e^{\delta t G^\dagger} - \rho_n)\end{aligned}$$

Connection with a CPTP Time Integrator

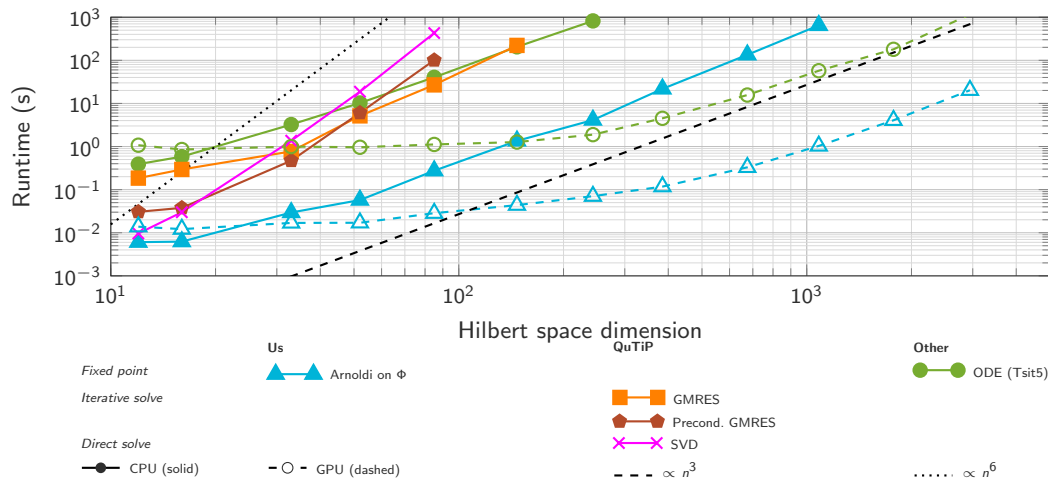
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- Scheme is **CPTP for any** δt : unconditionally stable.
- Fixed points as $\delta t \rightarrow +\infty$: **not** ρ_∞ **directly**, but in relation through $-\mathcal{L}_{\text{NJ}}^{-1}$.

Runtime to find ρ_∞ to tolerance 10^{-8} . CPU (solid, filled) and GPU (dashed, open). Reference slopes: $\propto n^3$ (- -), $\propto n^6$ (····). Ongoing work.



Some open problems and future directions

On-going work:

- Fully discrete error bound: $\|\rho(t) - \Phi_{N,\Delta t}^{t/\Delta t}(P_N \rho_0 P_N)\|_1 \leq C(t, \rho_0)(\Delta t^p + N^{-r})$
- Preconditioner for low lying eigenvalues of $\mathcal{L}$ in finite dimension.
- Implicit schemes based on the Lyapunov equation solver
- Implementation in `dynamiqs` (H. Hutin)

Further directions:

- Convergence of the spectrum of the Galerkin approximation $\mathcal{L}_N$ to that of $\mathcal{L}$
- Error estimate on the steady-state of $\mathcal{L}$ from that of $\mathcal{L}_N$
- New schemes? New methods for steady states?
- Stochastic methods for both deterministic and stochastic Lindblad equations
- Non-linear approximations (e.g. low-rank, tensor networks, shifted Fock, ...) after the Galerkin truncation
- ...

Thank you for your attention!
