Krylov-enhanced parallel integrators for linear problems

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Outline

1. Motivation
2. The Parareal Algorithm
3. Linear Problems
   - Exponential Integration
   - Chebyshev Method
   - Load Balancing
4. Numerical Example

Motivation

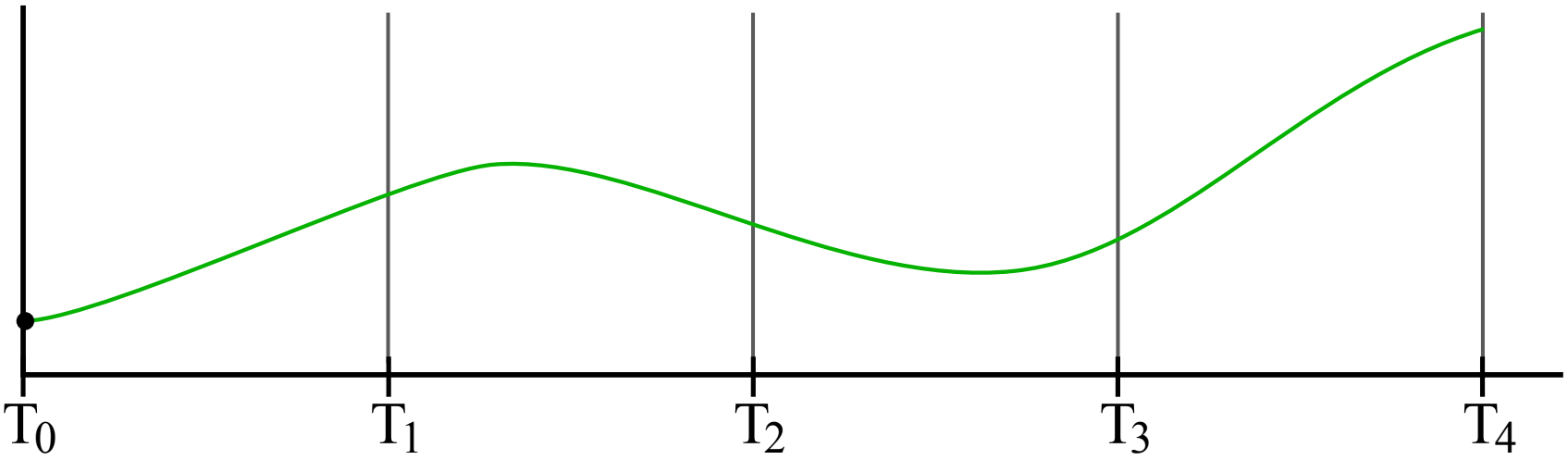
Want to solve the initial value problem

$$u'(t) = f(t, u), \quad t \in [0, T], \quad u(0) = u_0.$$

Usual approach:

Discretize the time interval at $0 = T_0 < T_1 < \cdots < T_N = T$ and compute approximations $U_n \approx u(T_n)$ by some time-stepping scheme

$$U_n = F(t, U_n, U_{n-1}, U_{n-2}, \ldots), \quad n = 1, 2, \ldots, N.$$



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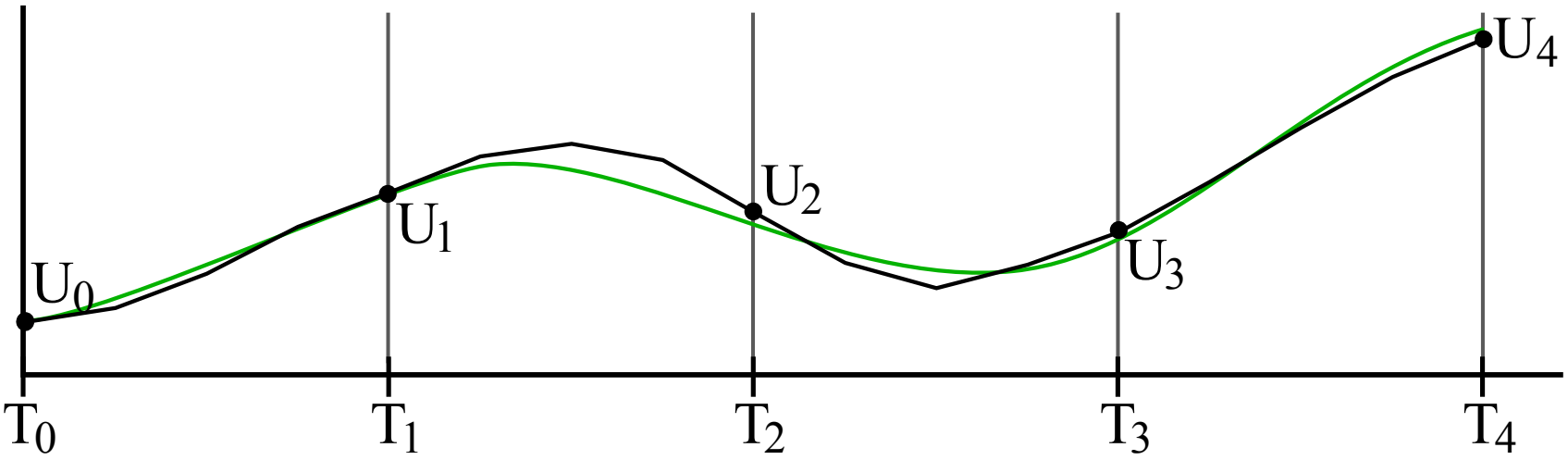

Time-parallel algorithms aim at computing approximations U_n^k without having obtained all previous $U_1^k, \ldots, U_{n-1}^k$ to fine accuracy.

Such algorithms are useful

- as another way toward more parallelism (sometimes as the only way),
- in realtime forecast applications (weather prediction),
- in realtime control problems (steering a rocket).

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The Parareal Algorithm (Parallel Realtime)

Introduced by [Lions, Maday & Turincini 01],
further studied by Bal, Chandesris, Farhat, Gander,
Hairer, Petcu, Minion, Vandewalle, Williams, Wu, ...

Idea: Partition the time domain $\Omega = [0, T]$ into N subdomains

$$\Omega_n = [T_{n-1}, T_n], \quad n = 1, 2, \ldots, N.$$

Also define

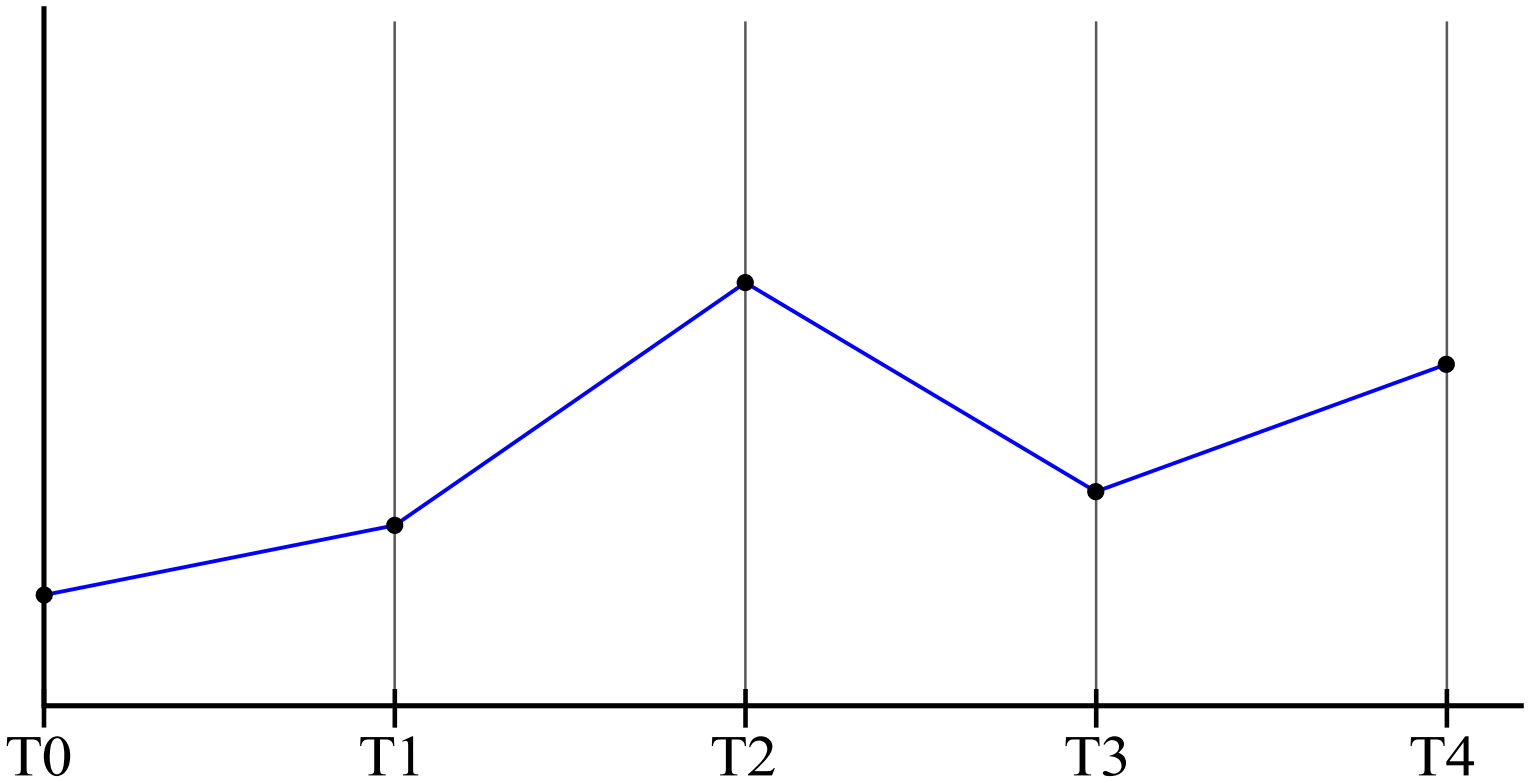
- a coarse propagator $\mathcal{G}(T_n, T_{n-1}, x)$, and
- a fine propagator $\mathcal{F}(T_n, T_{n-1}, x)$,

both of which return approximations U_n of $U(T_n)$ satisfying

$$U'(t) = f(t, U(t)), \quad U(T_{n-1}) = x.$$

In iteration $k = 1$ propagate coarsely

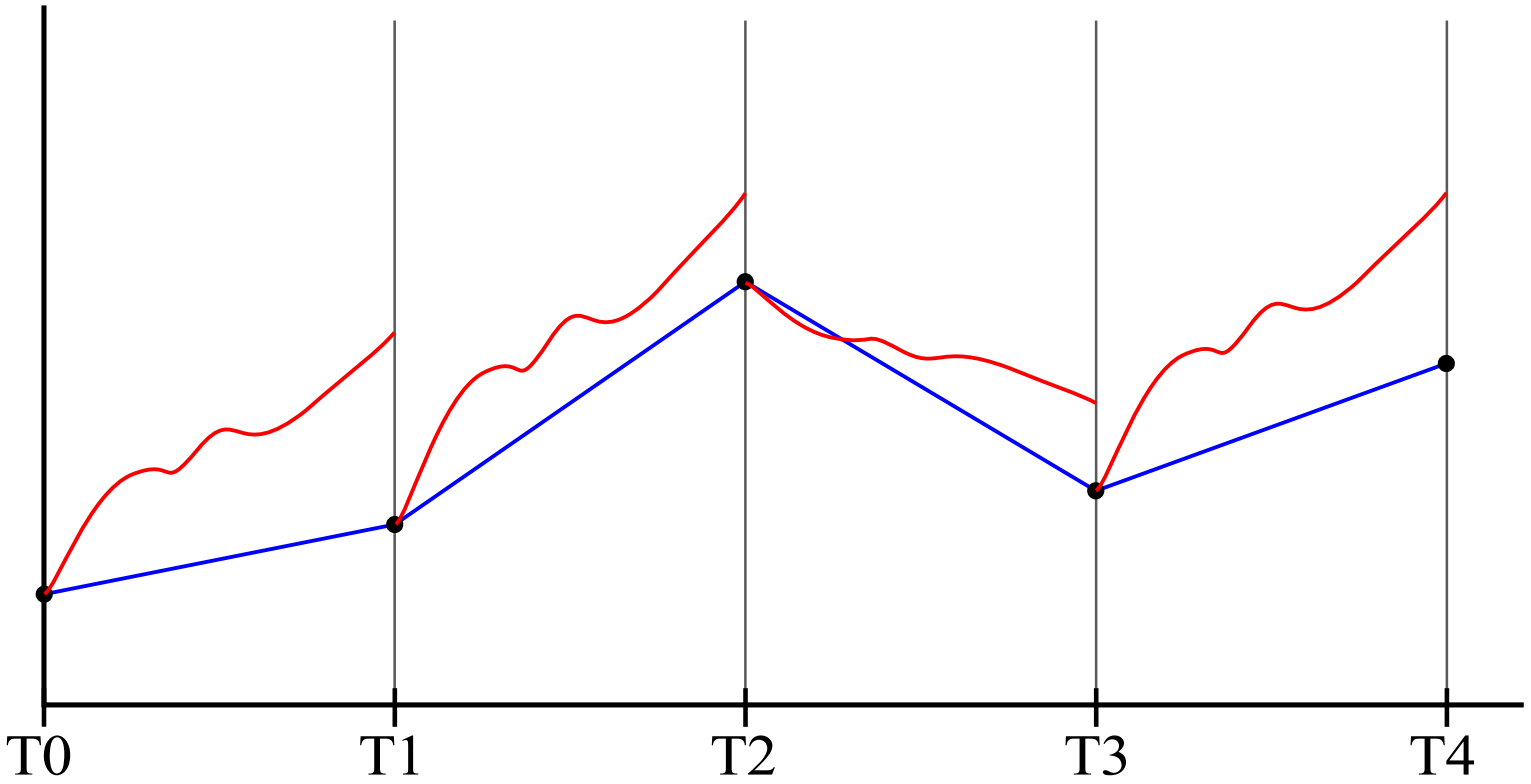
$$U_0^1 = u_0$$
$$U_n^1 = \mathcal{G}(T_n, T_{n-1}, U_{n-1}^1), \quad n = 1, 2, \ldots, N.$$



Now, an initial condition for the fine propagator is available on all subdomains Ω_n, hence

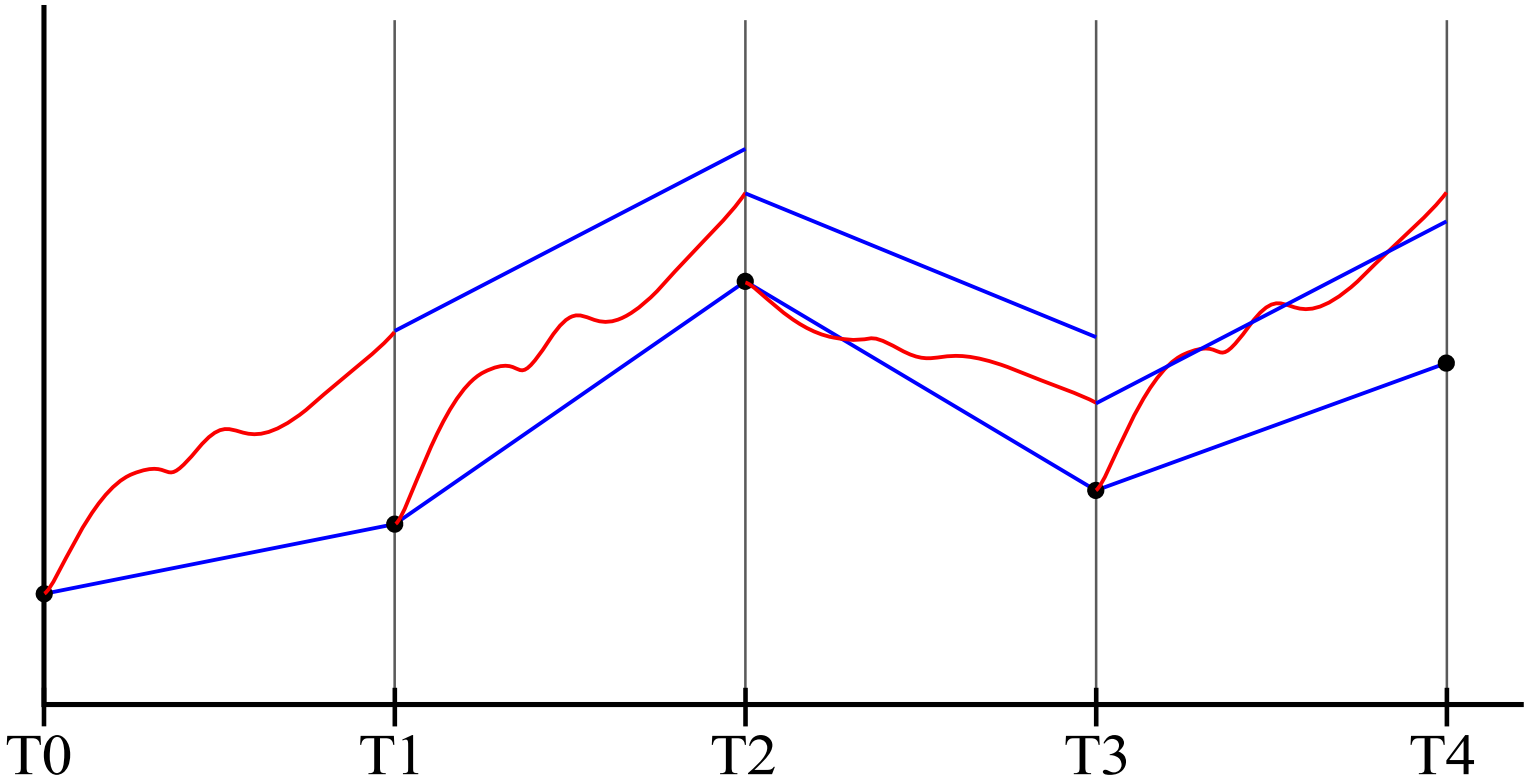
$$\mathcal{F}(T_n, T_{n-1}, U_{n-1}^1), \quad n = 1, 2, \ldots, N,$$

can be computed in parallel.



This yields an initial guess better than U_{n-1}^k, which we propagate coarsely, resulting in a correction ($n = 1, 2, \ldots, N$)

$$U_n^{k+1} = \mathcal{F}(T_n, T_{n-1}, U_{n-1}^k) + \mathcal{G}(T_n, T_{n-1}, U_{n-1}^{k+1}) - \mathcal{G}(T_n, T_{n-1}, U_{n-1}^k).$$



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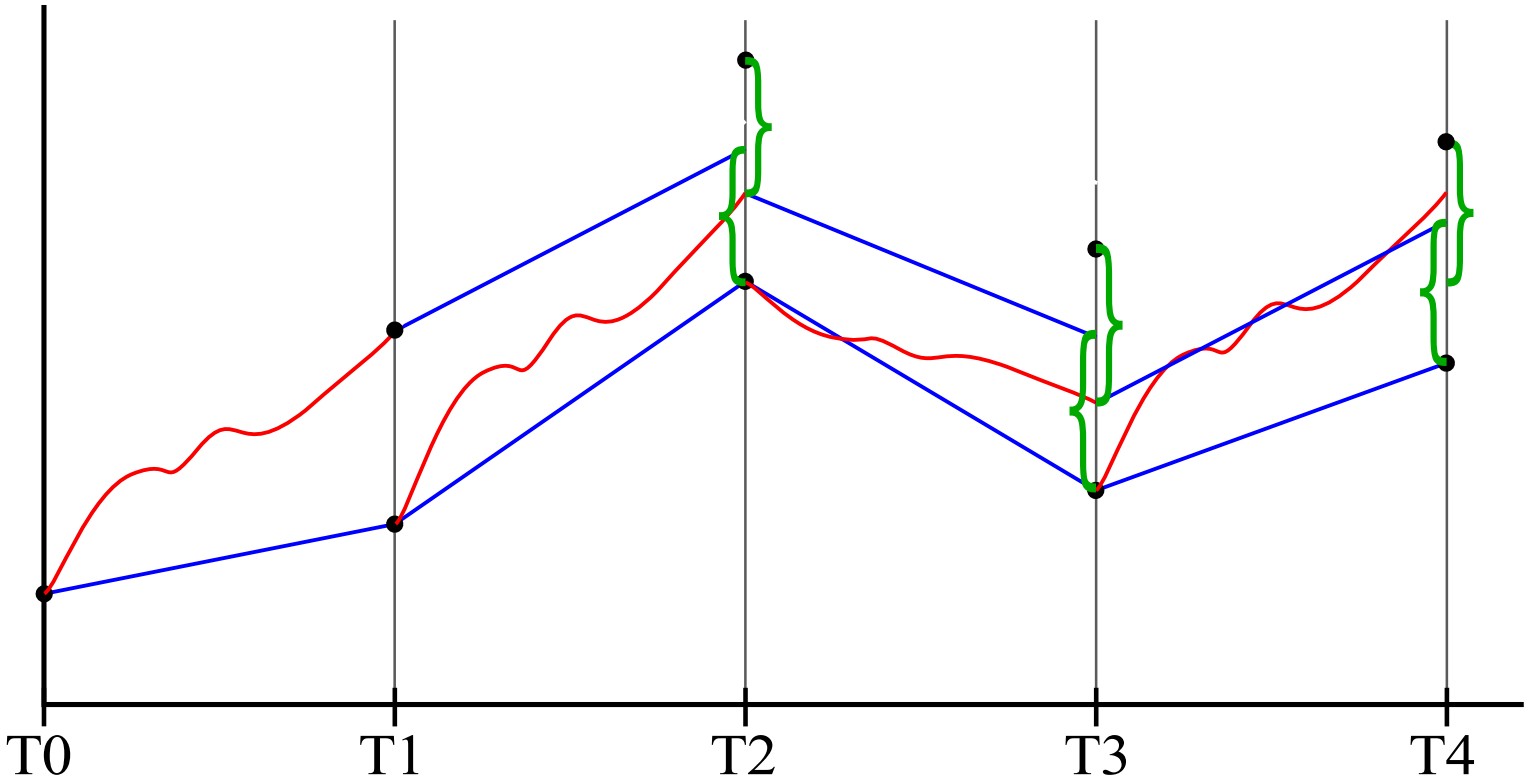

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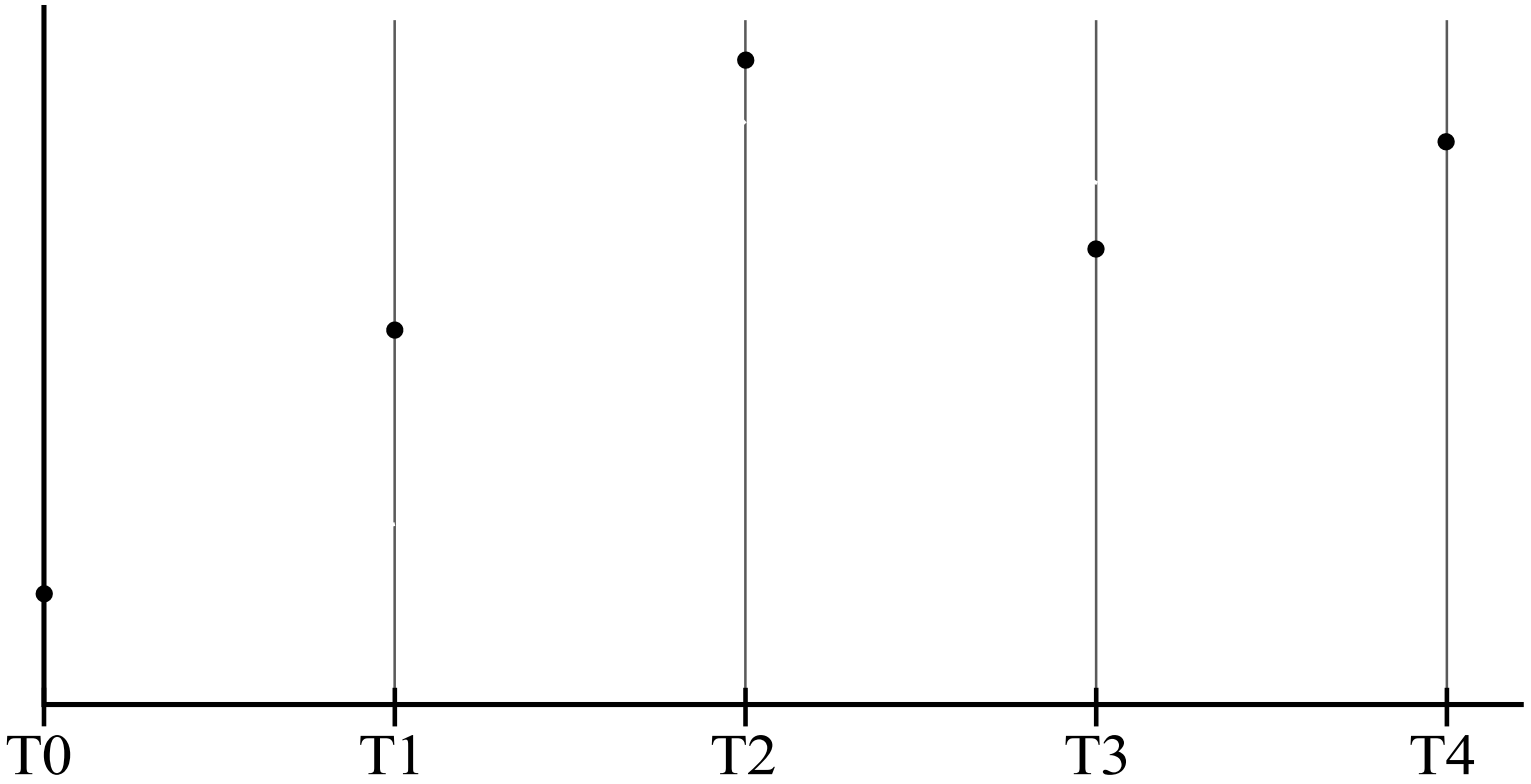

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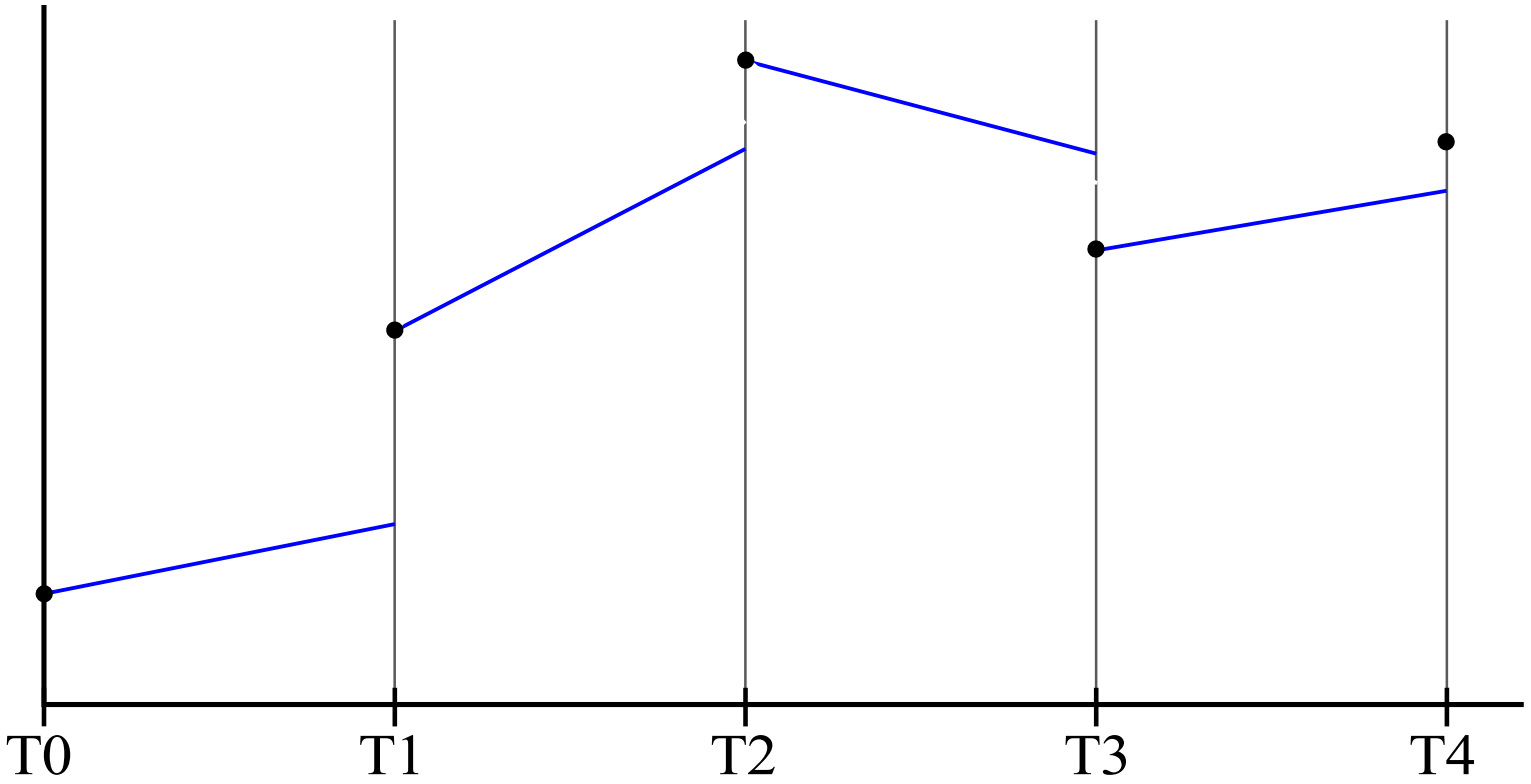

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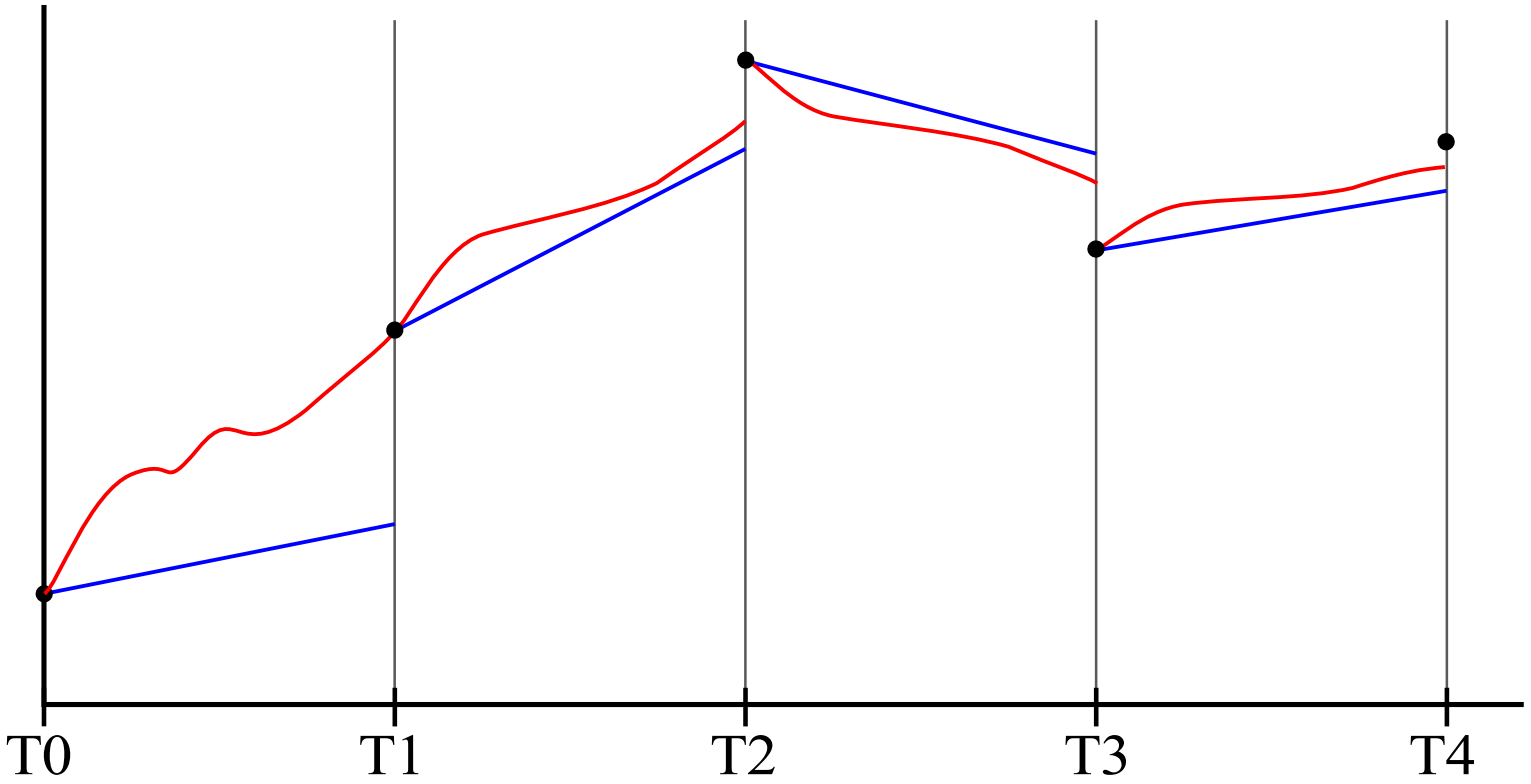

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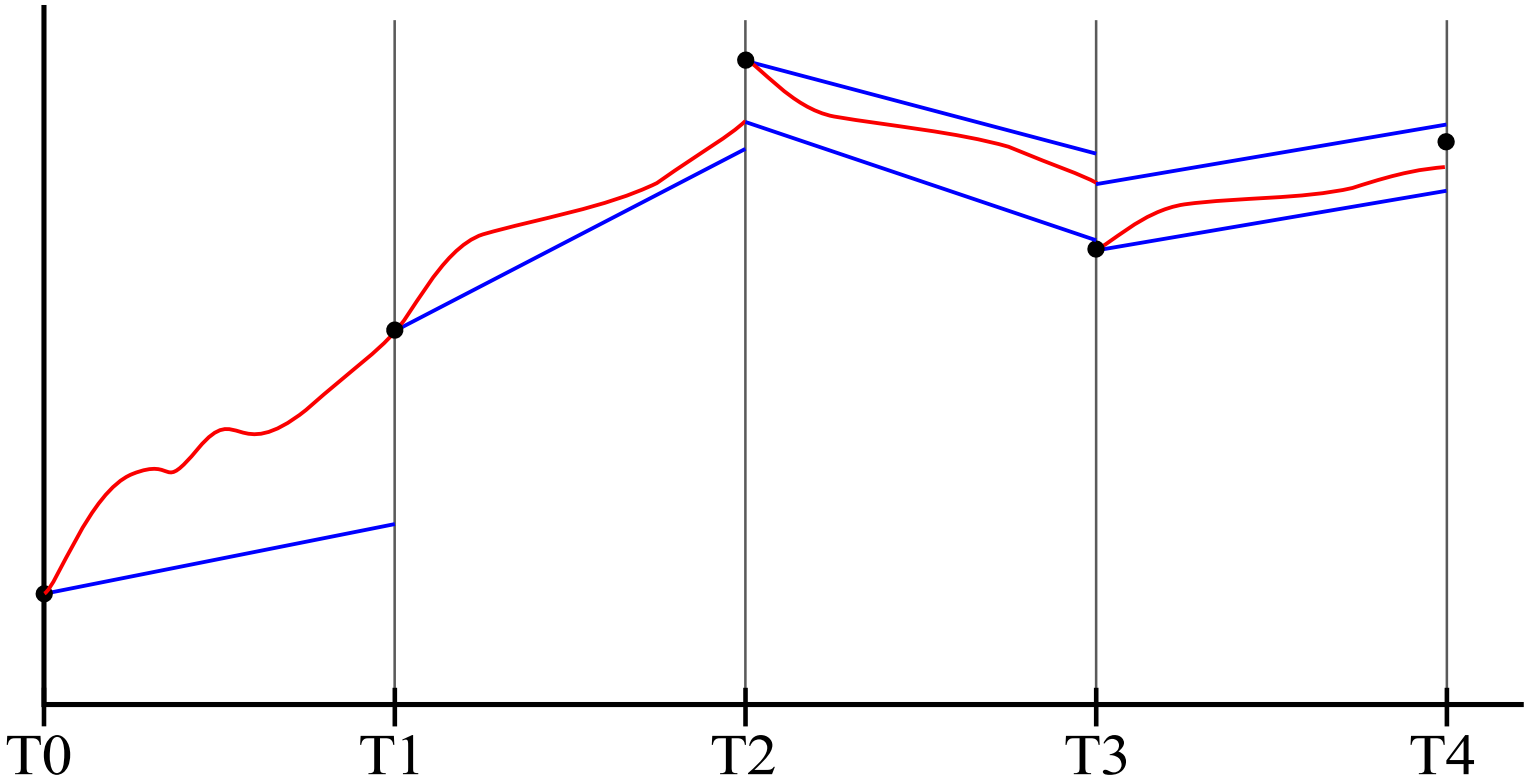

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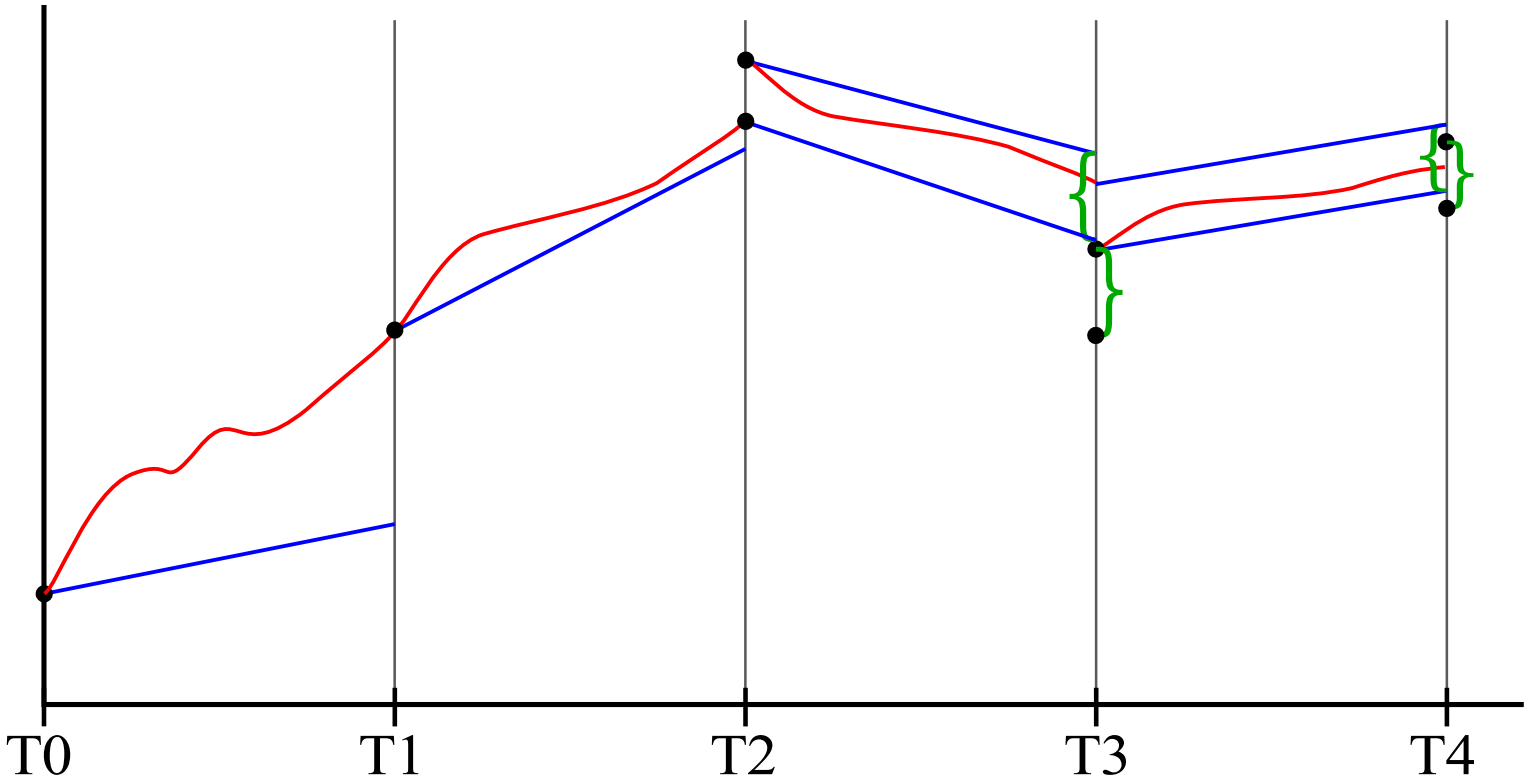

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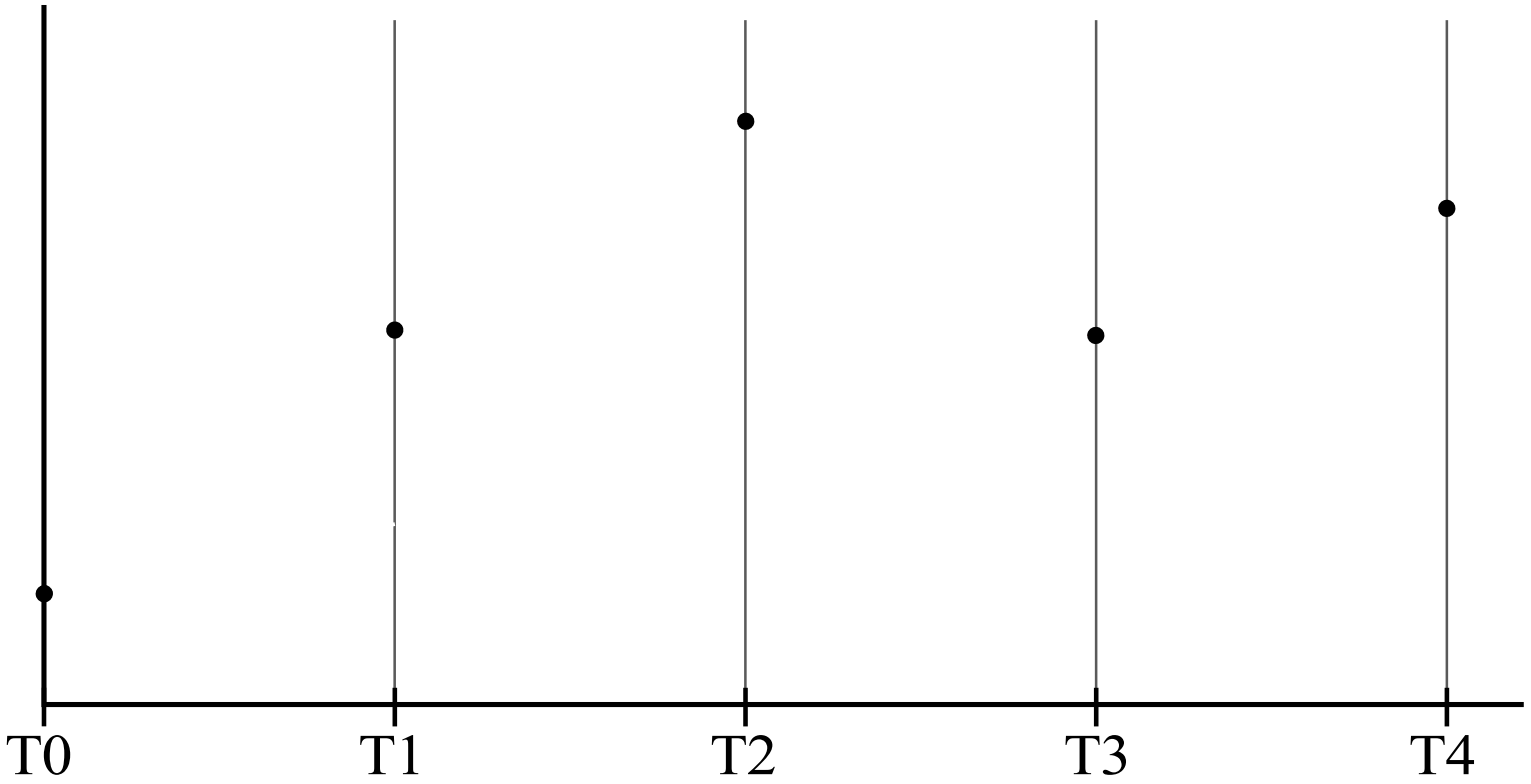

Convergence of Parareal

Theorem (Gander & Hairer 08)

Assume that all $T_n - T_{n-1} = \Delta T$, $\mathcal{F}$ *is an exact propagator and*

$$\mathcal{F}(T_n, T_{n-1}, x) - \mathcal{G}(T_n, T_{n-1}, x) = c_{p+1}(x)\Delta T^{p+1} + c_{p+2}(x)\Delta T^{p+2} + \cdots$$

with all $c_{p+j}(x)$ *being continuously differentiable. Moreover, assume that*

$$\|\mathcal{G}(t + \Delta T, t, x) - \mathcal{G}(t + \Delta T, t, y)\| \leq (1 + C_2\Delta T)\|x - y\|.$$

Then

$$\|u(T_n) - U_n^k\| \leq \frac{C_3}{C_1} \frac{(C_1 T_n)^{k+1}}{(k+1)!} e^{C_2(T_n - T_{k+1})} \Delta T^{p(k+1)}.$$

Linear Problems

We now consider

$$u'(t) = \mathbf{A}u(t) + g(t), \quad t \in [0, T], \quad u(0) = u_0,$$

with $\mathbf{A} \in \mathbb{C}^{d\times d}$ and $g : [0, T] \to \mathbb{C}^d$.

Aim: Exploit linearity to speed up convergence of parareal.

Idea: [Farhat et al. 06] [Gander & Petcu 08] On each interval solve

$$\begin{aligned} V_n'(t) &= \mathbf{A}V_n(t) + g(t), & t \in [T_{n-1}, T_n], \quad V_n(T_{n-1}) &= 0, \\ W_n^{k\prime}(t) &= \mathbf{A}W_n^k(t), & t \in [T_{n-1}, T_n], \quad W_n^k(T_{n-1}) &= U_{n-1}^k, \\ U_n^k(t) &= V_n(t) + W_n^k(t). \end{aligned}$$

The first subproblem needs to be solved only once.
The second subproblem is linear homogeneous, but depends on U_{n-1}^k.

At iteration k of parareal, on interval $[T_{n-1}, T_n]$, we have to solve

$$W_n^{k\prime}(t) = \mathbf{A} W_n^k(t), \quad t \in [T_{n-1}, T_n], \quad W_n^k(T_{n-1}) = U_{n-1}^k$$

with the homogeneous coarse and fine propagator ($\mathcal{G}^H$ and $\mathcal{F}^H$).

At this point, fine evaluations for previous initial conditions U_i^j are available:

$$F_i^j = \mathcal{F}^H(T_i, T_{i-1}, U_i^j).$$

If all U_i^j and F_i^j are collected columnwise in matrices $\mathbf{U}$ and $\mathbf{F}$, then

$$\mathbf{F}\mathbf{U}^\dagger U_{n-1}^k + \mathcal{G}^H(T_i, T_{i-1}, (I - \mathbf{U}\mathbf{U}^\dagger) U_{n-1}^k)$$

is an improvement to the coarse propagator $\mathcal{G}^H(T_i, T_{i-1}, U_{n-1}^k)$.

Remarks

- In a practical implementation, one orthonormalizes the columns of $\mathbf{U}$ such that $\mathbf{U}\mathbf{U}^\dagger = \mathbf{U}\mathbf{U}^*$. This is done by a modified Gram–Schmidt procedure to easily append new initial conditions to $\mathbf{U}$.
- One has to prevent loss of orthogonality by reorthogonalization, otherwise $\mathbf{U}\mathbf{U}^\dagger \neq \mathbf{U}\mathbf{U}^*$ and the method becomes unstable.
- The matrices $\mathbf{U}$ and $\mathbf{F}$ increase in size with every parareal iteration. Orthogonalization, projection, and storage become expensive.

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Claim: The columns of $\mathbf{U}$ and $\mathbf{F}$ are contained in a Krylov space generated by $\mathbf{A}$ because ...

Virtually every method available to integrate

$$W'(t) = \mathbf{A}W(t), \quad t \in [T_0, T_1], \quad W(T_0) = W^{[0]}$$

can be written as

$$W^{[m]} = p_m(h\mathbf{A})W^{[0]} \approx W(T_1)$$

for a polynomial (or rational function) $p_m(z)$.

Examples

- Forward Euler: $W^{[m]} = W^{[m-1]} + h\mathbf{A}W^{[m-1]} \Rightarrow p_m(z) = (1+z)^m$.
- Backward Euler: $W^{[m]} = W^{[m-1]} + h\mathbf{A}W^{[m]} \Rightarrow p_m(z) = (1-z)^{-m}$.
- Runge–Kutta: $p_m(z) = \left(1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4\right)^m$.
- SDC: interpolating polynomial.

Hence: At any iteration of parareal the degree of $W^{[m]}$ as a function in $\mathbf{A}$ will not exceed the degree we could generate with 1 processor!

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Exponential Integration (Paraexp)

We now decompose

$$u'(t) = \mathbf{A}u(t) + g(t), \quad t \in [0, T], \quad u(0) = u_0,$$

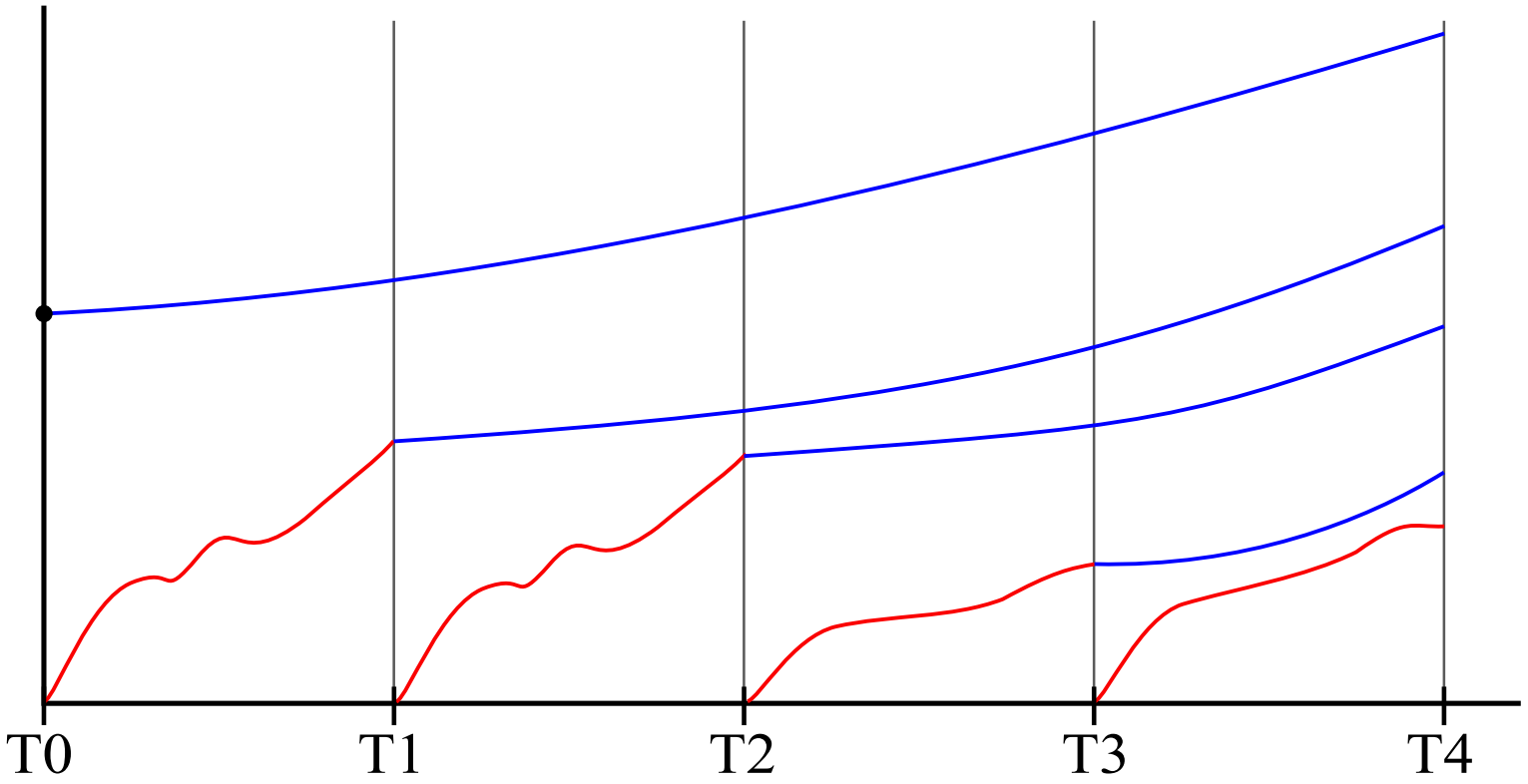
into N decoupled problems

$$\begin{aligned} V_n'(t) &= \mathbf{A}V_n(t) + g(t), & t \in [T_{n-1}, T_n], \quad V_n(T_{n-1}) &= 0, \\ W_n'(t) &= \mathbf{A}W_n(t), & t \in [T_{n-1}, T_N], \quad W_n(T_{n-1}) &= V_{n-1}(T_{n-1}), \end{aligned}$$

where $V_0(T_0) = u_0$, such that

$$u(t) = \sum_{n=1}^{N} V_n(t) + W_n(t).$$

If processor $P(n)$ computes $V_{n-1}(t)$ and $W_n(t)$, this summation is the only communication point.



1. On processor $P(n)$ compute $V_{n-1}(T_{n-1}) = \mathcal{F}(T_{n-1}, T_{n-2}, 0)$.
2. On processor $P(n)$ compute $W_n(t) = e^{(t-T_{n-1})\mathbf{A}} V_{n-1}(T_{n-1})$.
3. Summation $U(T_j) = \sum_{n=1}^{N} V_n(T_j) + W_n(T_j)$ at desired T_j.

To compute the matrix exponential in

$$W_n(t) = e^{(t-T_{n-1})\mathbf{A}} v, \quad v = V_{n-1}(T_{n-1}),$$

we can directly use a polynomial Krylov method to select approximations from an m-dimensional polynomial Krylov space

$$W_n(t) \approx W_n^m(t) \in \mathcal{K}_m(\mathbf{A}, v) := \text{span}\{v, \mathbf{A}v, \mathbf{A}^2 v, \ldots, \mathbf{A}^{m-1} v\}.$$

In what follows: **Chebyshev method**

[Druskin & Knizhnerman 89] [Schaefer 90]

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Chebyshev Method

Aim: Approximation of $e^{\tau \mathbf{A}} v$ for symmetric $\mathbf{A} \in \mathbb{C}^{d \times d}$, $\Lambda(\mathbf{A}) \in [-1, 1]$, without computing $e^{\tau \mathbf{A}}$.

The Chebyshev method is based on the polynomial expansion

$$e^{\tau x} = \sum_{j=0}^{\infty} \gamma_j C_j(x), \quad x \in [-1, 1],$$

where $C_0 \equiv 1$, $C_1(x) = x$, $C_j(x) = 2xC_{j-1}(x) - C_{j-2}(x)$.

Chebyshev polynomials $C_j(x)$ are orthogonal w.r.t. the inner product

$$\langle f(x), g(x) \rangle := \int_{-1}^{1} \frac{f(x)g(x)}{\sqrt{1-x^2}} \, \mathrm{d}x$$

and the γ_j are the coordinates of $e^{\tau x}$, i.e.,

$$\gamma_j := \langle e^{\tau x}, C_j(x) \rangle.$$

The truncated Chebyshev sum

$$S_m(x) := \sum_{j=0}^{m-1} \gamma_j C_j(x), \quad x \in [-1,1],$$

is the best approximation of $f(x) = e^{\tau x}$ from $\mathcal{P}_{m-1} \subset L^2_w([-1,1])$, and $\|e^{\tau x} - S_m(x)\|_{L^2_w([-1,1])} \to 0$ superlinearly as $m \to \infty$.

Note that $\|C_j\|_\infty := \max\{|C_j(x)| : x \in [-1,1]\} = 1$ and $C_j(1) = 1$.

Moreover, we have $\gamma_j > 0$ for all j. Hence

$$\|e^{\tau x} - S_m(x)\|_\infty = \left\| \sum_{j=m}^{\infty} \gamma_j C_j(x) \right\|_\infty = \sum_{j=m}^{\infty} \gamma_j C_j(1) = e - S_m(1).$$

A practical method for computing $S_m(\mathbf{A})v \approx e^{\tau \mathbf{A}} v$ is

- Initialize $C_0 = v$, $C_1 = \mathbf{A}v$.
- Set $S_2 = \gamma_0 C_0 + \gamma_1 C_1$.
- For $j = 2, \ldots, m-1$ compute $C_j = 2\mathbf{A}C_{j-1} - C_{j-2}$ and set $S_{j+1} = S_j + \gamma_j C_j$.

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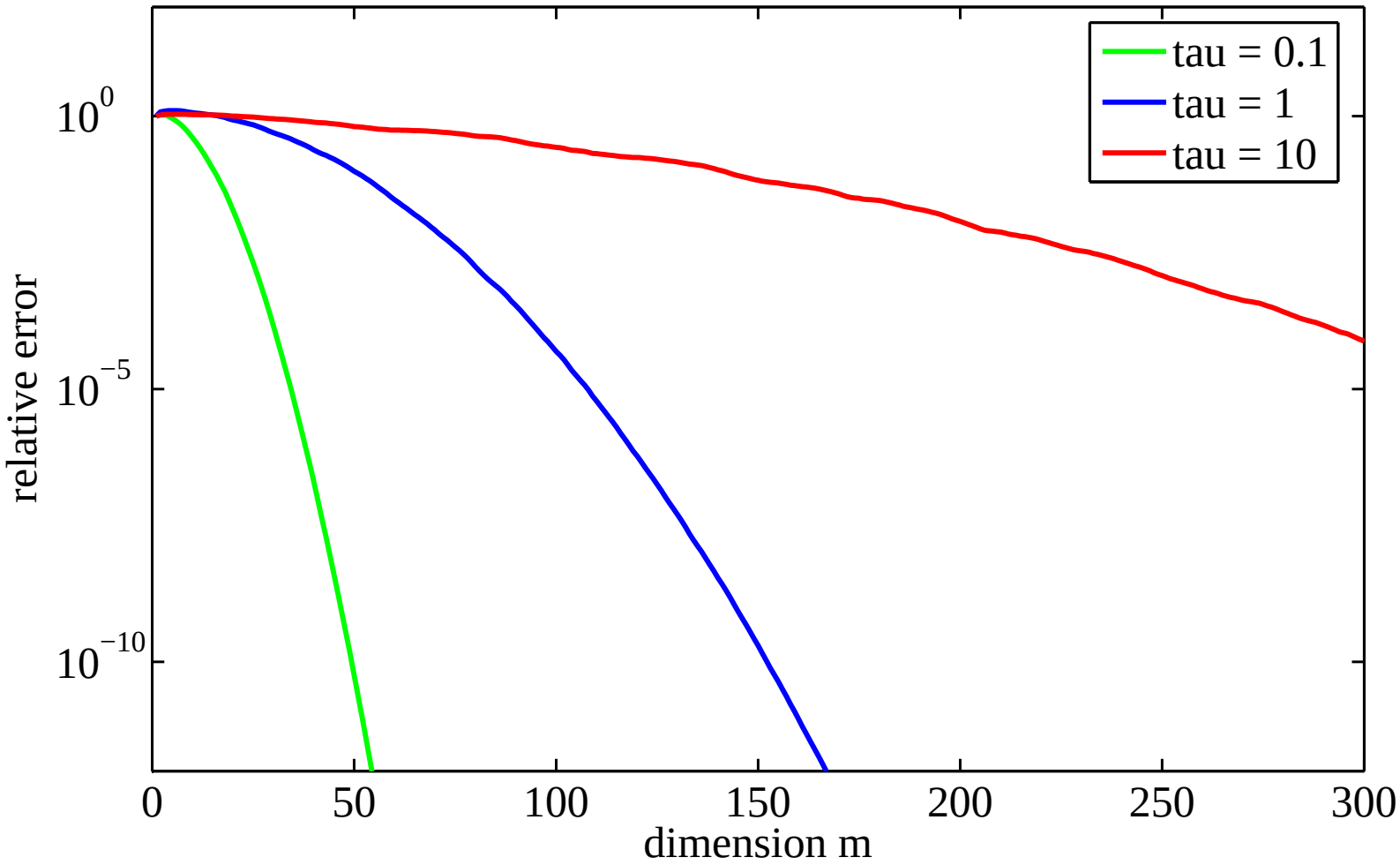
Remarks: Storage for only 3 vectors needed. We have the bound

$$\|e^{\tau \mathbf{A}} v - S_m(\mathbf{A})v\|_2 \leq \|e^{\tau x} - S_m(x)\|_\infty \|v\|_2 = (e - S_m(1))\|v\|_2.$$

A practical error estimate is

$$\|e^{\tau \mathbf{A}} v - S_m(\mathbf{A})v\|_2 \approx \|\gamma_m C_m + \gamma_{m+1} C_{m+1}\|_2.$$

Example: $\mathbf{A} = \mathrm{diag}(-1000, -999, \ldots, 0)$, $v = \mathrm{randn}$, compute $e^{\tau \mathbf{A}} v$.



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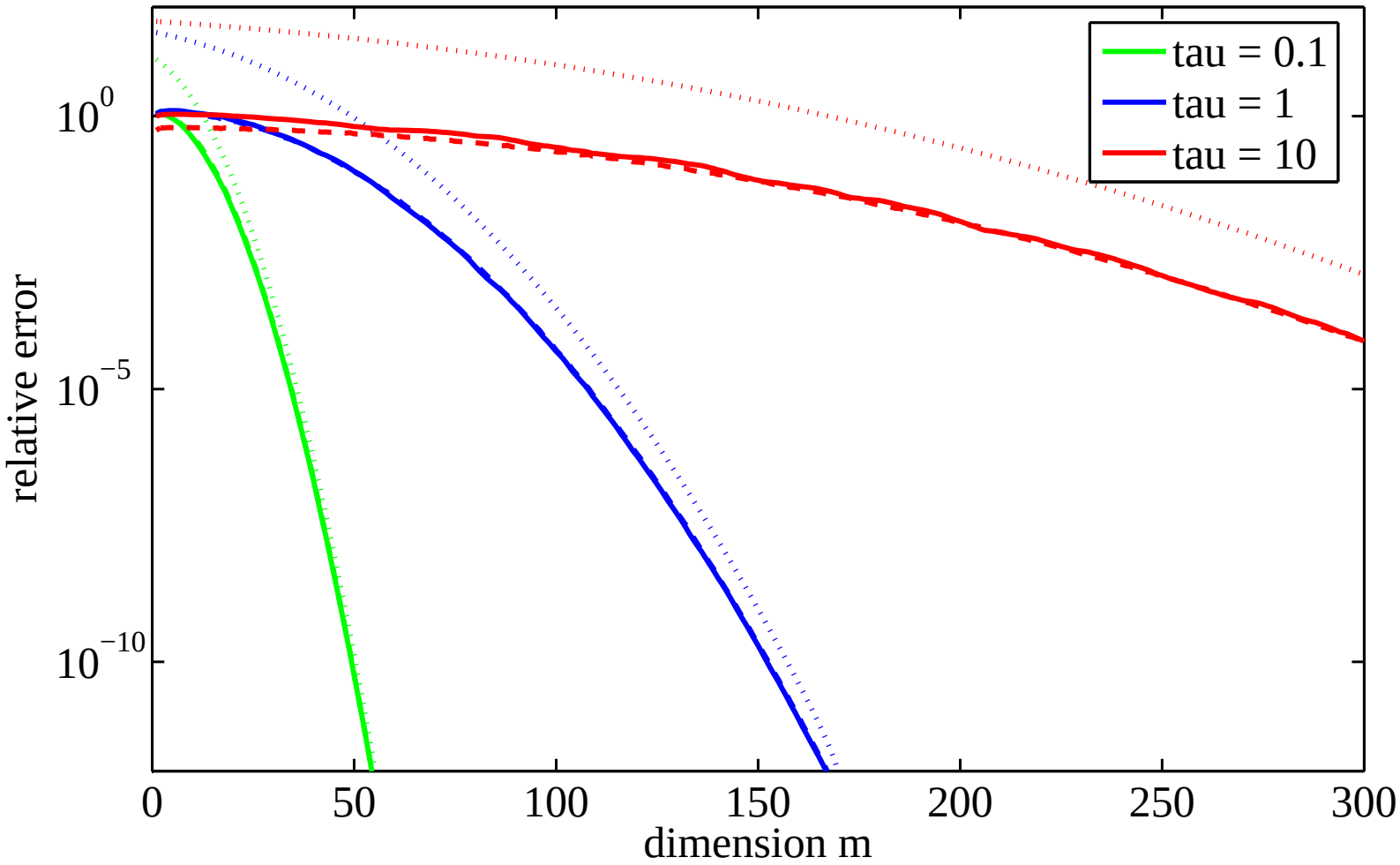

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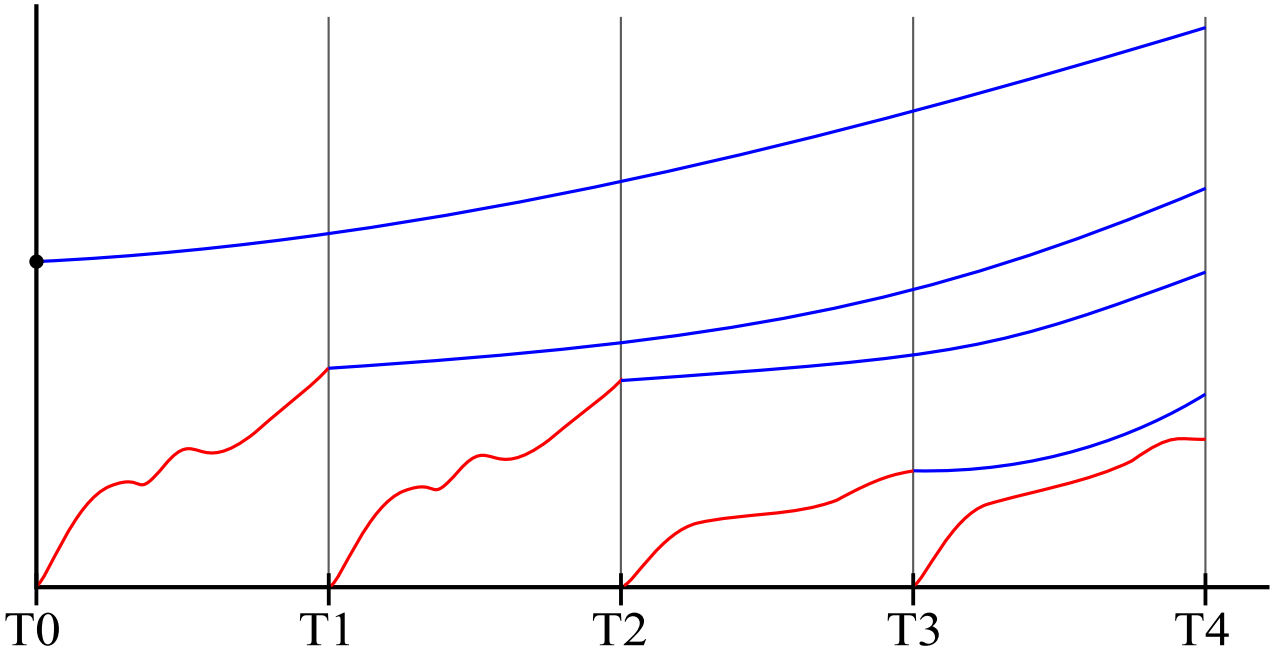

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3. Summation $U(T_j) = \sum_{n=1}^{N} V_n(T_j) + W_n(T_j)$ at desired T_j.

Idea: Choose $T_1, \ldots, T_{N-1}$ such that steps 1 & 2 end synchronously.

Numerical Example

1D heat equation with homogeneous Dirichlet boundary condition and "oscillating hat" source (half-width $w = 0.05$, height $h = 50$, frequency $f = 23$):

$$\begin{aligned} \partial_t u(t,x) &= \partial_{xx} u(t,x) + q(t,x) && \text{on } x \in (0,1), \\ u(t,0) &= u(t,1) = 0, \\ u(0,x) &= u_0(x) = x(1-x), \\ q(t,x) &= h \max\{1 - |c-x|/w, 0\}, && c = .5 + (.5 - w)\sin(2\pi f t). \end{aligned}$$

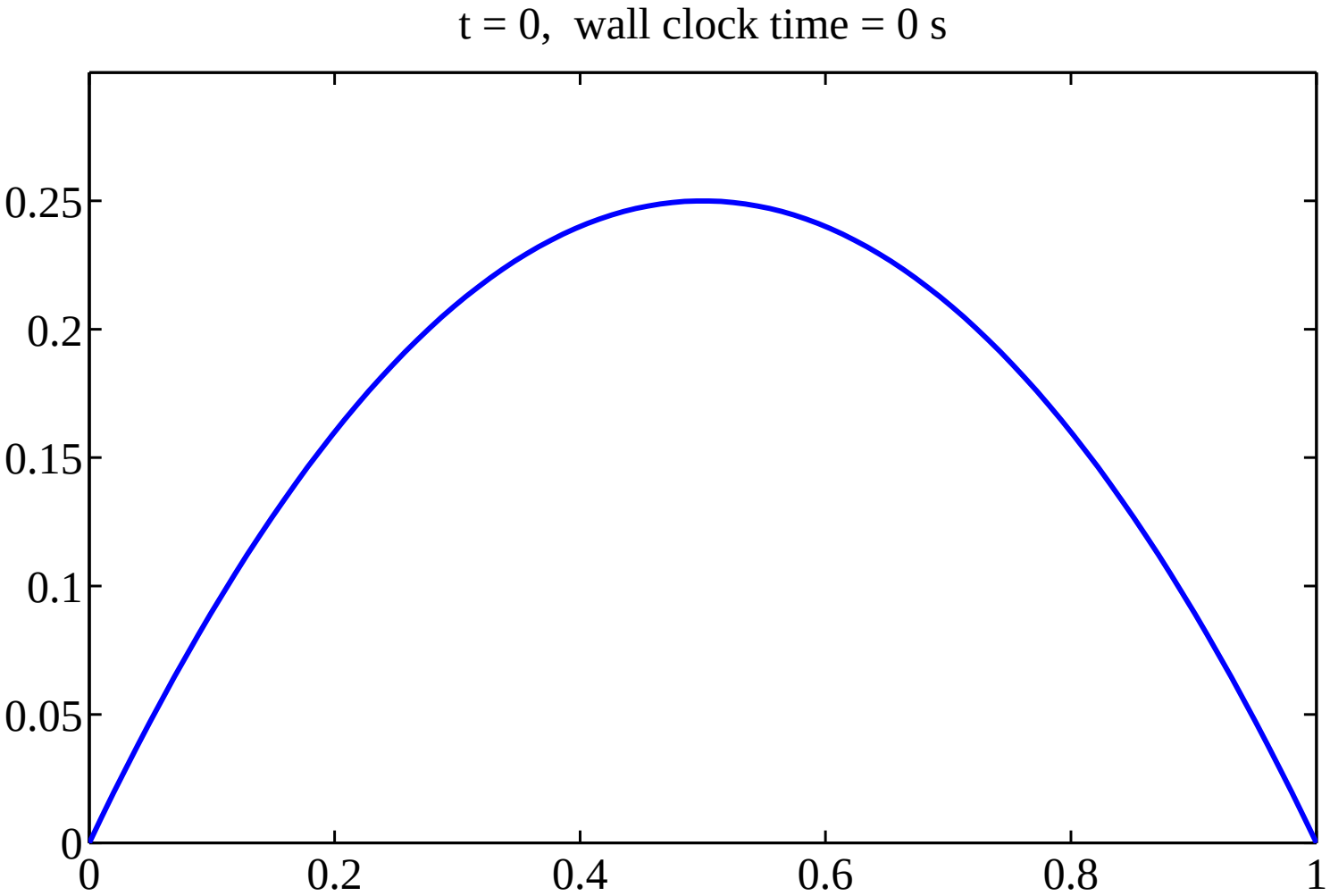
Finite-difference discretization in space yields

$$u'(t) = \mathbf{A}u(t) + q(t), \quad u(0) = u_0,$$

where $\mathbf{A} = (d+1)^2 \text{ tridiag}(1, -2, 1) \in \mathbb{R}^{d \times d}$, $d = 100$.

Serial integration

We integrate for $t \in [0, 1]$ using `ode15s` with error tolerance 10^{-3}.
Overall computation time: 5.2 s



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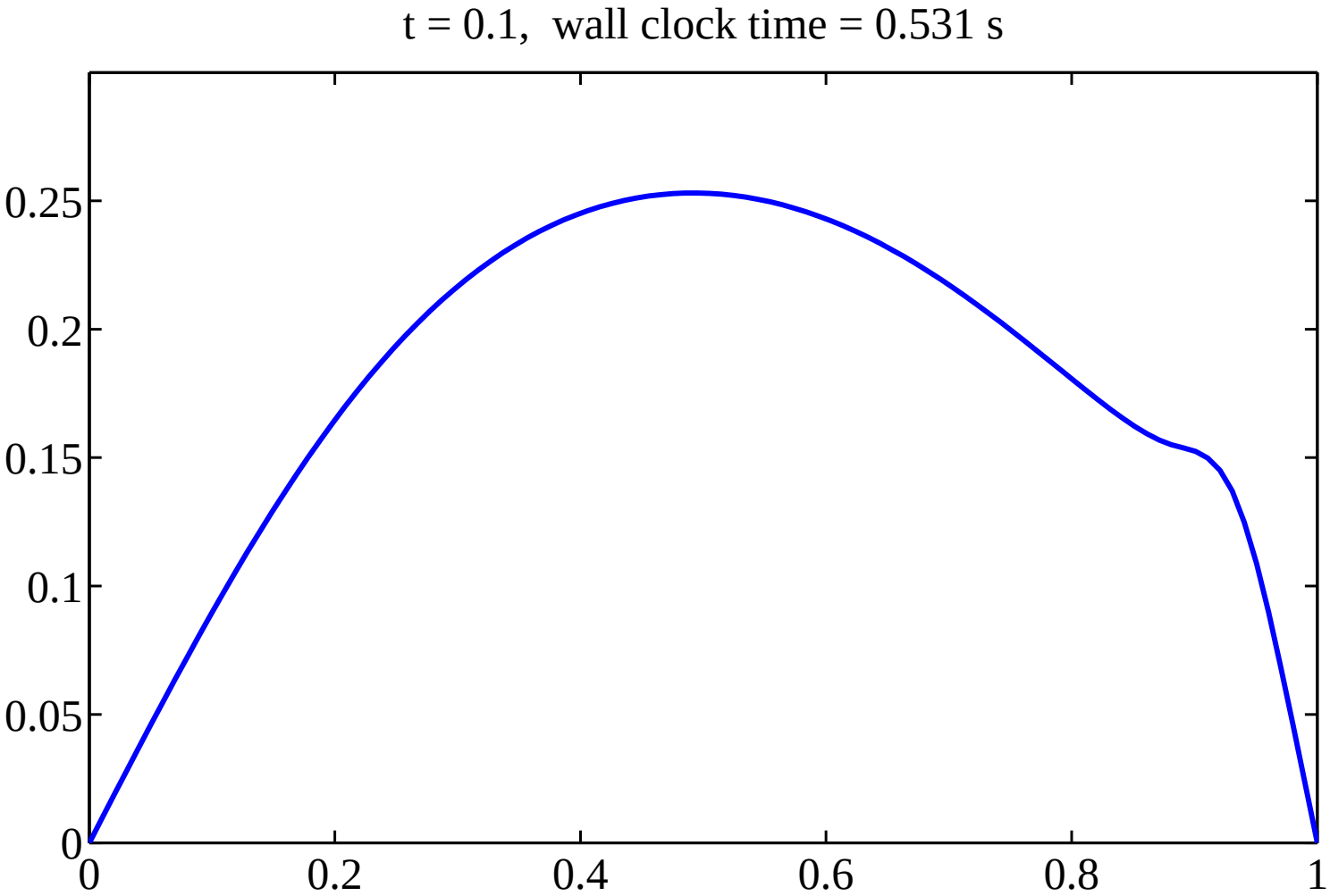
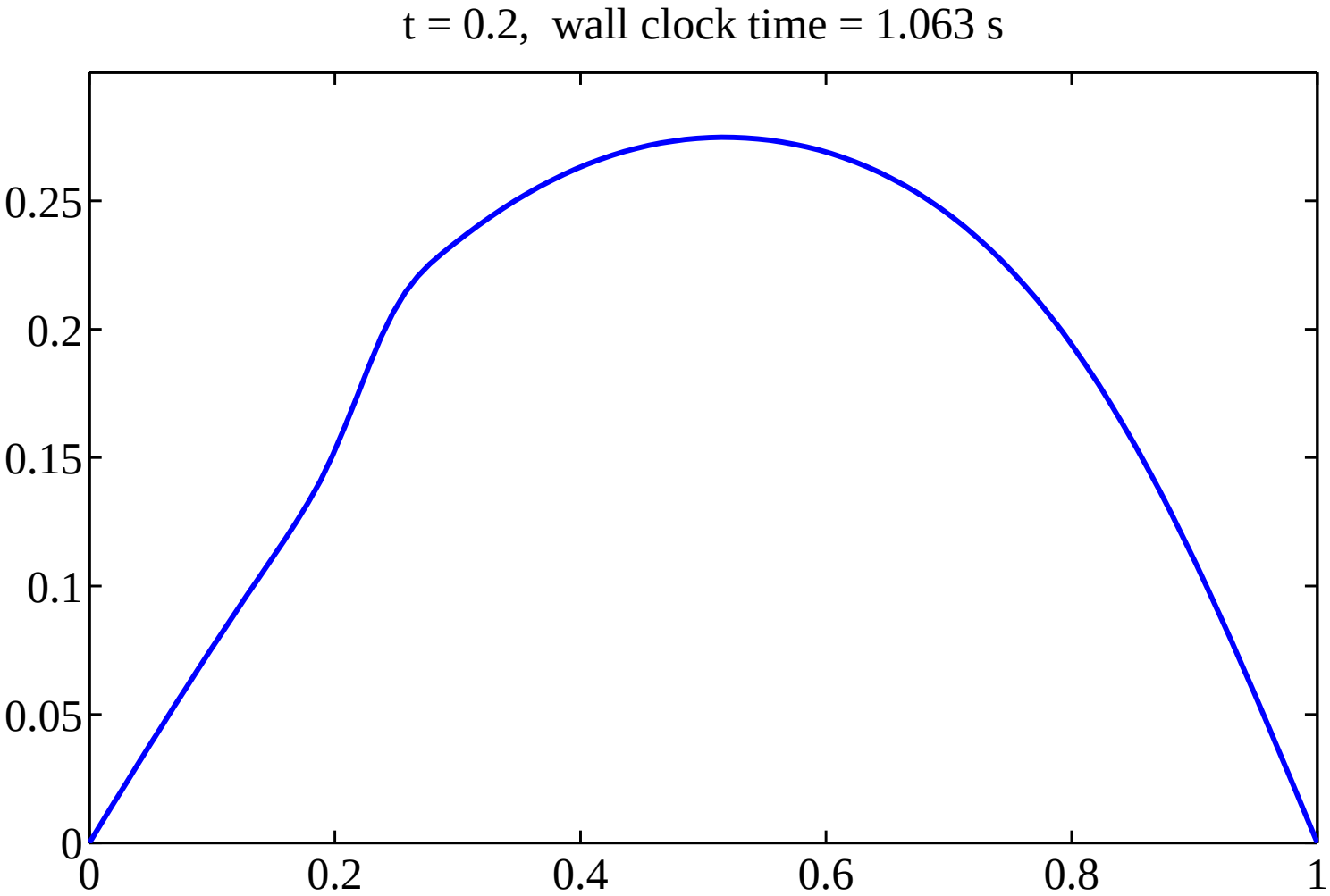


Serial integration

We integrate for $t \in [0, 1]$ using `ode15s` with error tolerance 10^{-3}.
Overall computation time: 5.2 s



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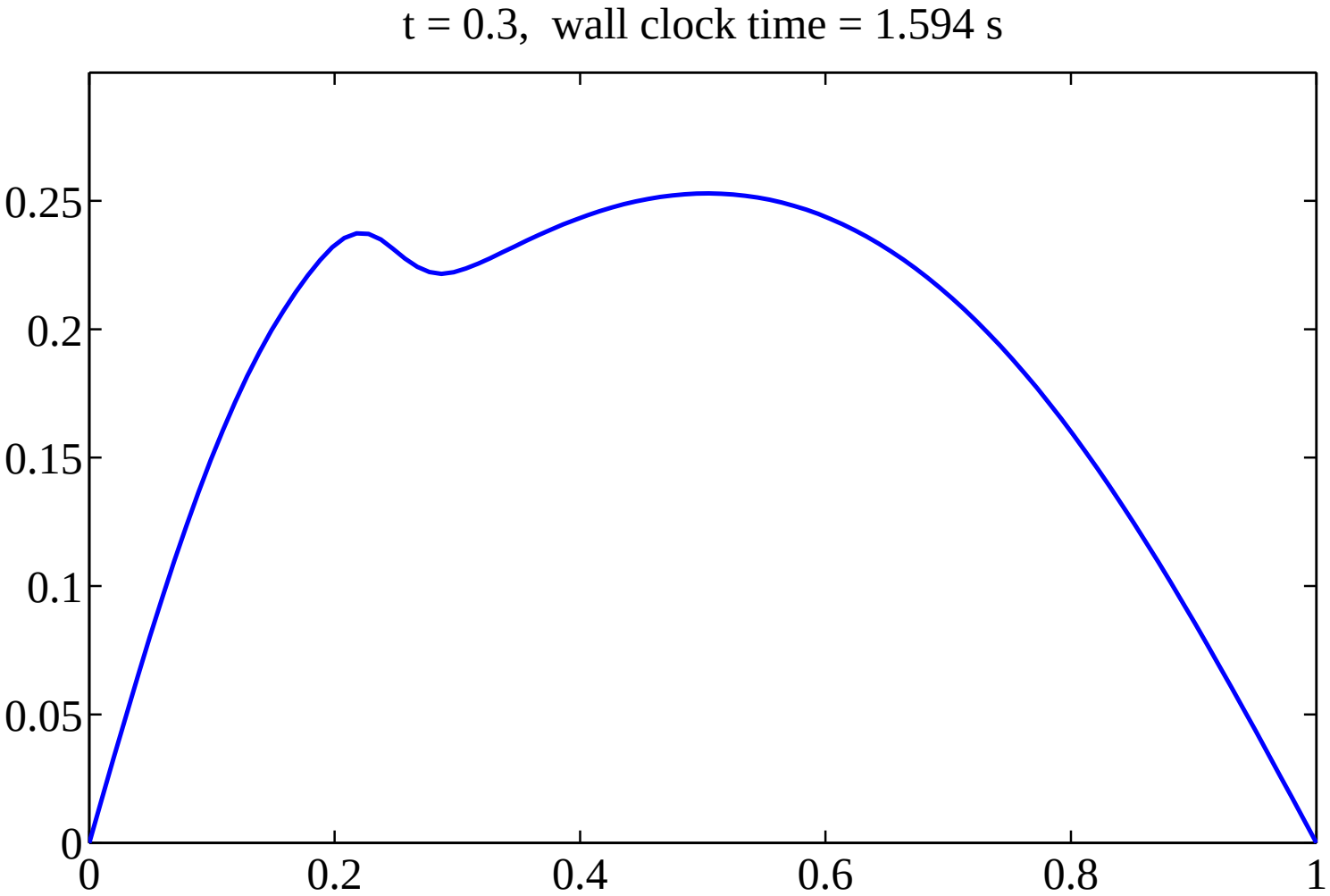

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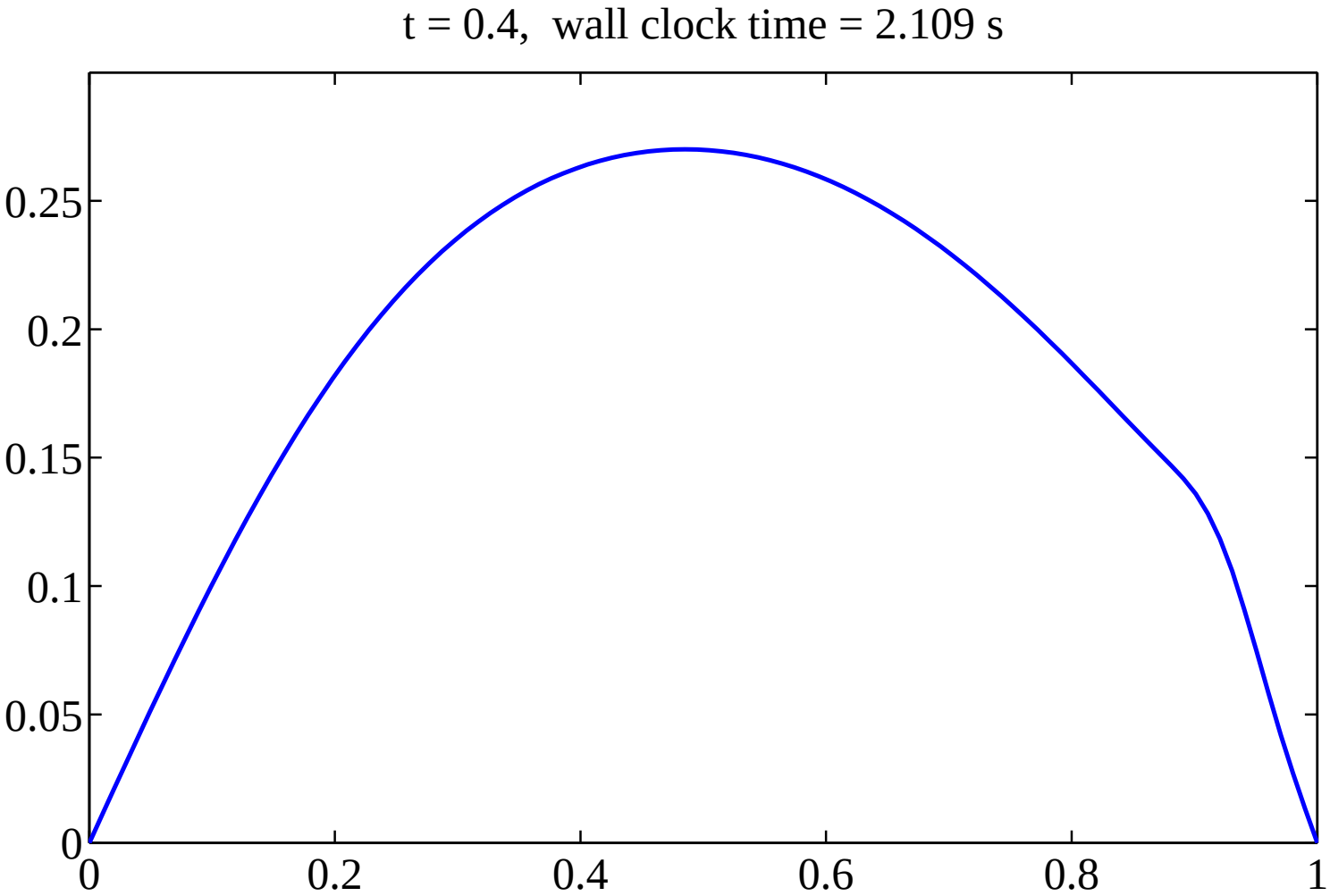

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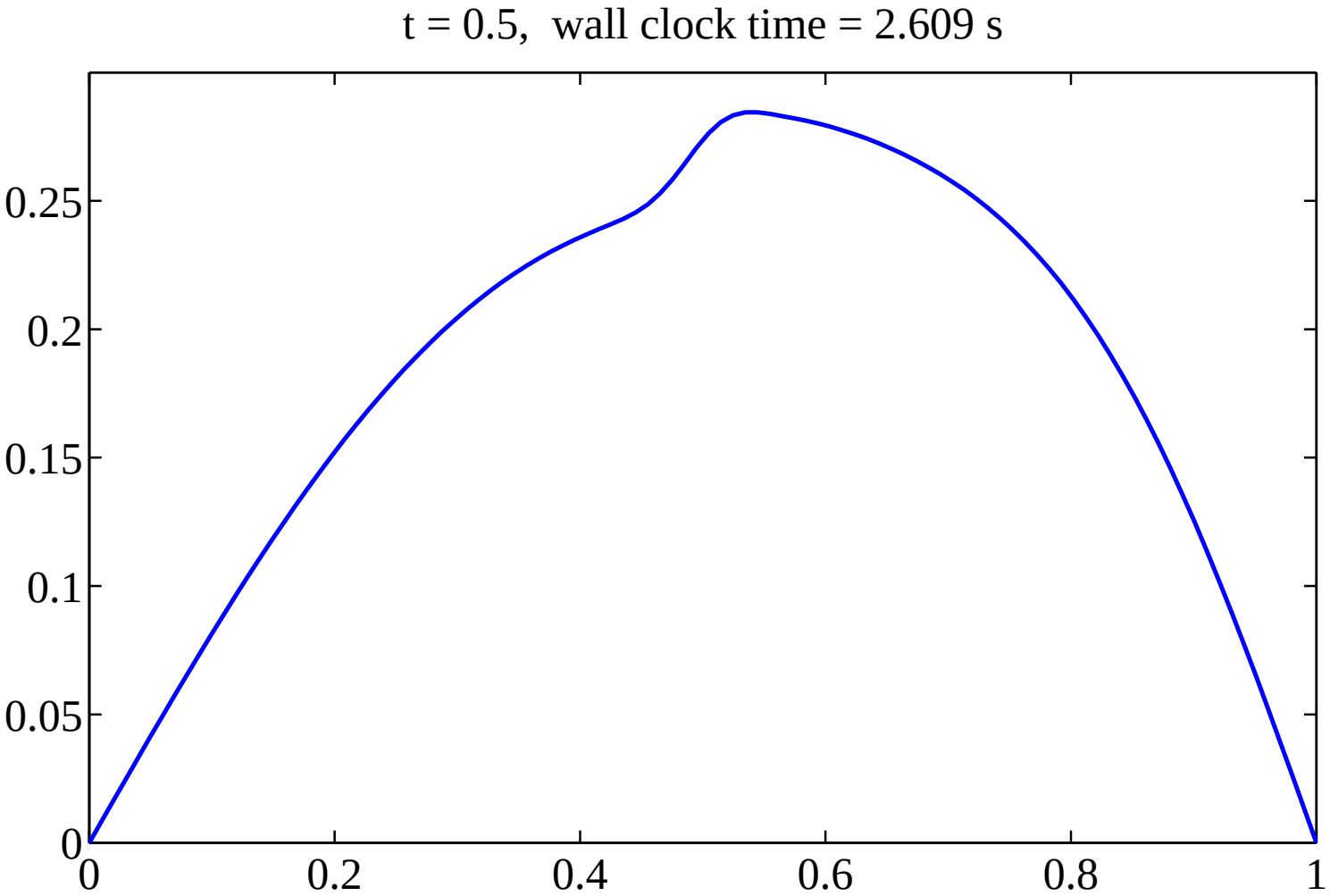

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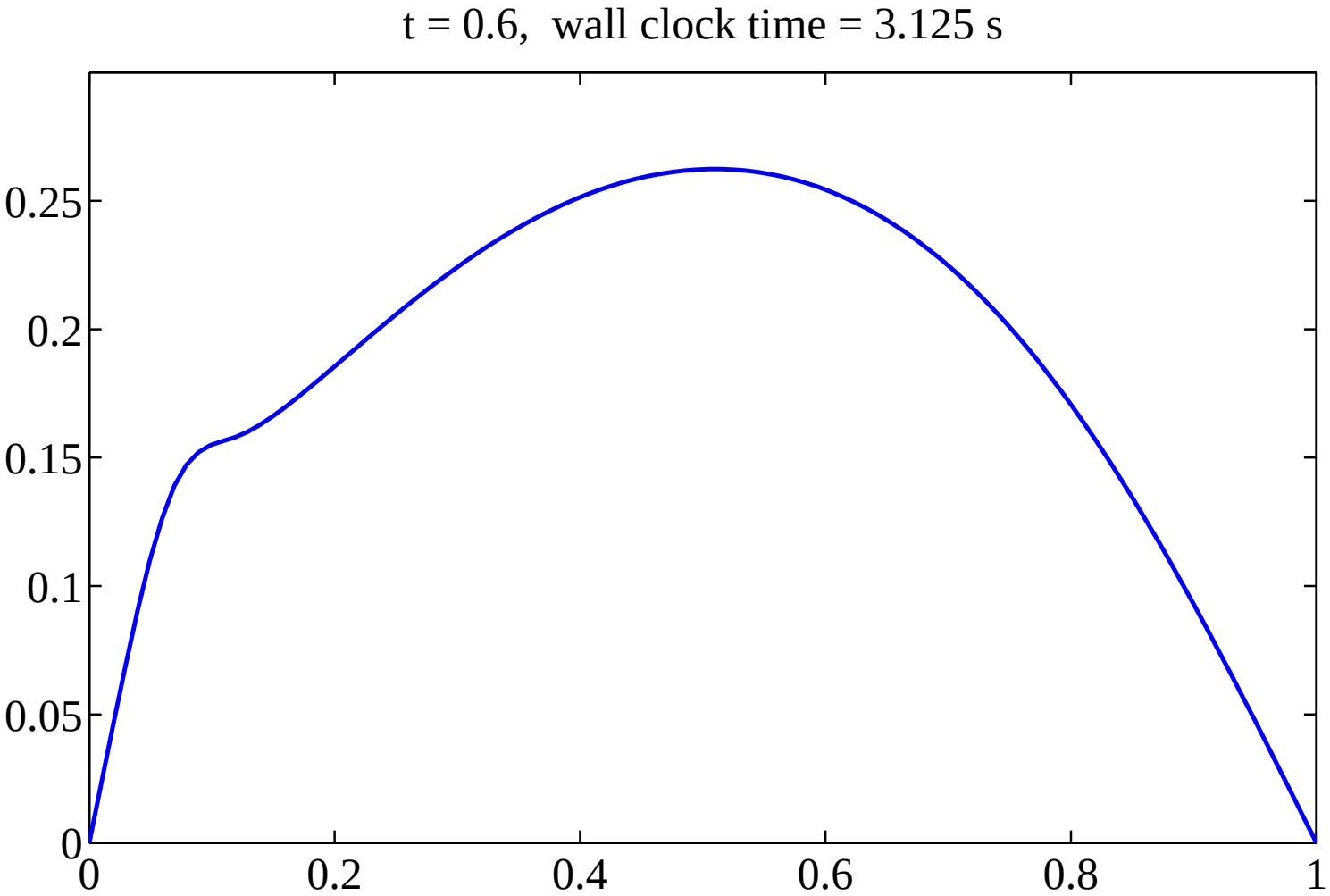

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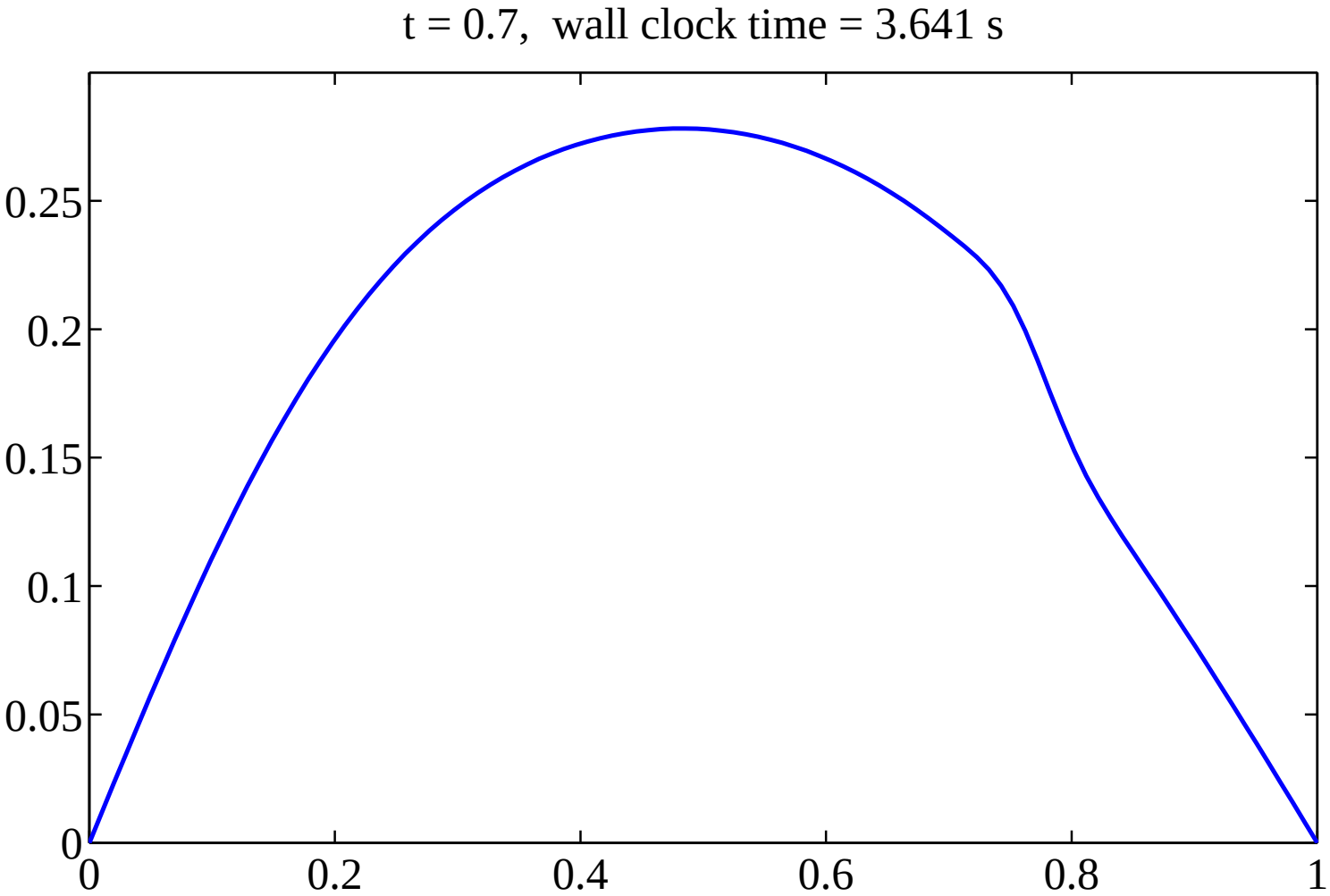

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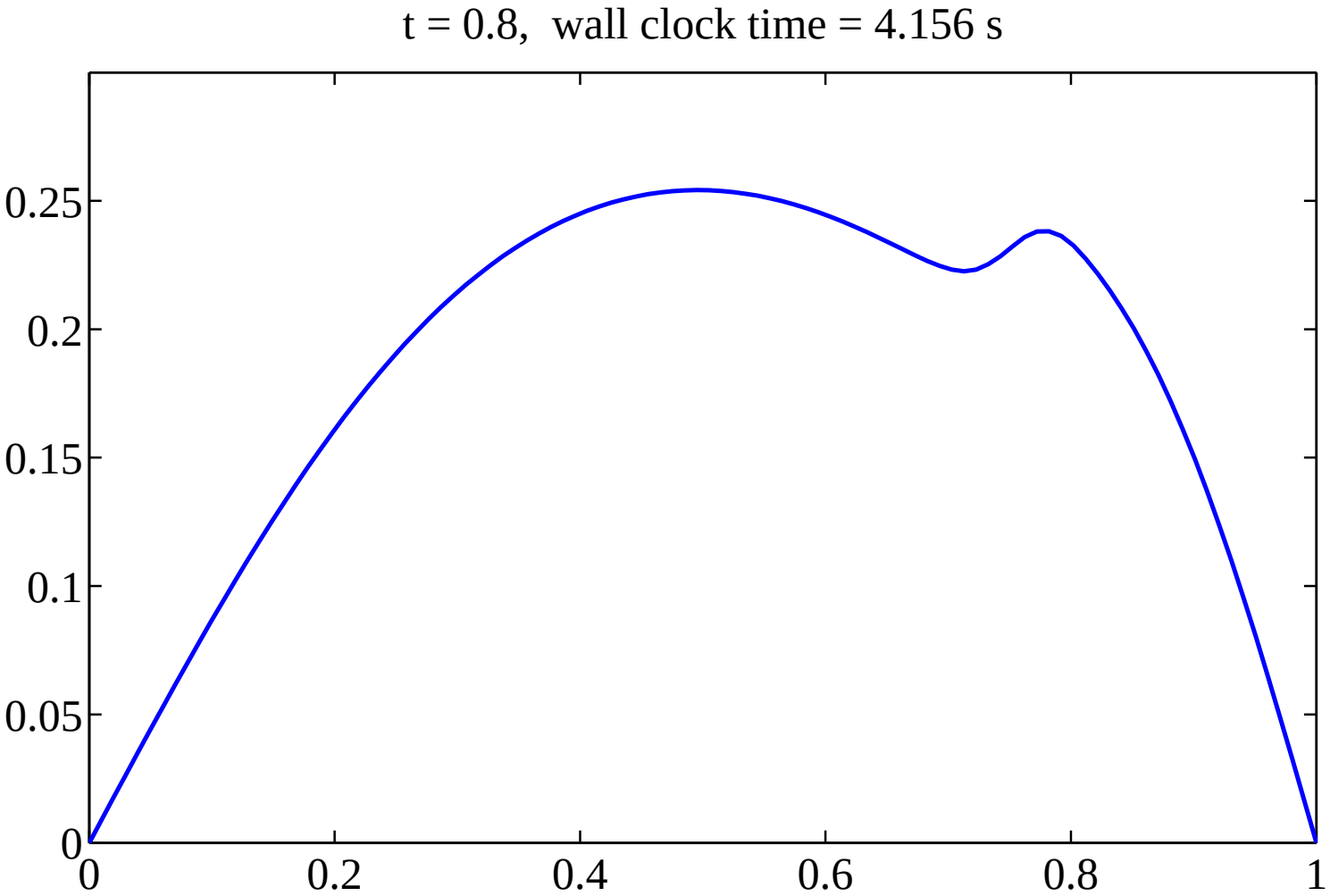

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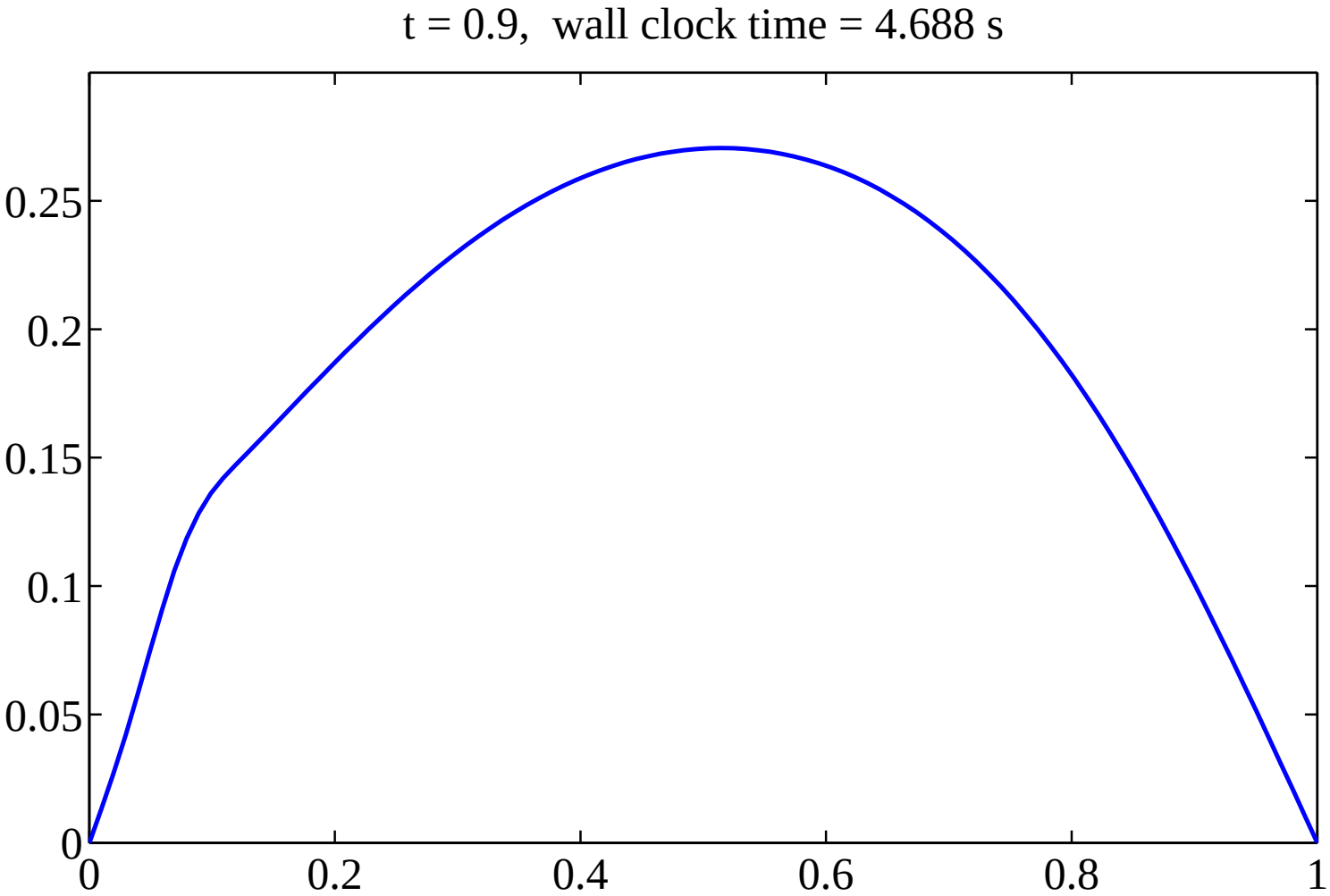

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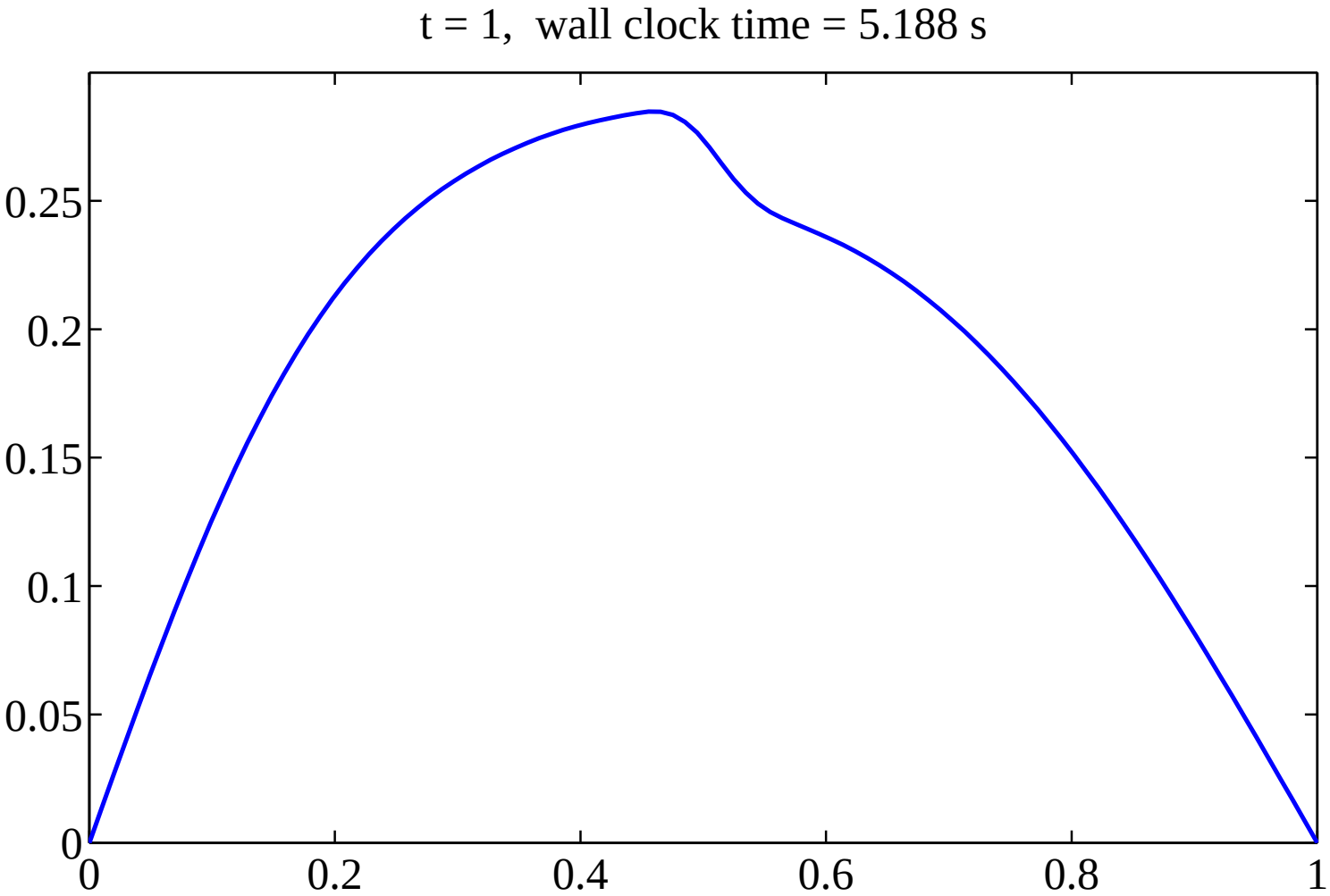
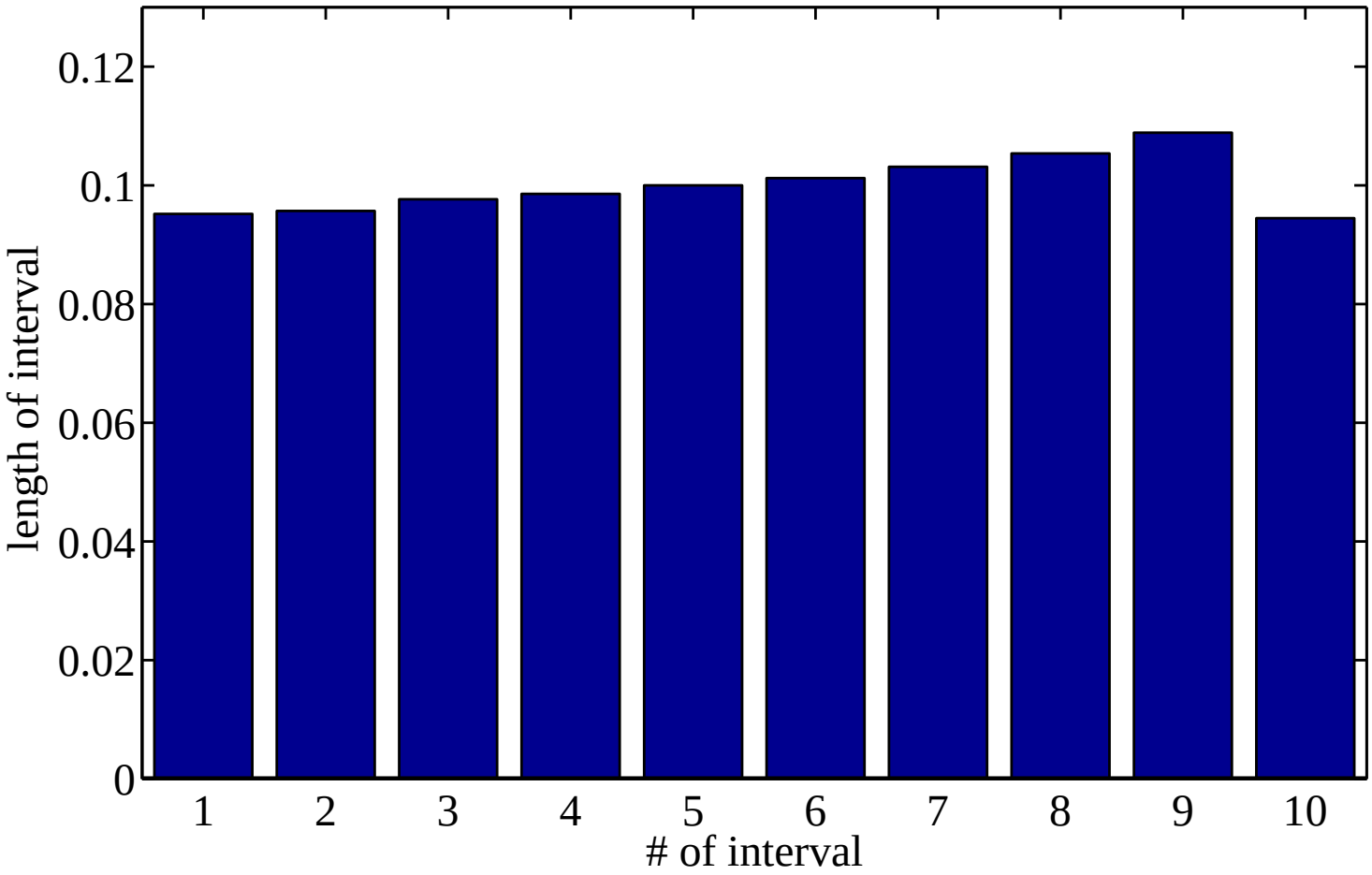
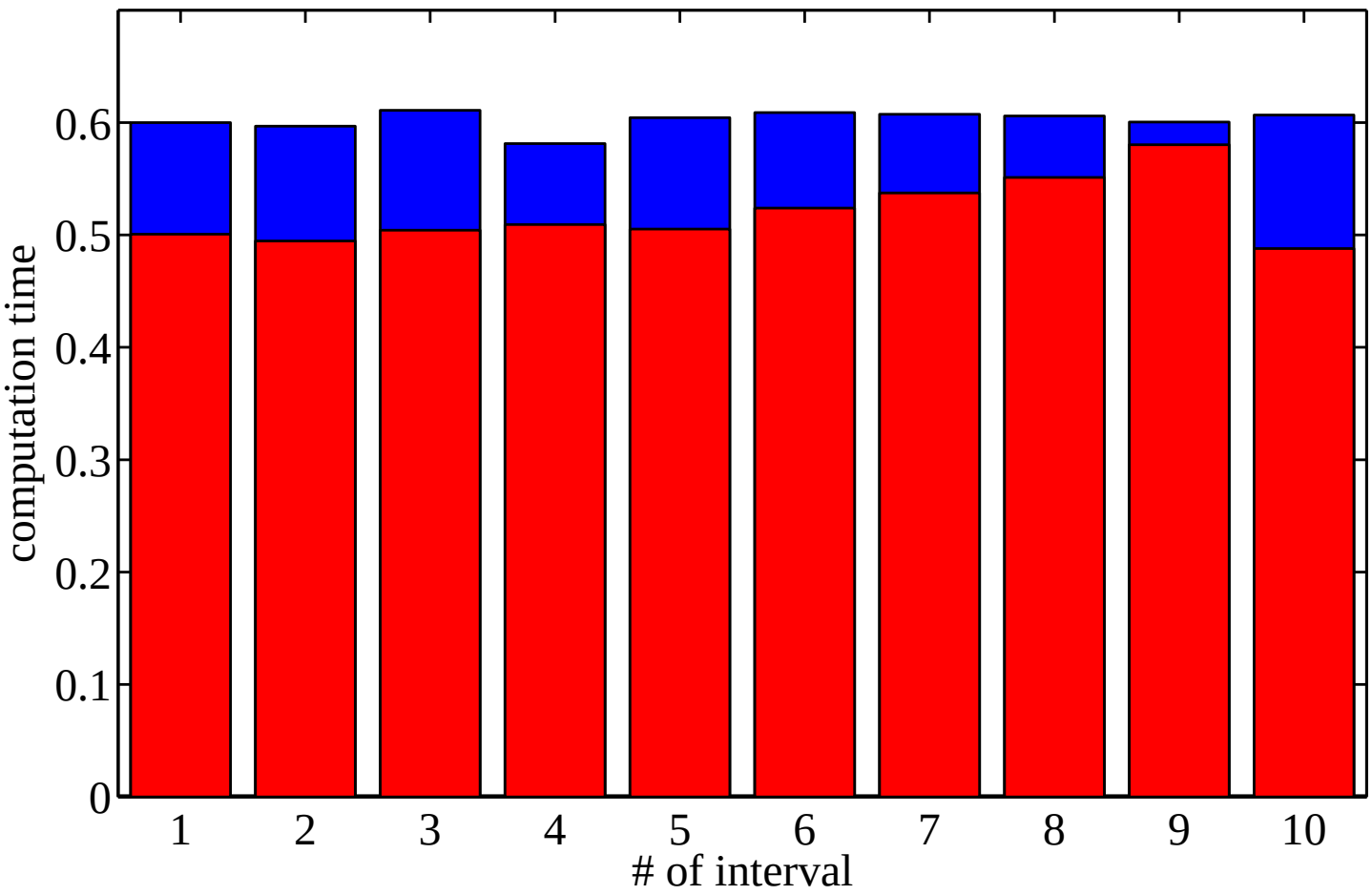
Overall computation time: 5.2 s



Optimized length of 10 integration intervals



Parallel computation time of paraexp (ode15s / cheby)



Speed up = 5.2 / 0.6 ≈ 8.7.

Summary

- For linear problems almost perfectly scaling methods can be derived by appropriate decomposition into homogeneous and inhomogeneous subproblems.
- Efficient (in fact, near-optimal) polynomial and rational Krylov methods are available to integrate the homogeneous subproblem.
- The proposed *paraexp method* requires almost no communication and converges superlinearly.
- For linear problems it is questionable whether a parareal iteration is actually necessary.
- For semilinear problems $u'(t) = \mathbf{A}u(t) + g(t, u(t))$ similar ideas can be applied. However, in this case a parareal-like iteration is indeed necessary.