Towards a PinT multirate explicit stabilized method with applications in electrophysiology

Giacomo Rosilho de Souza, Simone Pezzuto, Rolf Krause

Università della Svizzera italiana

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Introduction to explicit stabilized methods

We want to solve, for instance,

$$y' = \nabla \cdot (A(y)\nabla y) + f(y).$$

We typically have:

Standard explicit solver: $\Delta t \leq Ch^2$,

Implicit solver: solves nonlinear problem.

With explicit stabilized methods:

- No step size Δt restrictions,
- No linear systems to solve.

Some differences with respect to standard explicit methods:

- Adaptive in the number of stages s,
- Given an order p, use an increased number of stages $s \geq p$,
- Gained freedom is used to optimise in the stability direction,
- Stability domain grows as $O(s^2)$,
- Work load scales as $O(\sqrt{\rho}) = O(h^{-1})$, not as $O(\rho) = O(h^{-2})$.

Literature Review (without deprecated methods)

For general dissipative problems $y' = f(y)$:

- RKC1, RKC2 (Van der Houwen & Sommeijer, 1980),
- ROCK2, ROCK4 (Abdulle & Medovikov, 2001),
- RKL1, RKL2 (Meyer, Balsara, Aslam, 2014).

For advection-diffusion-reaction

- PRKC (Zbinden, 2011),
- PIROCK (Abdulle & Vilmart, 2013),
- IMPRKC (Tang & Xiao, 2020),
- ARKC (Almuslimani, 2022).

For multirate problems $y' = f_F(y) + f_S(y)$:

- mRKC (Abdulle, Rosilho, Grote, 2021).

In mixed precision arithmetic:

- MP-mRKC (Croci, Rosilho, 2022).

For SDEs $\mathrm{d}X = f(X)\mathrm{d}t + g(X)\mathrm{d}W$:

- SK-ROCK (Abdulle, Vilmart, Almuslimani, 2018).

$f_F(X)\mathrm{d}t + f_S(X)\mathrm{d}t + g(X)\mathrm{d}W$:

Rosilho, 2021).

For chemical kinetics $S_1 \rightleftharpoons S_2 \rightharpoonup S_3$:

- SK-τ-ROCK (Abdulle, Rosilho, Gander, 2021),

For jump SDEs $\mathrm{d}X = f(X)\mathrm{d}t + g(X)\mathrm{d}W + \int h(X)\mathrm{d}N$:

- SK-JD-ROCK (Chanay, Rosilho, 2021).

Missing: PinT method

Example of practical application

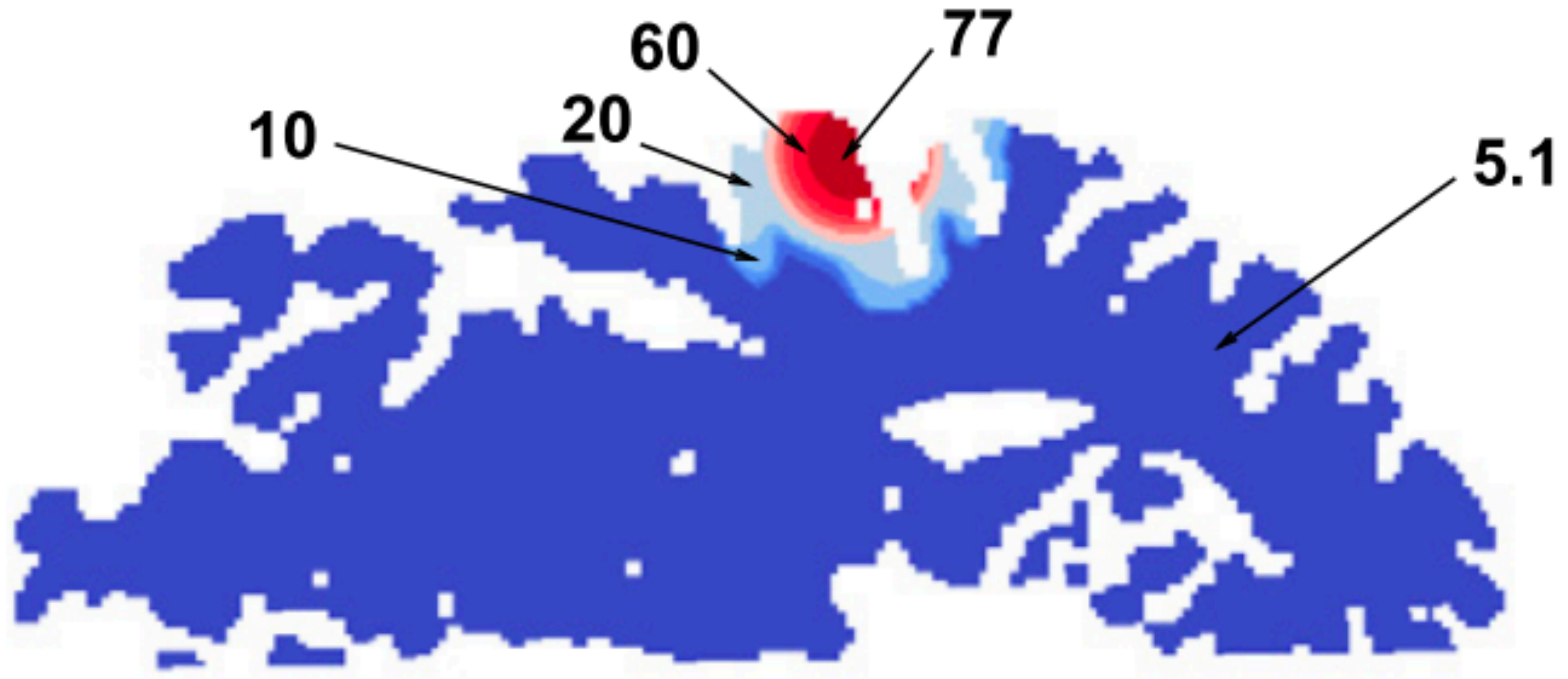
Human ischemic stroke in 3D (Dumont et al., 2013)

System of 15 reaction-diffusion PDEs, plus 4 reactions

$$y' = Ay + F(y),$$

ROCK4 for diffusion and RADAU5 for reaction.

Due to the explicit stabilized method no large linear system is solved and realistic simulations can be run on a workstation.



T. Dumont et al. / Commun Nonlinear Sci Numer Simulat 18 (2013) 1539–1557

Construction of explicit stabilized methods for $y' = f(y)$

1. Search for a family of polynomials $P_s : [-\omega_0, \omega_0] \to [-P_s(\omega_0), P_s(\omega_0)]$
2. with $P_s'(\omega_0)/P_s(\omega_0)$ large and increasing in s. Typically $P_s'(\omega_0)/P_s(\omega_0) = O(s^2)$.
3. Set $R_s(z) = P_s(\omega_0)^{-1} P_s\left(\omega_0 + \frac{P_s(\omega_0)}{P_s'(\omega_0)} z\right)$,
4. then $R_s(0) = R_s'(0) = 1$ and yields a first-order method.
5. Also, $|R_s(z)| \leq 1$ for $|z| \leq \ell_s := 2\omega_0 \dfrac{P_s'(\omega_0)}{P_s(\omega_0)} = O(s^2)$.
6. Find a Runge-Kutta method having $R_s(z)$ as stability polynomial.
   Warning: due to the high number of stages, internal stability is a concern.

Example: Runge-Kutta-Chebyshev (RKC) method

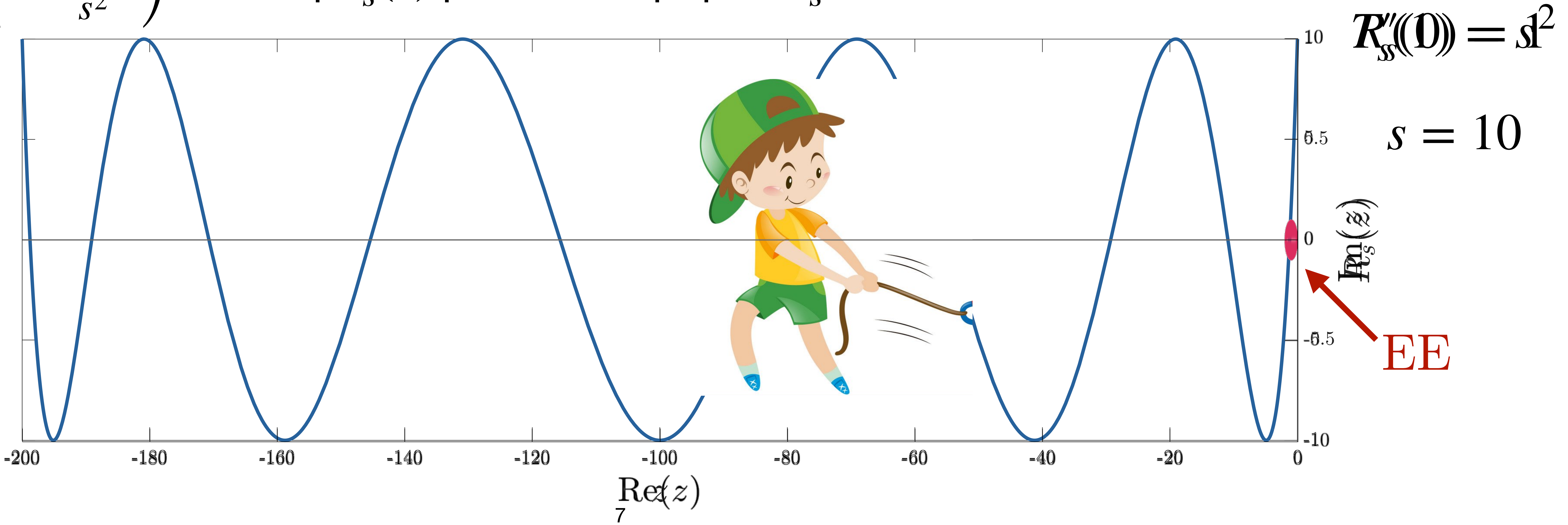
1. Let $\omega_0 = 1$ and consider Chebyshev polynomials

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

   that satisfy $T_s : [-1,1] \to [-1,1]$, $T_s(1) = 1$ and $T_s'(1) = s^2$.

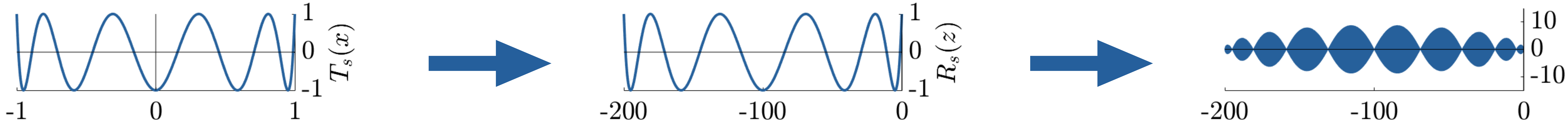
2. Hence $T_s'(1)/T_s(1) = s^2$

3. And $R_s(z) = T_s\left(1 + \frac{1}{s^2} z\right)$ with $|R_s(z)| \leq 1$ for $|z| \leq \ell_s = 2s^2$.

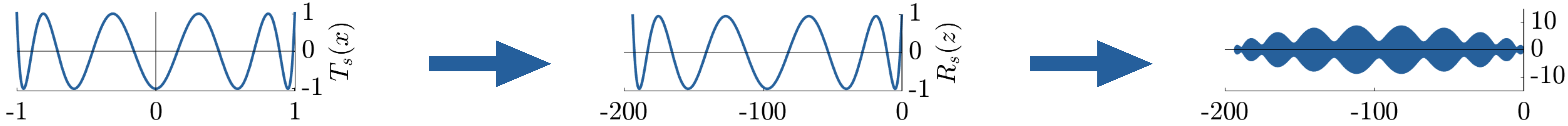


Considering different values for ω_0

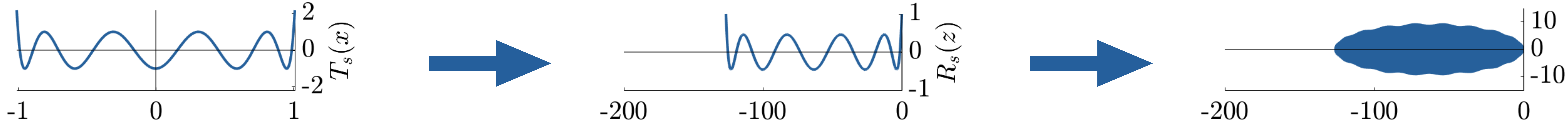
1. With $s = 10$, $\omega_0 = 1$:



2. With $s = 10$, $\omega_0 = 1 + \varepsilon/s^2, \varepsilon = 0.05$:

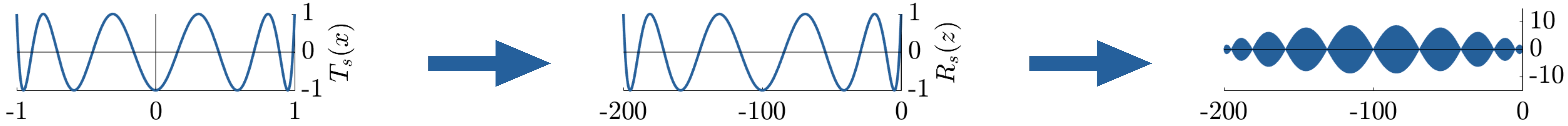


3. With $s = 10$, $\omega_0 = 1 + \varepsilon/s^2, \varepsilon = 1$:

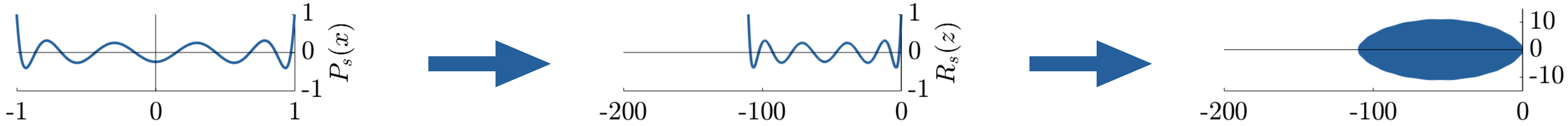


Considering different polynomials

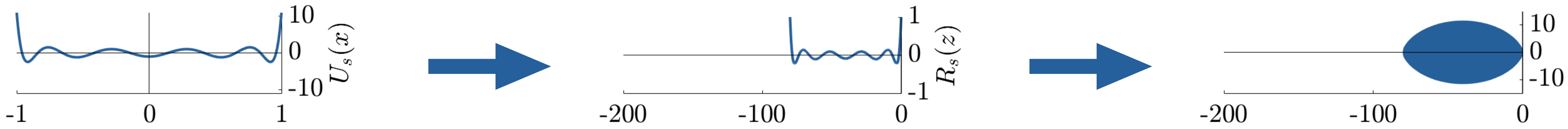
1. With $s = 10$, $\omega_0 = 1$ and first kind Chebyshev polynomials (RKC, 1980)



2. With $s = 10$, $\omega_0 = 1$ and Legendre polynomials (RKL, 2014)



3. With $s = 10$, $\omega_0 = 1$ and second kind Chebyshev polynomials (RKU, April 2022)



Explicit stabilized Runge-Kutta method

It remains to find a Runge-Kutta method with $R_s(z)$ as stability polynomial.

Explicit stabilized methods with good internal stability properties rely on the recursive formula (typical of orthogonal polynomials) for $P_s(x)$:

$$P_0(x) = 1, \quad P_1(x) = a_1 x, \quad P_n(x) = (a_n x + b_n) P_{n-1}(x) + c_n P_{n-2}(x)$$

Then a Runge-Kutta method

$$\begin{aligned} k_0 &= y_n, \qquad k_1 = k_0 + \mu_1 \Delta t\, f(k_0), \\ k_j &= \mu_j \Delta t\, f(k_{j-1}) + \nu_j\, k_{j-1} + \kappa_j\, k_{j-2}, \quad j = 2, \dots, s, \\ y_{n+1} &= k_s \end{aligned}$$

with $R_s(z)$ as stability polynomial exists.

Number of stages s is chosen according to $\Delta t \rho \le \ell_s$, with $\rho = \rho(\partial f / \partial y)$.

Parareal with explicit stabilized methods

The Parareal scheme for parallel in time integration is:

- Compute a first coarse solution $\{y_n^0\}_{n=0}^N$

  $$y_{n+1}^0 = G(y_n^0, t_n, t_{n+1}),$$

  with G providing a rough approximation of $y(t_{n+1})$, with $y' = f(y)$, $y(t_n) = y_n^0$.

- Iterate and correct the solutions:

  $$\begin{aligned} y_{n+1}^{k+1} = F(y_n^k, t_n, t_{n+1}) \\ +G(y_n^{k+1}, t_n, t_{n+1}) - G(y_n^k, t_n, t_{n+1}), \end{aligned}$$

  with F providing a fine approximation.

We define the propagators F, G as RKC schemes (Chebyshev polynomials), where

- $G(y_n, t_n, t_{n+1})$ employs step size Δt_c and the number of stages s_c is chosen according to $\Delta t_c \rho \leq \ell_s \approx 2s^2$.
- $F(y_n, t_n, t_{n+1})$ employs step size $\Delta t_f \ll \Delta t_c$. Number of stages s_f is according to $\Delta t_f \rho \leq \ell_s$.

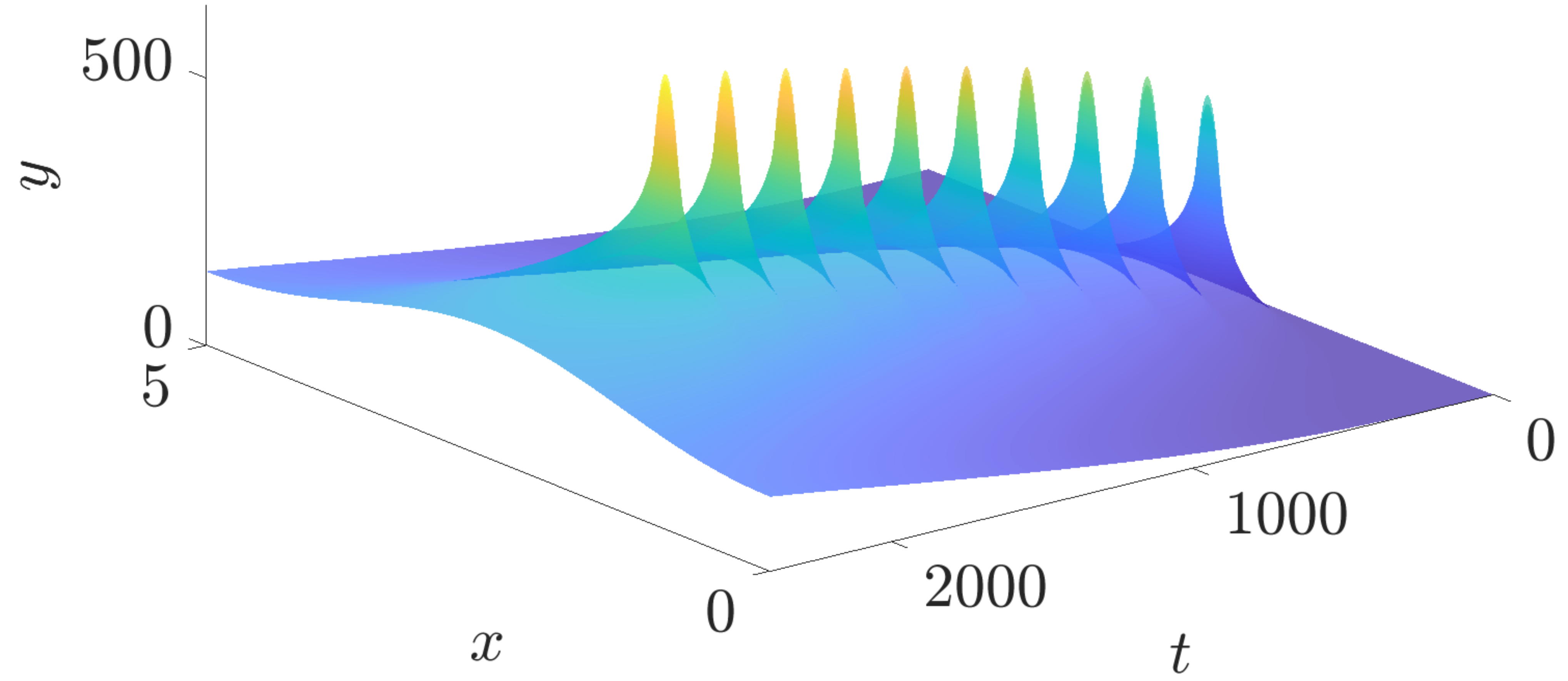
Similar PinT schemes are defined using RKL (Legendre) or RKU (second kind Chebyshev).

Numerical experiment: heat equation

Consider $\Omega = [0,5]cm$, $T = 2400ms$ and

$$\begin{aligned} \partial_t y &= \nu \Delta y + I_s(t), && \text{in } \Omega \times [0,T] \\ \nabla y \cdot \mathbf{n} &= 0, && \text{on } \partial\Omega \times [0,T], \\ y &= 0, && \text{in } \Omega \times \{0\}, \end{aligned}$$

$\nu = 10^{-3}$ and $I_s(t)$ a stimulus.



We discretise with FD and $\Delta x = 0.01$, then solve the problem with

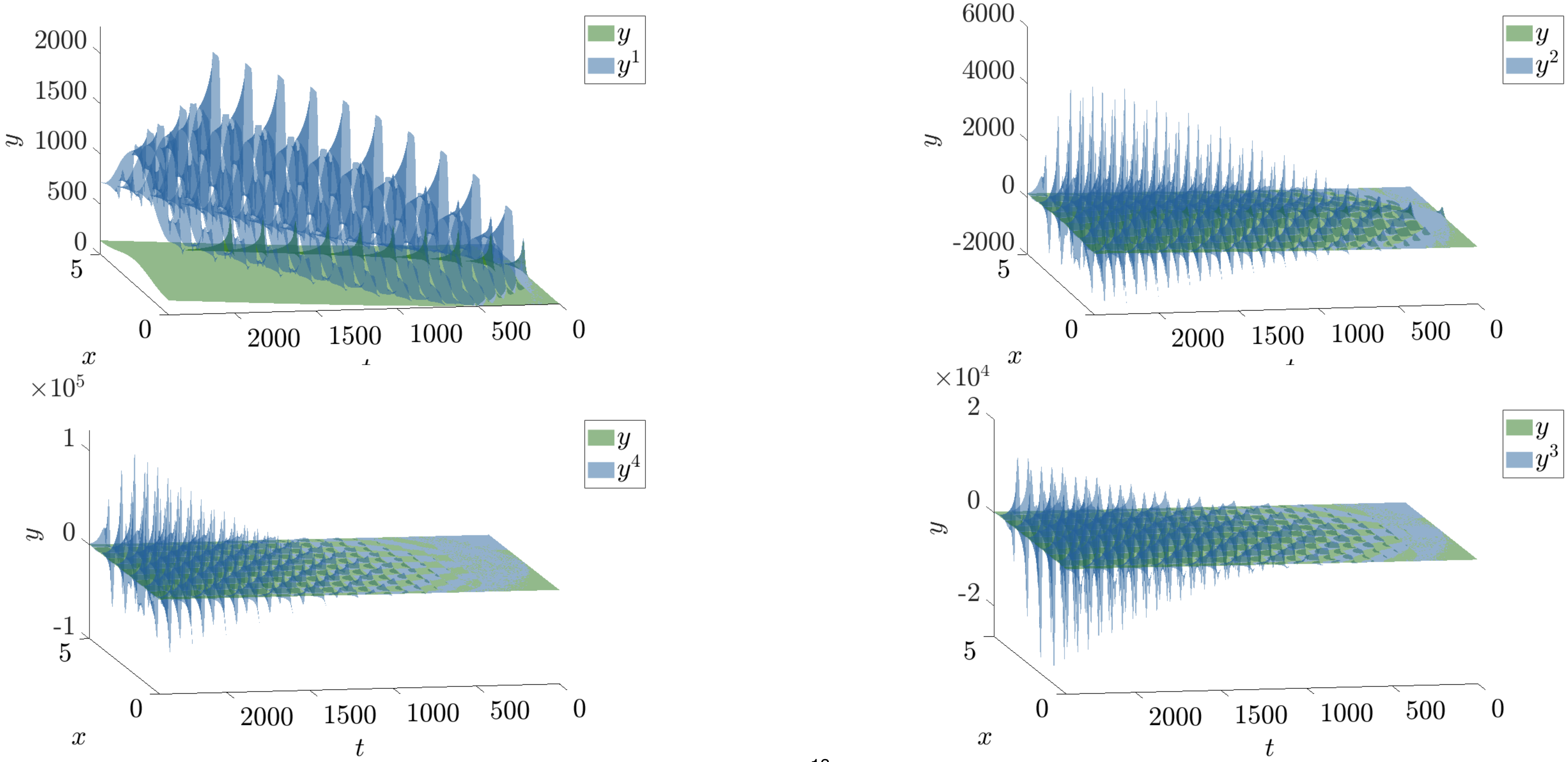
- $N = 24$ threads,
- $\Delta t_c = T/N = 100ms$,
- $\Delta t_f = 0.1ms$.

Note:

- For explicit Euler $\Delta t \leq 0.05$,
- Implicit Euler do not capture the stimulus.

PinT-RKC on heat equation

We set $\omega_0 = 1 + \varepsilon/s^2$, $\varepsilon = 0.05$. The number of stages are $s_c = 47$, $s_f = 2$.



Parareal convergence factor

From the results of

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Vol. 29, No. 2, pp. 556–578

ANALYSIS OF THE PARAREAL TIME-PARALLEL TIME-INTEGRATION METHOD*

MARTIN J. GANDER[†] AND STEFAN VANDEWALLE[‡]

We know that the convergence factor of Parareal is

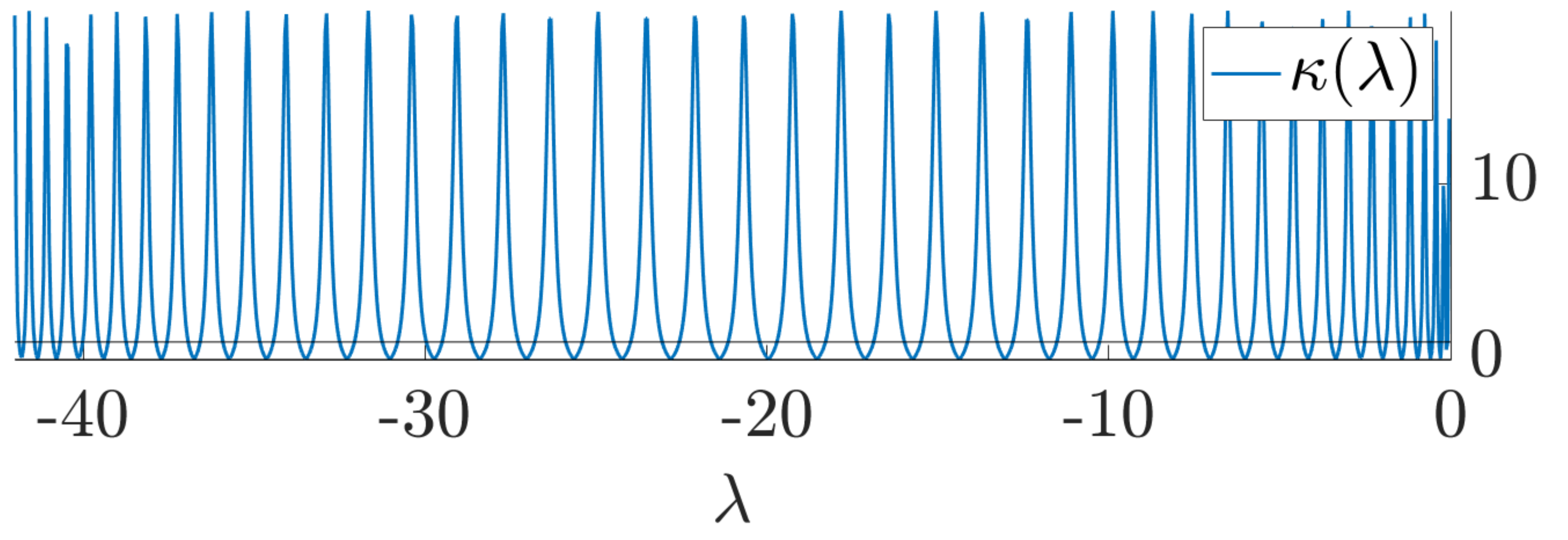
$$\kappa(\lambda) = \frac{|R_f(\Delta t_f \lambda) - R_c(\Delta t_c \lambda)|}{1 - |R_c(\Delta t_c \lambda)|}$$

Here

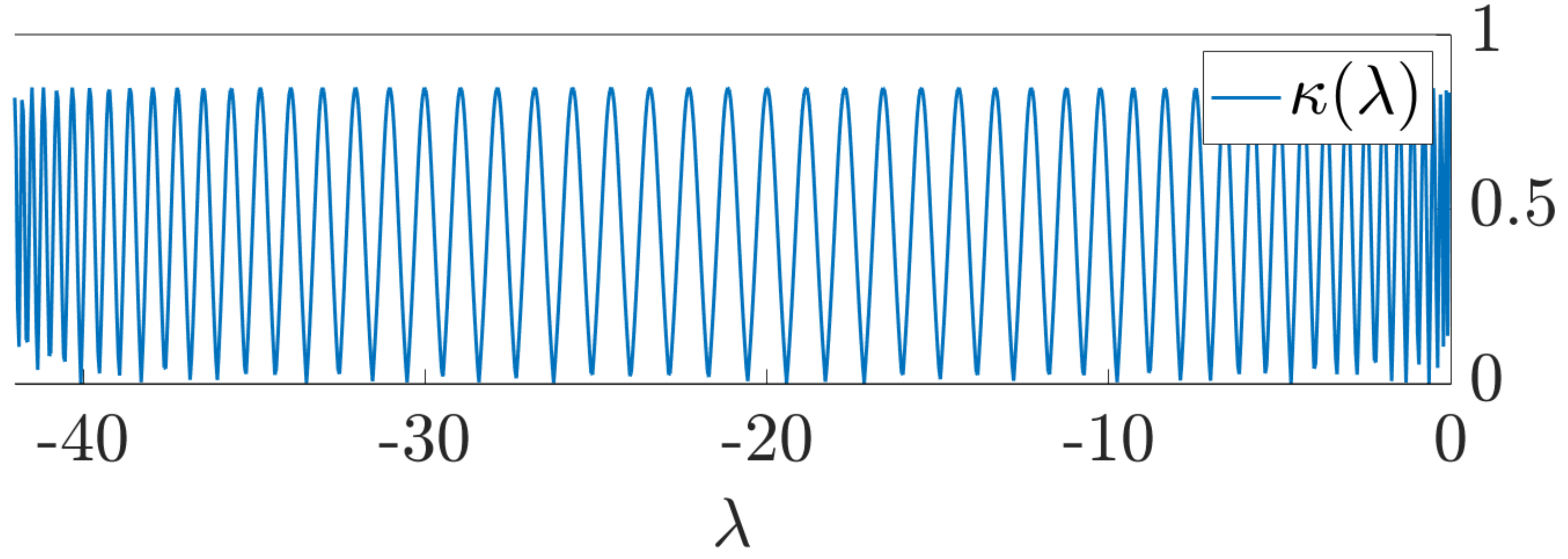
$$R_c(z) = R_{s_c}(z) \quad \text{and} \quad R_f(z) = R_{s_f}(z)^{\Delta t_c/\Delta t_f}.$$

PinT-RKC convergence factor

The convergence factor of RKC with $\omega_0 = 1 + \varepsilon/s^2$, $\varepsilon = 0.05$ is:

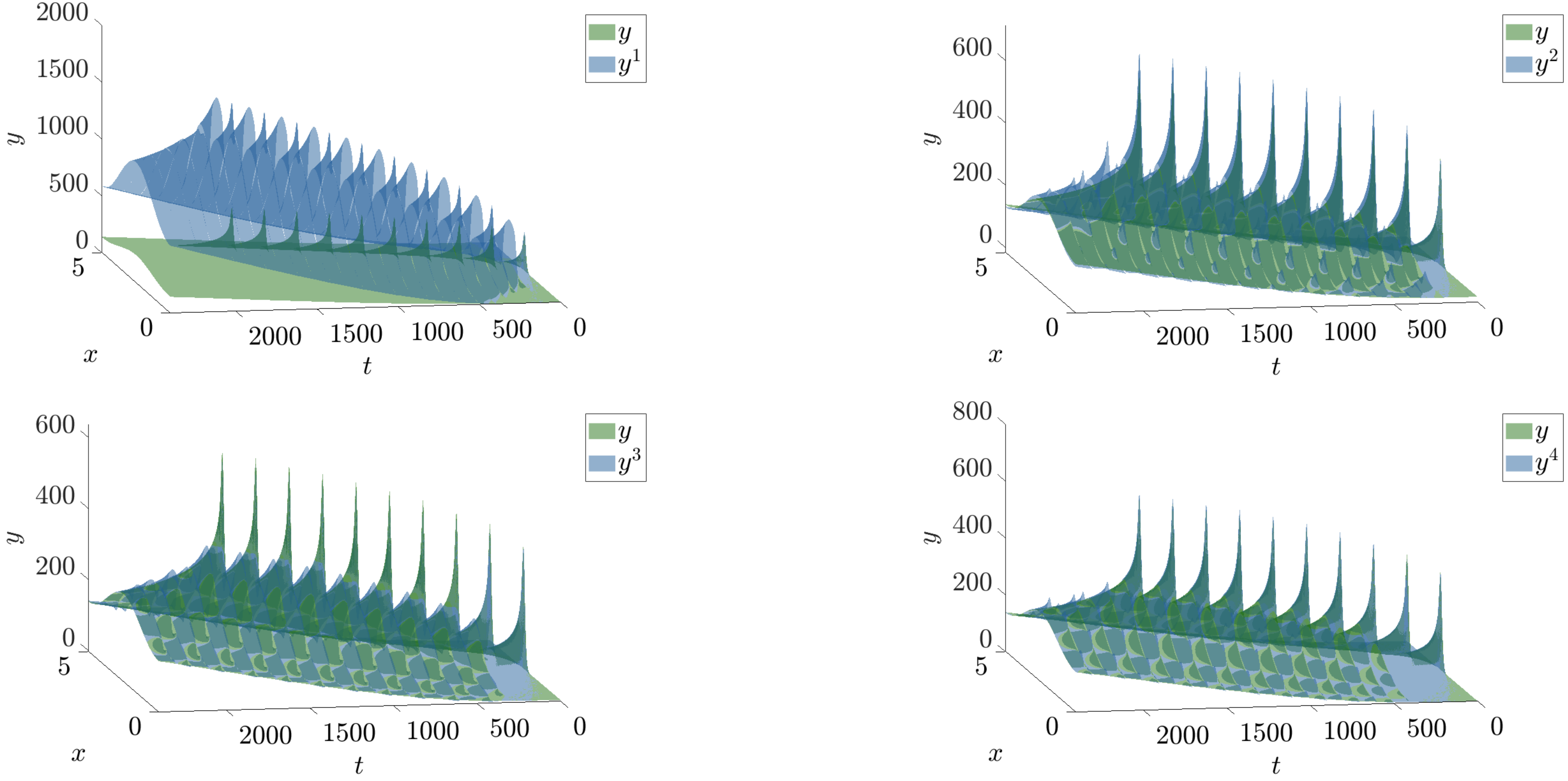


The convergence factor of RKC with $\omega_0 = 1 + \varepsilon/s^2$, $\varepsilon = 1$ is:



PinT-RKC on heat equation

We set $\omega_0 = 1 + \varepsilon/s^2$, $\varepsilon = 1$. The number of stages are $s_c = 58$, $s_f = 2$.



Numerical experiment: Monodomain model

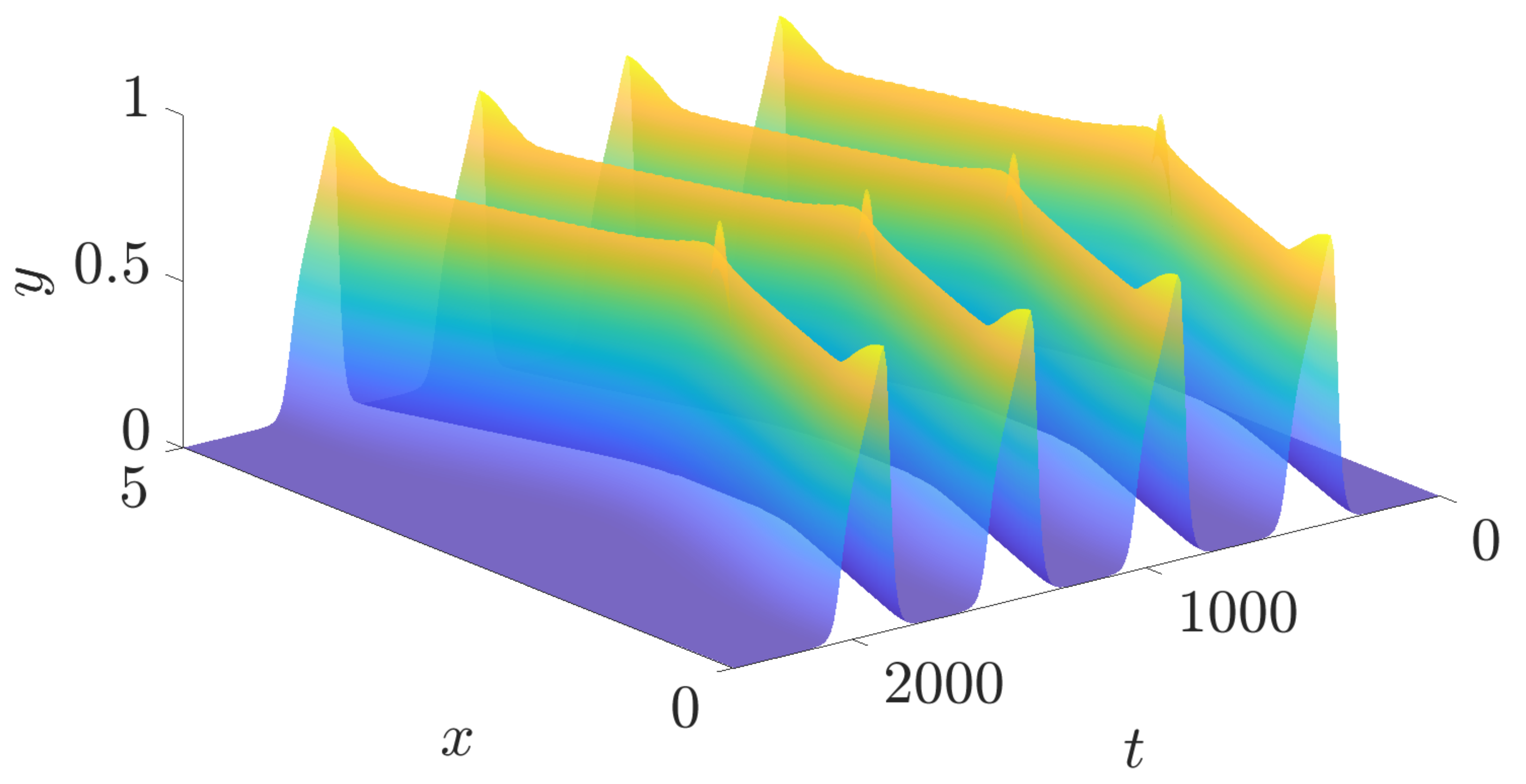
Consider $\Omega = [0,5]cm$, $T = 2400ms$ and

$$
\begin{aligned}
\partial_t y &= \nu \Delta y - I_{ion}(y,z) + I_s(t), && \text{in } \Omega \times [0,T] \\
z' &= g(y,z), && \text{in } \Omega \times [0,T] \\
\nabla y \cdot \mathbf{n} &= 0, && \text{on } \partial\Omega \times [0,T], \\
y &= 0, && \text{in } \Omega \times \{0\}, \\
z &= 0, && \text{in } \Omega \times \{0\},
\end{aligned}
$$

$\nu = 10^{-3}$, $I_s(t)$ a stimulus, I_{ion}, g an ionic model and z its state variables:

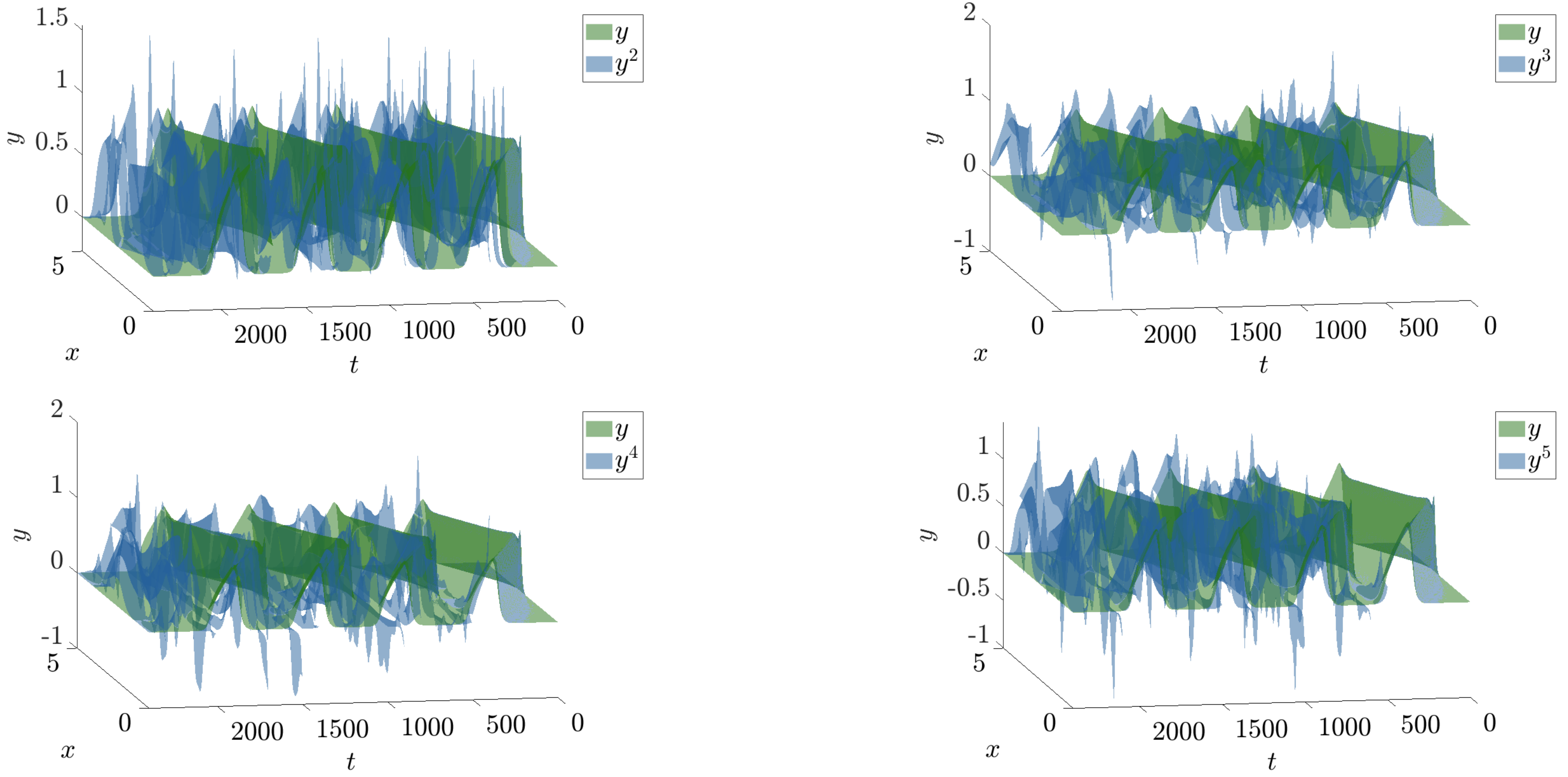
$$
\begin{aligned}
I_{ion}(y,z) &= -a_1 y(y-a_2)(1-y) + a_3 yz, \\
g(y,z) &= b_1(y - b_2 z)\,.
\end{aligned}
$$

We again discretise with FD and solve the problem with $N = 24$ threads, $\Delta t_c = 100ms$, $\Delta t_f = 0.1ms$.



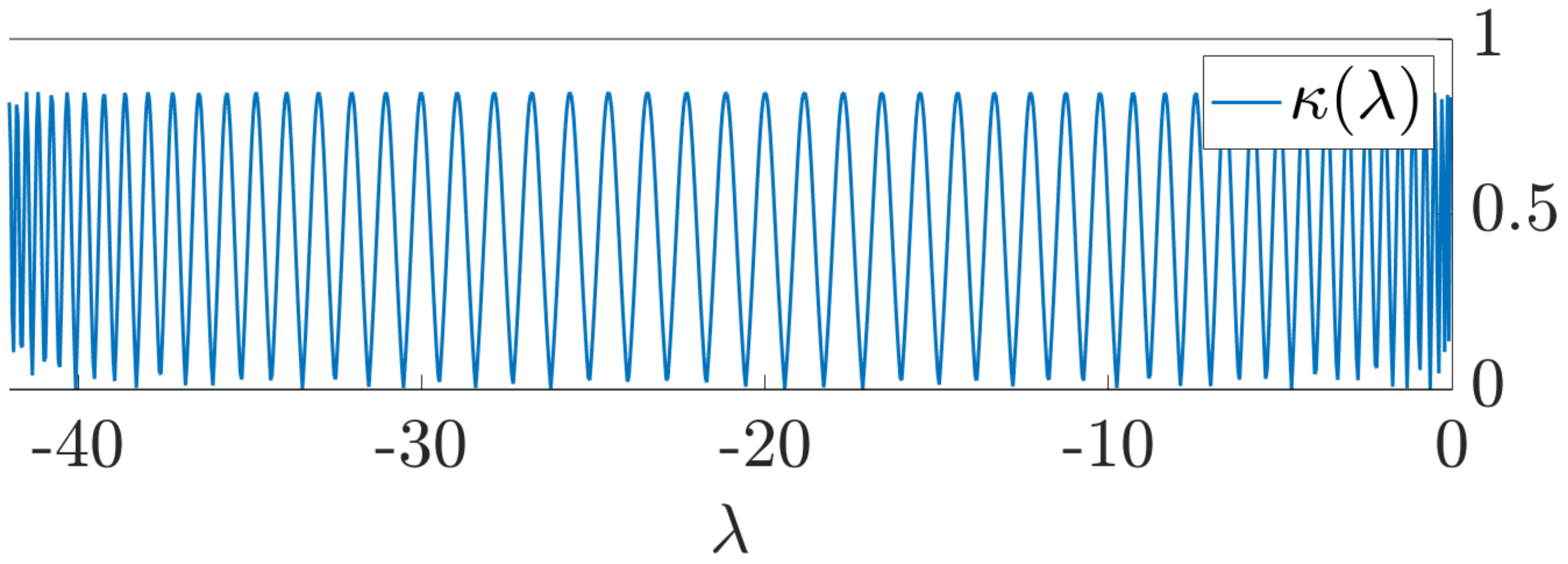
PinT-RKC on Monodomain model

We set $\omega_0 = 1 + \varepsilon/s^2$, $\varepsilon = 1$. The number of stages are $s_c = 58$, $s_f = 2$.

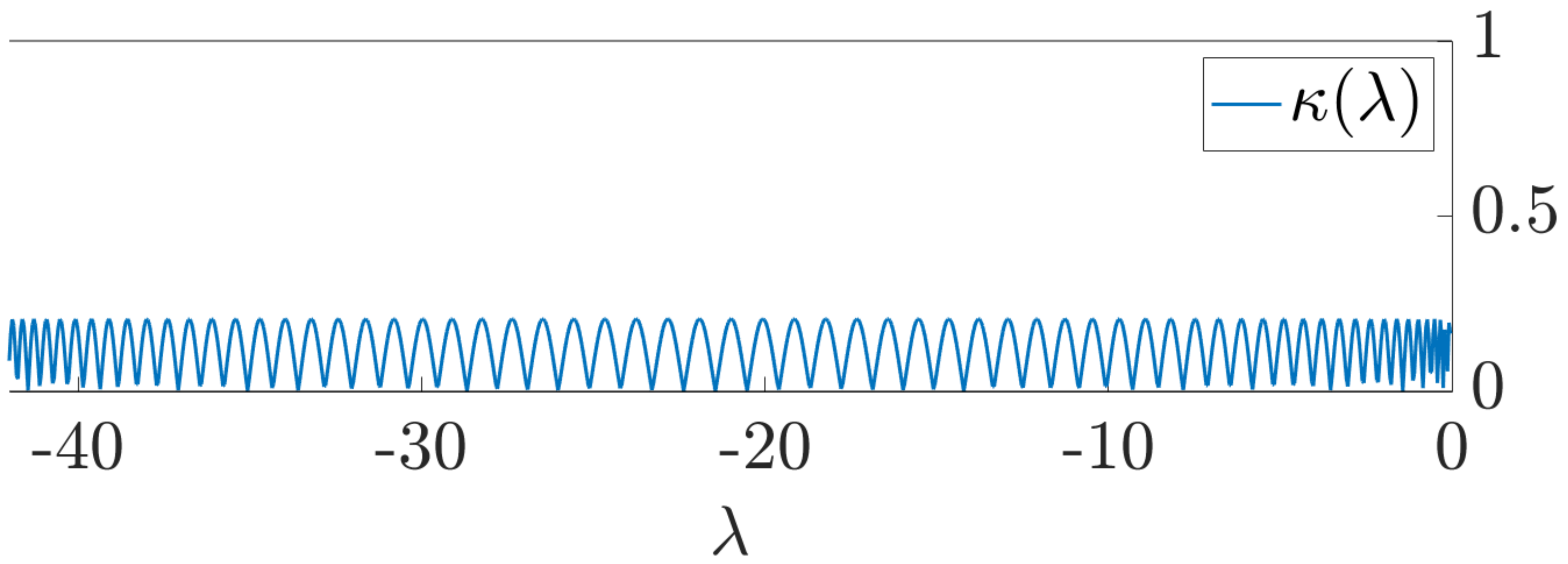


PinT-RKC convergence factor

The convergence factor of RKC with $\omega_0 = 1 + \varepsilon/s^2$, $\varepsilon = 1$ is:

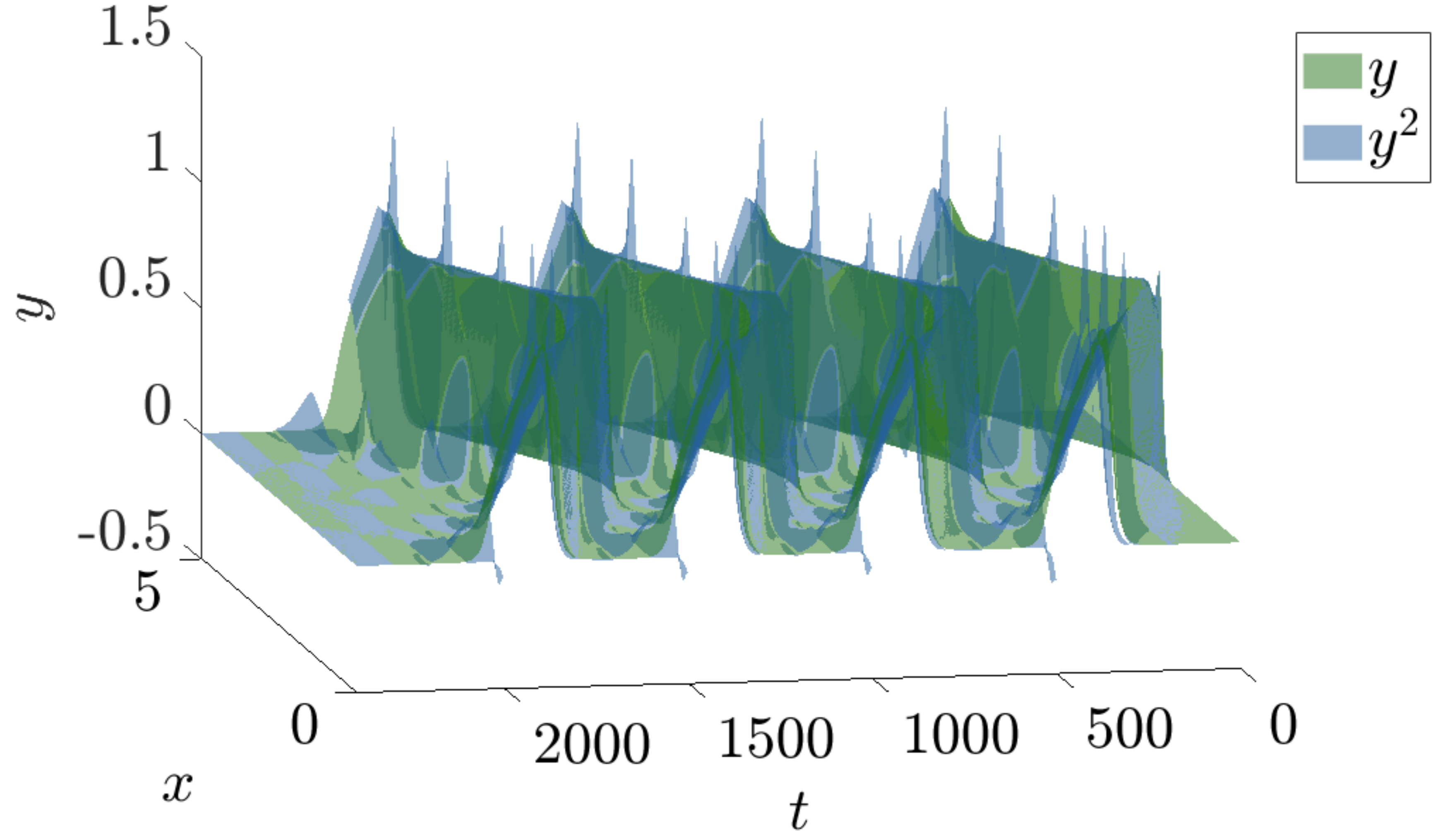


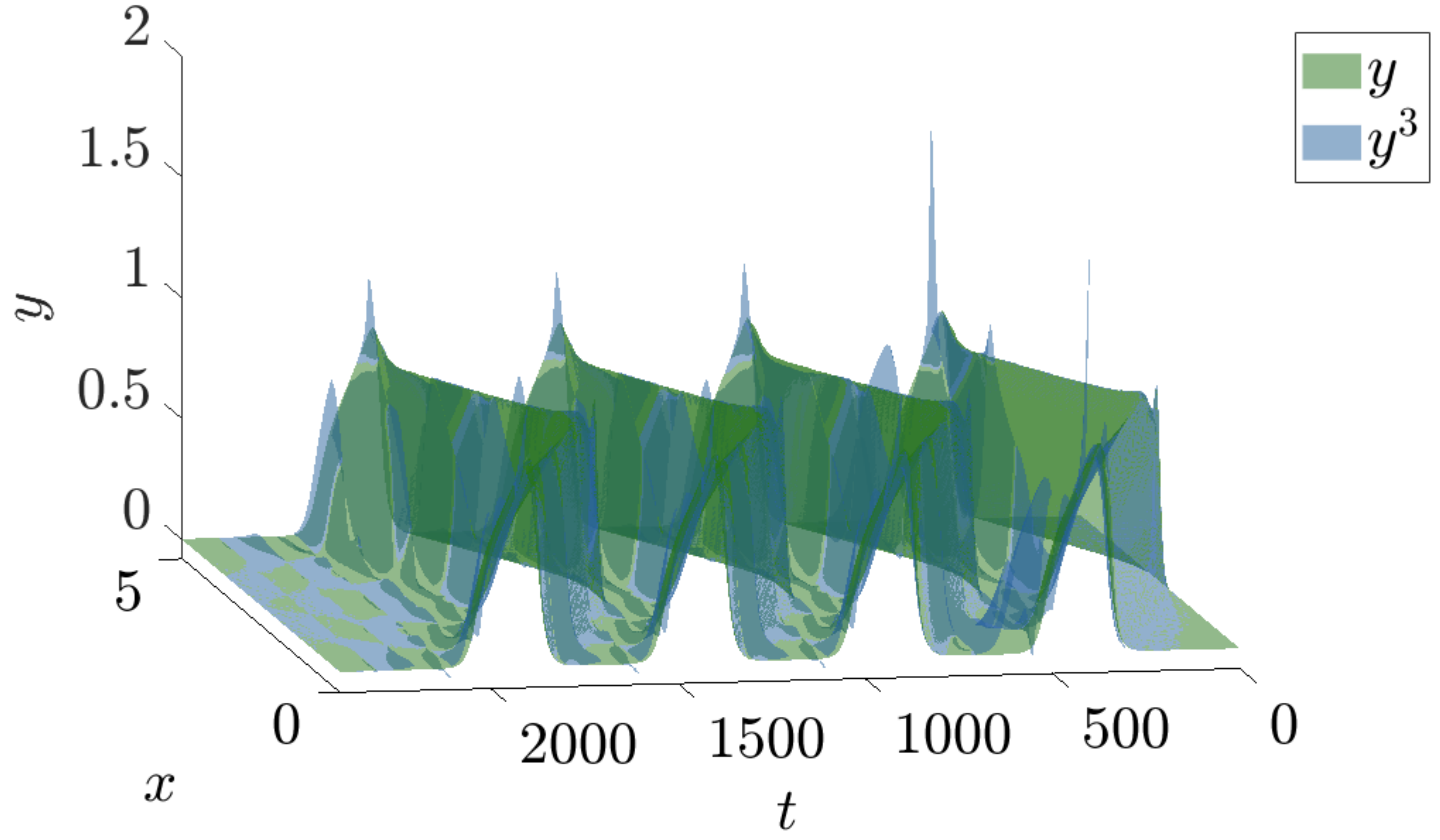
The convergence factor of RKC with $\omega_0 = 1 + \varepsilon/s^2$, $\varepsilon = 3$ is:

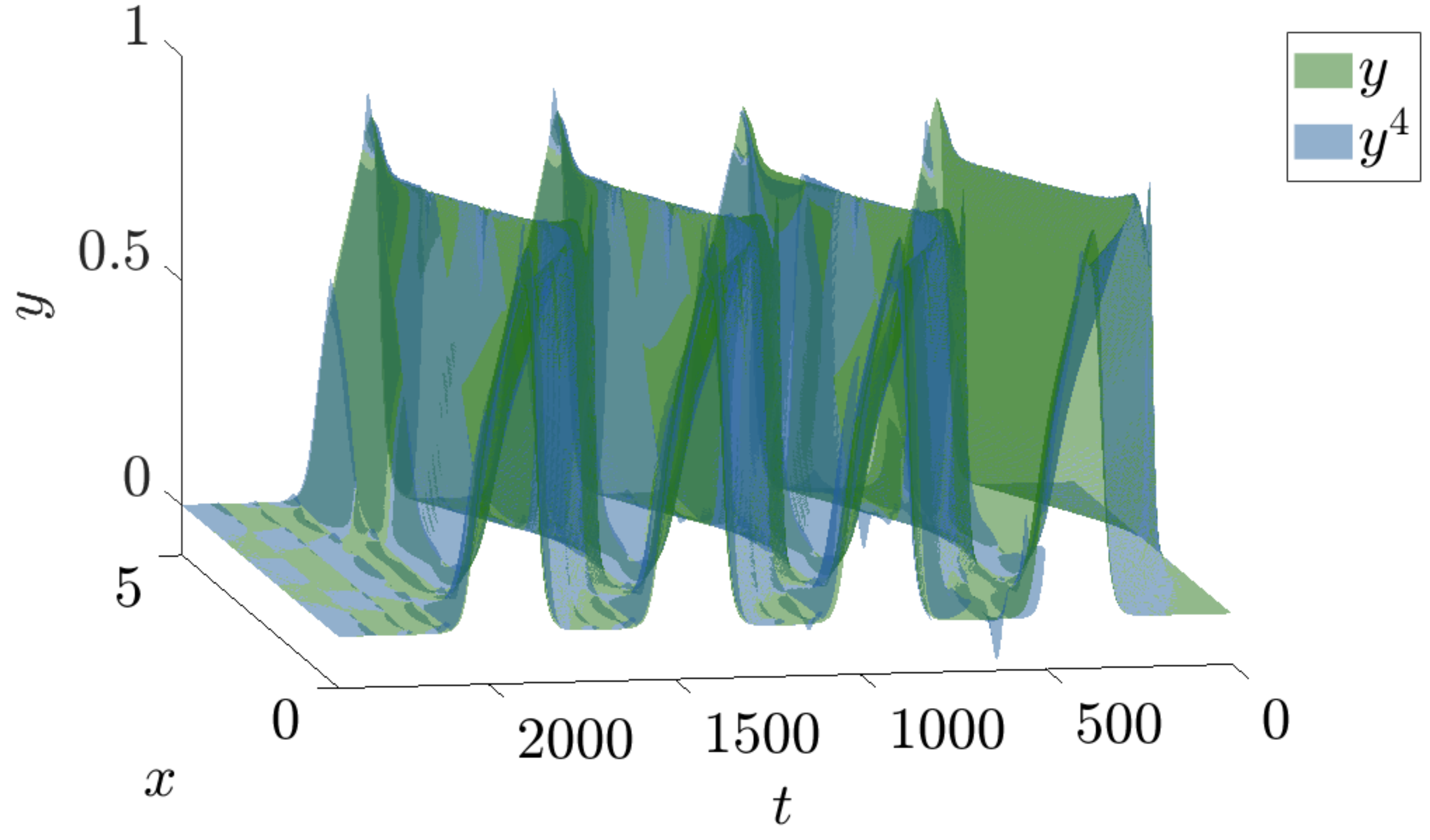


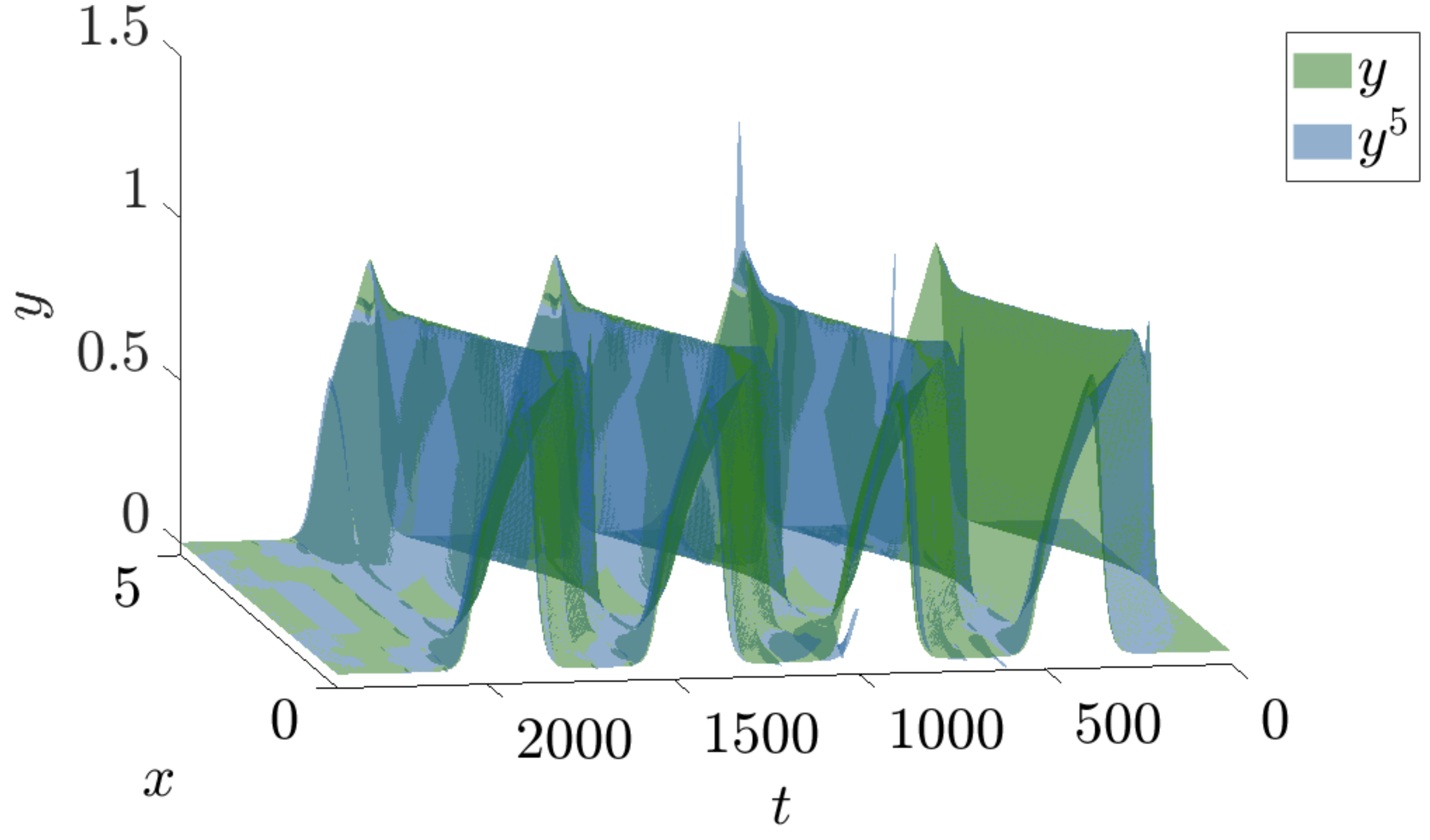
PinT-RKC on Monodomain model

We set $\omega_0 = 1 + \varepsilon/s^2$, $\varepsilon = 3$. The number of stages are $s_c = 73$, $s_f = 2$.



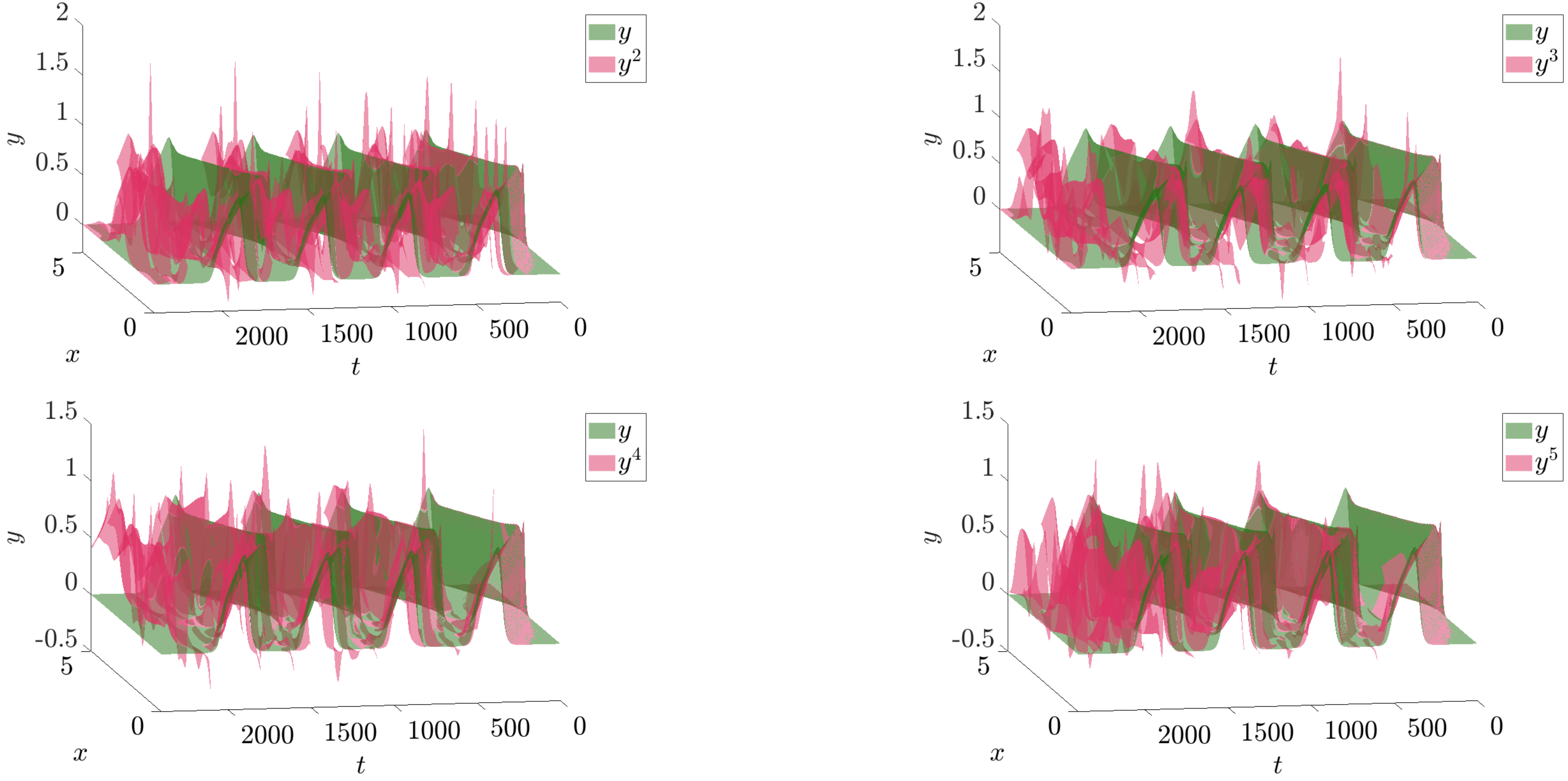






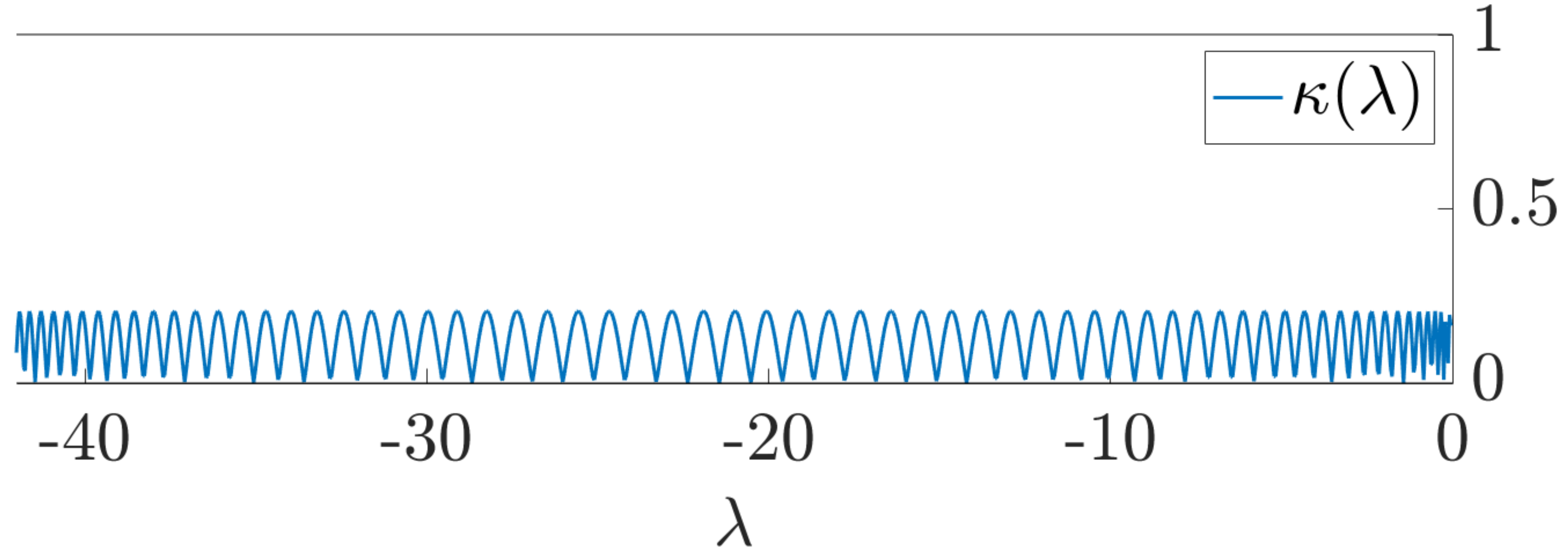
PinT-RKL on Monodomain model

We set $\omega_0 = 1$. The number of stages are $s_c = 73$, $s_f = 2$.

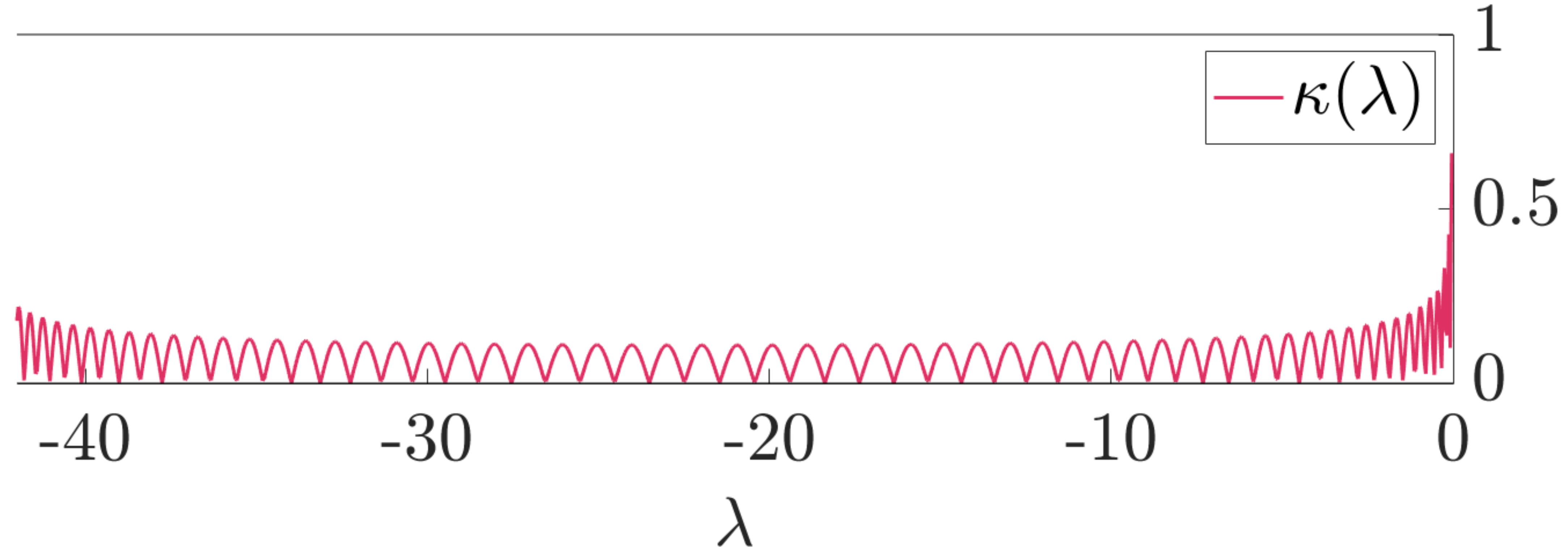


PinT-RKC and RKL convergence factors

The convergence factor of RKC with $\omega_0 = 1 + \varepsilon/s^2$, $\varepsilon = 3$ is:

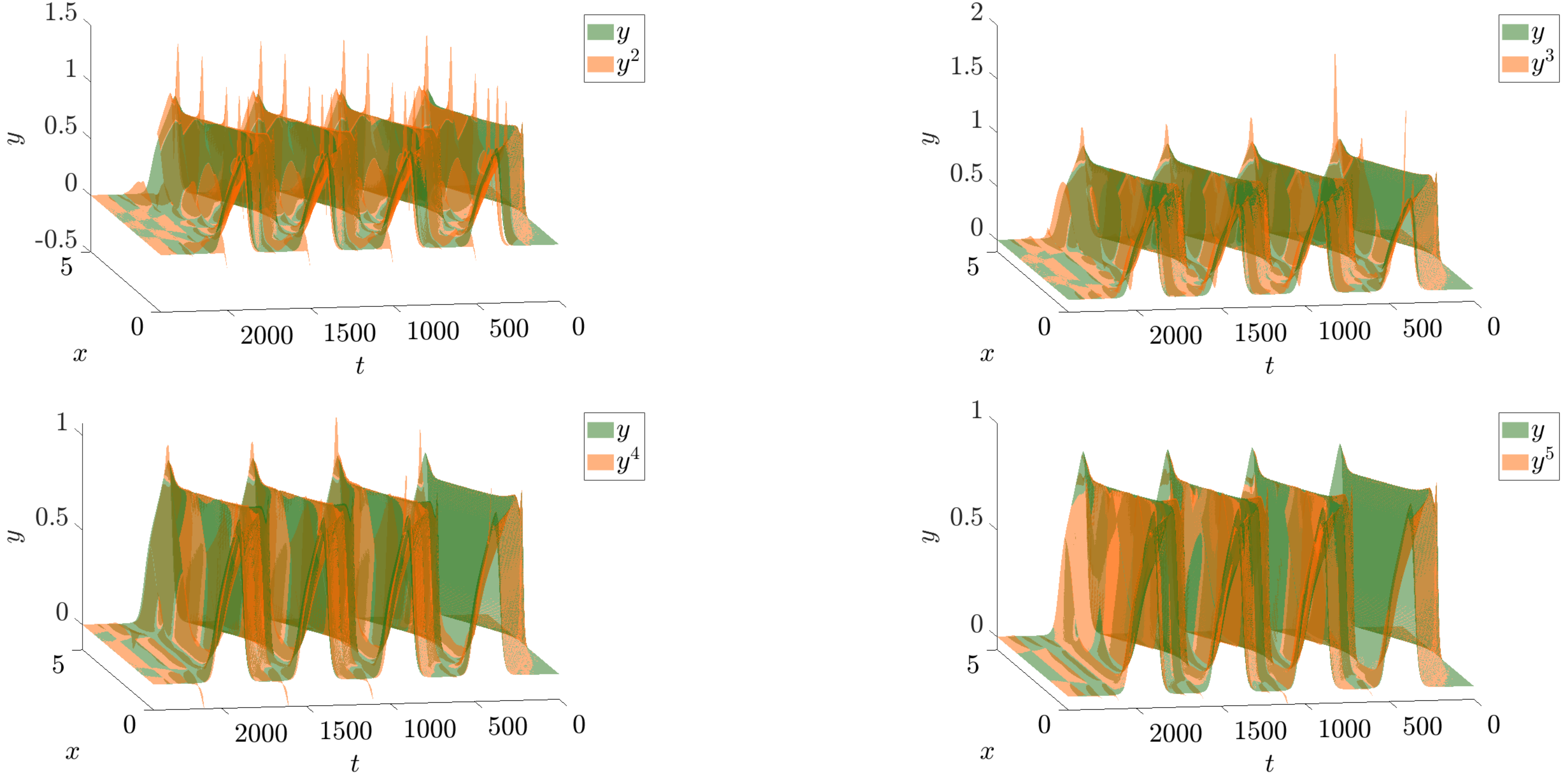


The convergence factor of RKL with $\omega_0 = 1$ is:



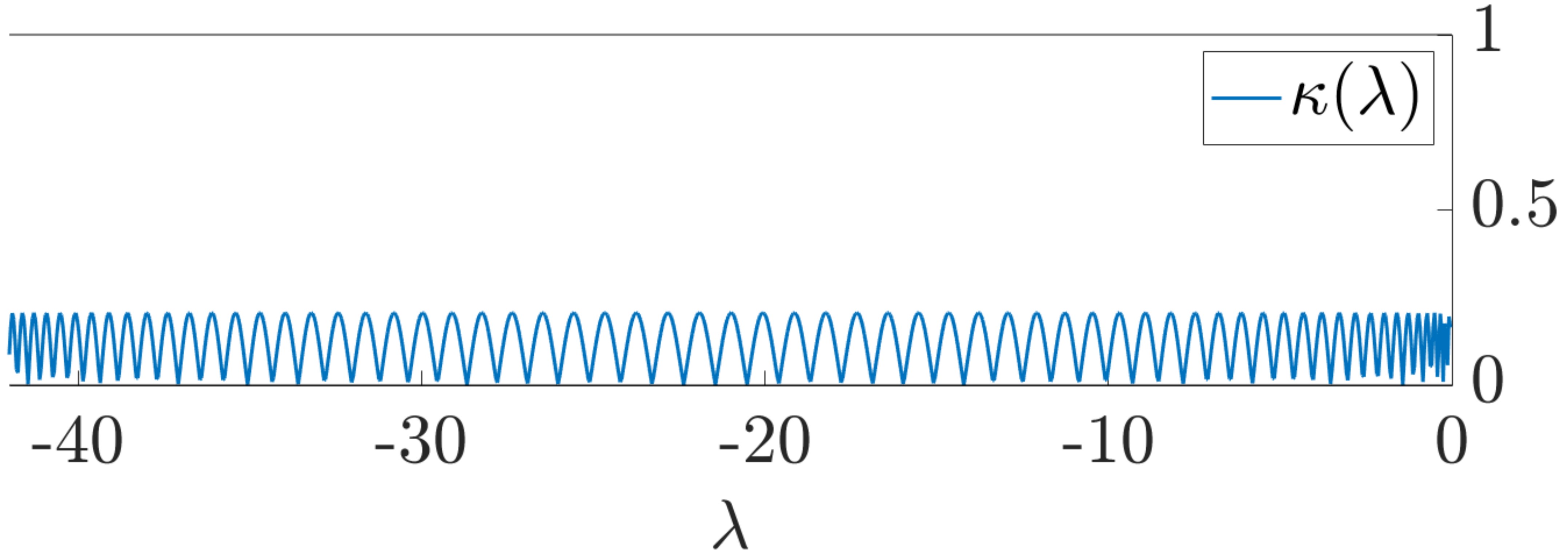
PinT-RKU on Monodomain model

We set $\omega_0 = 1$. The number of stages are $s_c = 79$, $s_f = 2$.

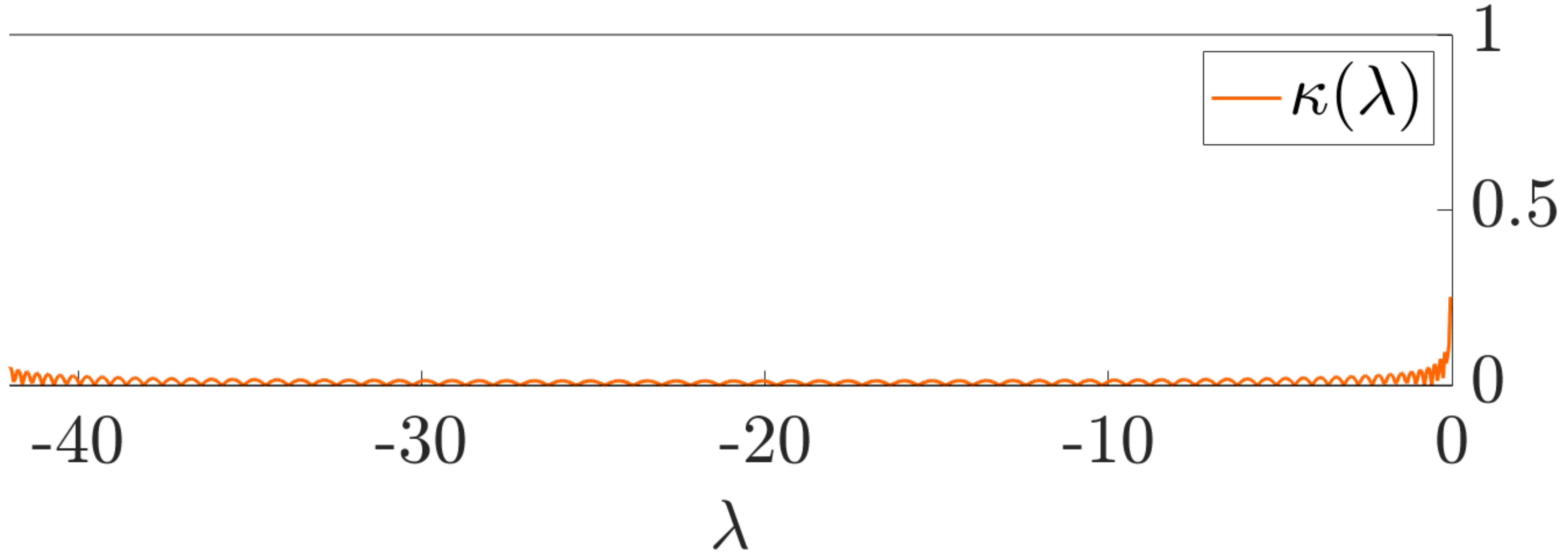


PinT-RKU convergence factor

The convergence factor of RKC with $\omega_0 = 1 + \varepsilon/s^2$, $\varepsilon = 3$ is:



The convergence factor of RKU with $\omega_0 = 1$ is:



TODOs

- Better understanding of stability properties of PinT explicit stabilized methods,
- Maybe consider different correction formula than $G(y_n^{k+1}, t_n, t_{n+1}) - G(y_n^k, t_n, t_{n+1})$?
- Ionic model I_{ion}, g is in general multiscale and stiff. Consider Rush-Larsen for some ionic variables.
- Not all stiffness is removed by Rush-Larsen. Hence we can consider a multirate version of explicit stabilized methods:

1. Replace $f(y) = f_S(y) + f_F(y)$ with a less stiff

$$f_\eta(y) = f_S(y) + \frac{1}{\eta}\int_0^\eta f_F(u)\mathrm{d}s = \frac{1}{\eta}(u(\eta) - y),$$

with $u' = f_S(y) + f_F(u)$, $u(0) = y$.

2. Solve $y' = f_\eta(y)$ instead of $y' = f_S(y) + f_F(y)$.

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Thank you!

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