Rational function surrogate modeling for the optimal control of parabolic systems

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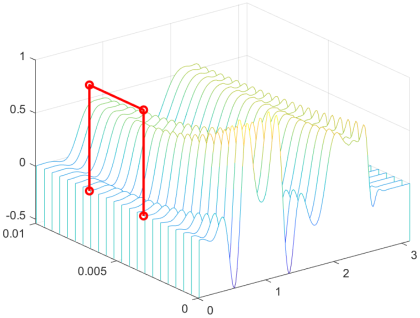
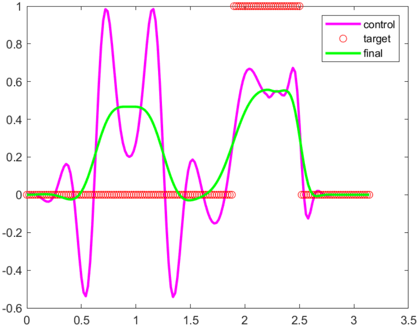
Outline in pictures





Controlability of dynamical systems I

Abstract parabolic problem

$$\begin{cases} y'(t) = Ay(t) + f(t), & t > 0, \\ y(0) = u. \end{cases} \tag{1}$$

Here,

- $\mathcal{H}$ is a Hilbert space and A is upper-bounded self–adjoint with an upper bound κ
- $(S_t)_{t \geq 0}$ is the semigroup generated by A, see (Engel and Nagel, 2000).

Problem (1) has the mild solution given by

$$y(t) = S_t u + \int_0^t S_\tau f(t - \tau) \mathrm{d}\tau, \quad t \geq 0.$$

Controlability of dynamical systems II

Controlability

We say that the system (1) is controllable to a target state $y^* \in \mathcal{H}$ in time $T > 0$ if there is $u \in \mathcal{H}$ such that

$$S_T u = y^* - \int_0^T S_\tau f(T - \tau)\mathrm{d}\tau.$$

Approximate controlability

We say that the system (1) is approximately controllable in time $T > 0$ if for all $y^* \in \mathcal{H}$ and all $\varepsilon > 0$ there exists $u \in \mathcal{H}$ such that

$$\|S_T u + \int_0^T S_\tau f(T - \tau)\mathrm{d}\tau - y^*\| \leq \varepsilon. \tag{2}$$

Optimization problem

Quadratic cost function

for ε, $T > 0$ and $y^* \in \mathcal{H}$ we introduce the problem

$$\min_{u \in \mathcal{H}} \left\{ J(u) \colon \|S_T u + \int_0^T S_\tau f(T-\tau)\mathrm{d}\tau - y^*\| \leq \varepsilon \right\} \tag{3}$$

where

$$J(u) = \frac{\alpha}{2}\|u\|^2 + \frac{1}{2}\int_0^T \beta(t) \left\| S_t u + \int_0^t S_\tau f(t-\tau)\mathrm{d}\tau - w(t) \right\|^2 \mathrm{d}t.$$

Here

- $\alpha > 0$ and $\beta \in L^\infty((0,T);[0,\infty))$ are weights of the cost
- $w \in L^2((0,T);\mathcal{H})$ is the target trajectory

Turning on the constraints I

Problem (3) can be restated as

$$\min_{u\in\mathcal{H}} \left\{ J(u) + I_{\bar{B}}\left(\mathcal{S}_T u + \int_0^T S_\tau f(T-\tau)\mathrm{d}\tau\right)\right\}, \tag{4}$$

where $\bar{B}$ stands for the closure of the ball $B_\varepsilon(y^*)$ of radius ε and center y^*, and $I_{\bar{B}}$ is the corresponding *indicator function* defined as

$$I_{\bar{B}}(y) = \begin{cases} 0 & \text{if } y \in \bar{B}, \\ +\infty & \text{else.} \end{cases}$$

Solvability

The function $u \to J(u) + I_{\bar{B}} \circ (\mathcal{S}_T u + \int_0^T S_\tau f(\tau)\mathrm{d}\tau)$ is proper, strongly convex and lower-semicontinuous, problem (3) has a unique solution, which we denote by u^{opt} (see, for instance, Peypouquet, 2015, Corollary 2.20).

Turning on the constraints II

Some further definitions

- The solution to the corresponding unconstrained problem

$$u^{\min} = \operatorname*{arg\,min}_{u \in \mathcal{H}} J(u),$$

- by

$$y^{\min} = S_T u^{\min} + \int_0^T S_\tau f(T-\tau)\mathrm{d}\tau$$

$$y^{\mathrm{opt}} = S_T u^{\mathrm{opt}} + \int_0^T S_\tau f(T-\tau)\mathrm{d}\tau$$

we denote optimal states obtained from $u^{\min}$ and u^{opt}, respectively.

Our approach

Joint work

Joint work with: I. Nakić, M. Lazar and M. Tautenhan.

- Our approach is an extension of the result from (Lazar, Molinari, and Peypouquet, 2017)
- We add stability analysis based on resolvent calculus
- Numerical resolvent calculus

RKFun

Further, we discuss the relationship between numerical rational function's calculus based on rational Krylov subspace representation (Berljafa and Güttel, 2017) and the approximation problem for the generalized exponential functions which appear as central for the study of the concrete numerical examples.

The main result I

Theorem

Let $T, \varepsilon > 0$, $y^* \in \mathcal{H}$. Then the optimal initial state u^{opt} is given by

$$u^{\mathrm{opt}} = (\mu^{\varepsilon} S_{2T} + \Psi)^{-1}(\mu^{\varepsilon} S_T y^{*,\mathrm{hom}} + \psi), \tag{5}$$

where

$$\Psi = \alpha\,\mathsf{Id} + \int_0^T \beta(t) S_{2t} \mathrm{d}t, \quad \psi = \int_0^T \beta(t) S_t w^{\mathrm{hom}}(t) \mathrm{d}t,$$

and $\mu^{\varepsilon} \geq 0$ is the unique solution of $\Phi(\mu) = \varepsilon$ for $\varepsilon < \|\Psi^{-1} S_T \psi - y^{*,\mathrm{hom}}\|$, and zero otherwise. Here $\Phi\colon [0,\infty) \to [0,\infty)$ is the function defined by

$$\Phi(\mu) = \|y^{*,\mathrm{hom}} - (\mu S_{2T} + \Psi)^{-1}(\mu S_{2T} y^{*,\mathrm{hom}} + S_T \psi)\|. \tag{6}$$

The main result II

Piece-wise constant constraints

For β the indicator function of the interval $[T_1, T_2]$, we have

$$\int_0^T \beta(t) S_t \, dt = A^{-1}(S_{T_2} - S_{T_1}) = \int \frac{e^{T_2 \lambda} - e^{T_1 \lambda}}{\lambda} \, dE(\lambda) \, .$$

Here $E(\cdot)$ is the spectral measure of the self-adjoint operator A.

Perturbed exponential functions

Functions g which can be represented as

$$g(x) = u_0(x) + u_1(x) \mathrm{e}^{ax}$$

where u_0 and $u_1 \neq 0$ are arbitrary rational functions and $a < 0$, are called perturbed exponential functions

Spectral calculus

Given a rational function r and a measurable function g we have

$$(v, g(A)v) - (v, r(A)v) = \int_{-\infty}^{0} \big(g(\lambda) - r(\lambda)\big)\, \mathrm{d}(E(\lambda)v, v), \tag{7}$$

where $E(\cdot)$ is the spectral measure (Reed and Simon, 1979; Kato, 1995). Then

$$\|g(A) - r(A)\|_{\mathcal{L}(\mathcal{H})} \leq \|g - r\|_{L^\infty\langle-\infty,0]}.$$

Best rational approximation

There exists a unique real rational function r_n^* such that

$$r_n^* = \arg\min\{\|g - r\|_{L^\infty} \ : \ r \text{ is a type } (n,n) \text{ rational function}\}$$

and further

$$\|g - r_n^*\|_{L^\infty} \leq CH^{-n}$$

where $C > 0$ is a constant independent of n and $H \approx 9.29$ is the Halphen constant, (Cody, Meinardus, and Varga, 1969; Walsh, 1931)

Constructing rational approximations I

For a continuous function f, and a contour Γ enclosing a point $z \in \mathbb{C}$ we have

$$f(z) = \frac{1}{2\pi \mathrm{i}} \int_\Gamma \frac{f(s)}{(s-z)}\, ds \approx \sum_{i=1}^{N} \omega_i \frac{f(s_i)}{s_i - z}$$

Quadratures turn Cauchy integrals into rational functions

Take

$$r(z) = \sum_{i=1}^{N} \omega_i \frac{f(s_i)}{s_i - z}$$

as a rational function surrogate.

- Start from trapezoid rule on an interval
- For infinite intervals use Moebius transforms (rational functions!)
- Talbot quadratures, Carathéodory-Fejér, and such approaches, (Trefethen, Weideman, and Schmelzer, 2006)

Constructing rational approximations II

Bromwich integral

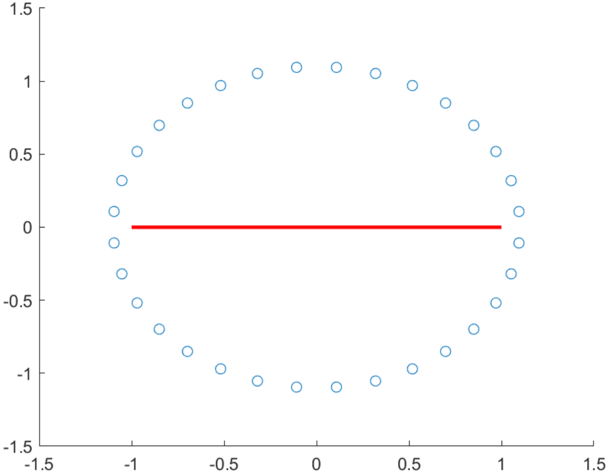
Inverse Laplace transform of a partial rational function $f(z) = 1/(z - a)$

$$e^a = \frac{1}{2\pi \mathrm{i}} \int_\Gamma \frac{e^z}{z - a} \, dz$$

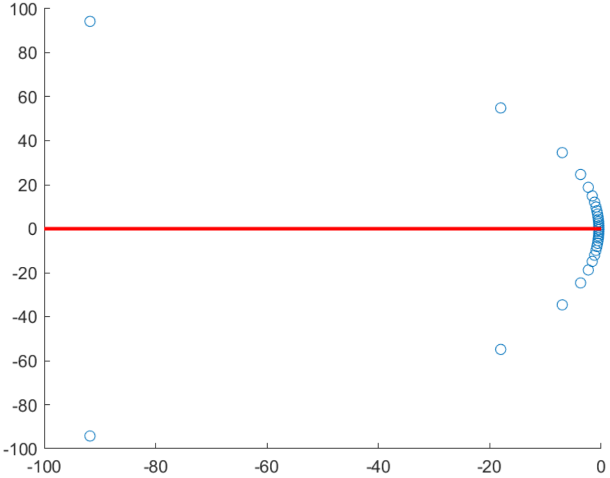
and in the case in which a is an operator

$$e^A = \frac{1}{2\pi \mathrm{i}} \int_\Gamma e^z (z - A)^{-1} \, dz \, .$$

Constructing rational approximations III



Constructing rational approximations IV



Rational Arnoldi decomposition

RAD

For $A \in \mathbb{C}^{n\times n}$ a relation of the form

$$AV_m K_m = V_m H_m,$$

for $V_m \in \mathbb{C}^{n\times m}$ of full column rank and $K_m, H_m \in \mathbb{C}^{(m+1)\times m}$ an unreduced Hessenberg pencil, is called the rational Arnoldi decomposition.

Let $H_m = (h_{ij})$ and $K_m = (k_{i,j})$

- The quotients $h_{j+1,j}/h_{j+1,j}$ are called the poles of the decomposition.
- Polynomials $q_1 = 1$, $q_j(z) = \prod_{i=1}^{j}(h_{i+1,i} - zk_{j+1,j}$ define rational Krylov spaces

$$\mathcal{V}_j = q_{j-1}(A)^{-1}\mathcal{K}_j(A, v)\ .$$

- We use $\mathcal{V}_j$ to parametrize a family of rational functions.

Galerkin approximations I

- Let $\mathcal{V}_h$ be the space of piece-wise linear, for a given triangular tessellation of Ω, and continuous functions on Ω.
- The Galerkin projection $A_h : \mathcal{V}_h \to \mathcal{V}_h$ is given by the formula

$$A_h = (A^{1/2} P_h)^* (A^{1/2} P_h),$$

  where P_h is the orthogonal projection onto $\mathcal{V}_h$.
- The resolvent estimate for A using the Galerkin projection A_h reads (see e.g. (Gopalakrishnan, Grubišić, and Ovall, 2020) for technical details)

$$\|(z - A)^{-1} v - (z - A_h)^{-1} v\|_{L^2(\Omega)} \leq C h^{2\nu} \|v\| \ , \tag{8}$$

  for $h < h_0$ and $v \in V_h$.

Galerkin approximations II

See also (Lasiecka and Triggiani, 2000, Section 5).
We will, however need this estimate solely for at most d poles $\tilde{\zeta}_i$, $i = 1, \cdots, d$ of the rational function r in the pole residue form, and so

For a rational function in partial fractions form

Let e.g.

$$r(z) = \sum_{i=1}^{N} \omega_i \frac{f(s_i)}{s_i - z} = \sum_{i=1}^{N} \frac{r_i}{s_i - z}$$

Then

$$\|r(A)v - r(A_h)v\|_{L^2(\Omega)} \leq d\ C\ h^{2\nu} \|v\|_{L^2}\ .$$

Finally, let $g(x) = u_0(x) + u_1(x)\mathrm{e}^{ax}$ be the perturbed exponential function. For a given rational function r and $v \in V_h$ we have the estimate

$$\begin{aligned} \|g(A)v - r(A_h)v\| &\leq \|g(A)v - r(A)v\| + \|r(A)v - r(A_h)v\| \\ &\leq \|g - r\|_{L^\infty(-\infty,0]}\|v\| + dCh^{2\nu}\|v\|\ . \end{aligned} \tag{9}$$

Galerkin approximations III

We can now construct the operator $r_{RK}(A) := r_0 I + \sum_{i=1}^{d} r_i (A - s_i)^{-1}$ such that

$$\|g(A) - r_{RK}(A)\|_{L(\mathcal{H})} \leq \mathtt{tol} \|g\|_{L^2(-\infty,0]} \,.$$

RKToolbox

We use lumped mass approximation of a differential operator!

Rational functions galore

With this setting and under additional assumption that the operator A is strictly negative, the operator Ψ and the vector ψ from the main theorem can be computed explicitly

$$\Psi = \alpha I + \frac{1}{2} A^{-1} S_{2T/3}(I - S_{2T/3}), \quad \psi = A^{-1} S_{T/3}(I - S_{T/3}) w. \tag{10}$$

We can now use spectral calculus to exemplary represent the operator Ψ as

$$\begin{aligned}\Psi &= \alpha I + \int_{\mathbb{R}} \mathrm{e}^{\lambda \ 2T/3} \ g(\lambda) \, \mathrm{d}E(\lambda) \\ &= \alpha I + \int_{\mathbb{R}} \mathrm{e}^{\lambda \ 2T/3} (1/\lambda - \mathrm{e}^{\lambda 2T/3}/\lambda) \, \mathrm{d}E(\lambda)\end{aligned}$$

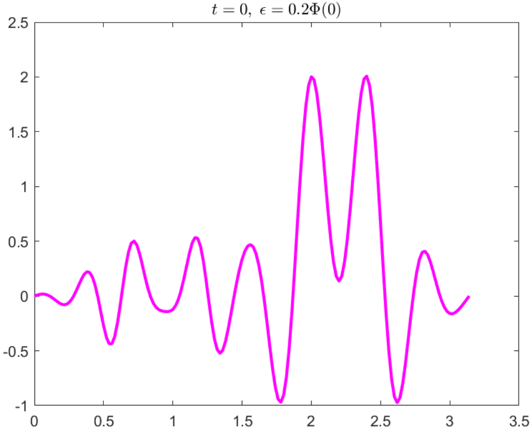
The function $g(\lambda) = (1/\lambda - \mathrm{e}^{\lambda \ 2T/3}/\lambda)$ is obviously the perturbed exponential function for which the rational approximation theory holds (there exists a small degree rational approximation).

Diffusion in an homogeneous material in 1D I

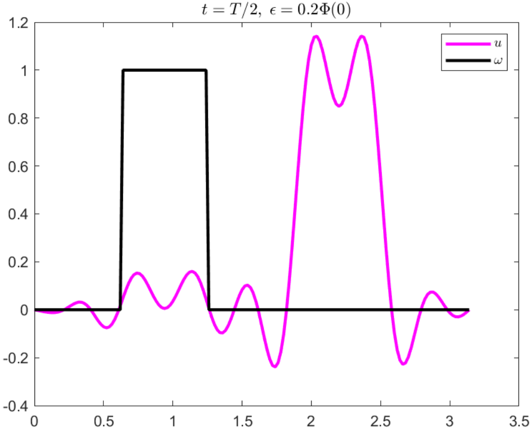
Example 1

Take $A = \partial_{xx}$. The initial control $u = y(0)$ (left), the computed solution at time $t = T/2$ compared with the desired trajectory ω(middle), and the optimal final state at $t = T$ compared with the target y^* (right) for three different values of the tolerance ε.

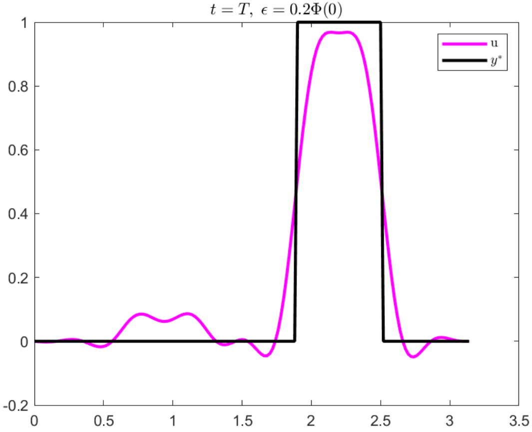
Diffusion in an homogeneous material in 1D II



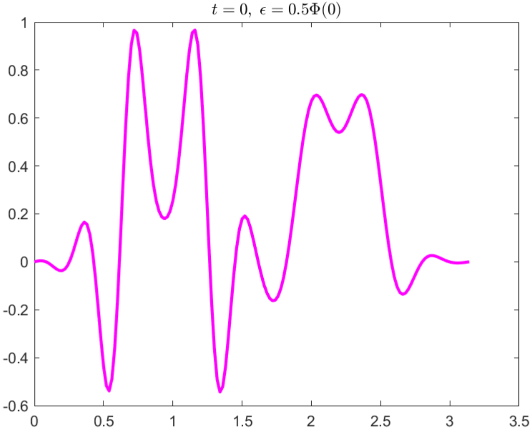
Diffusion in an homogeneous material in 1D III



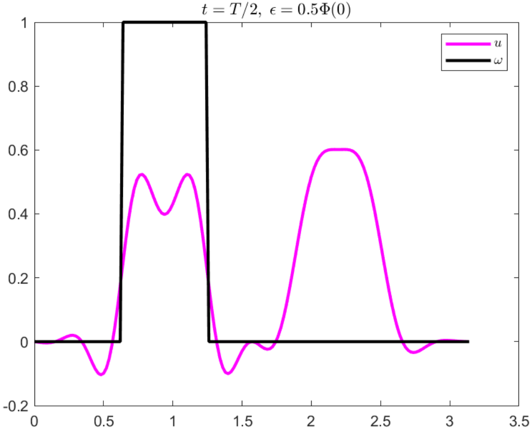
Diffusion in an homogeneous material in 1D IV



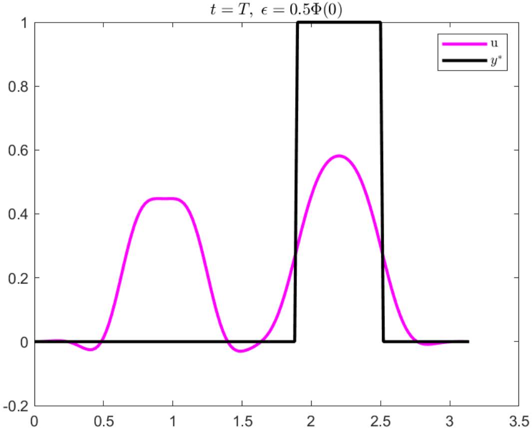
Diffusion in an homogeneous material in 1D V



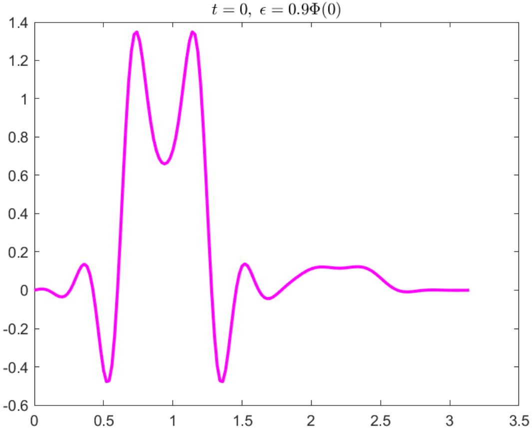
Diffusion in an homogeneous material in 1D VI



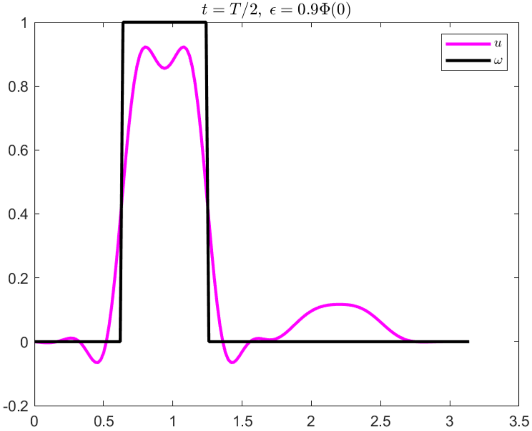
Diffusion in an homogeneous material in 1D VII



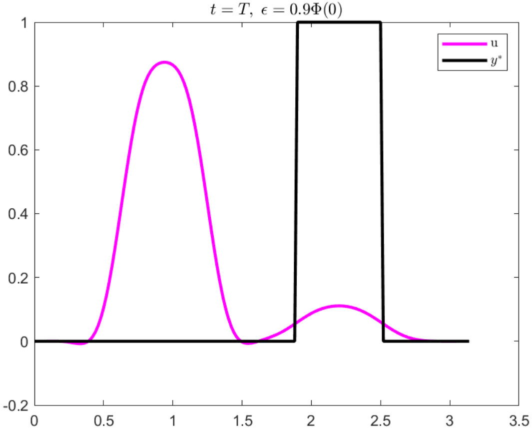
Diffusion in an homogeneous material in 1D VIII



Diffusion in an homogeneous material in 1D IX



Diffusion in an homogeneous material in 1D X



Diffusion in an in-homogeneous material in 1D I

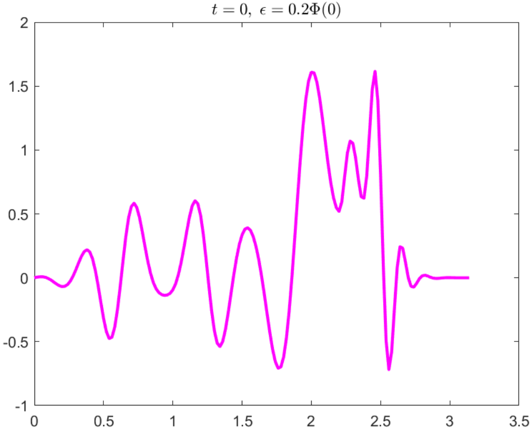
Example 2: In-homogeneous material

The operator A is taken of the form

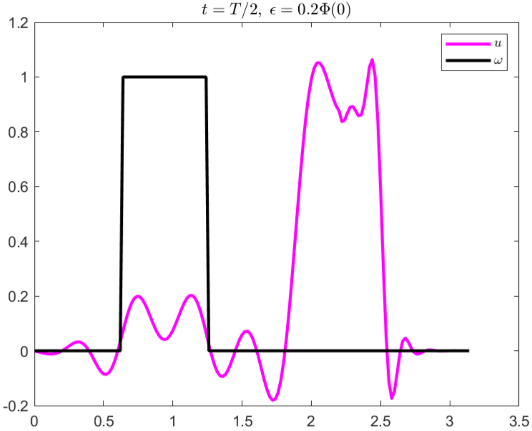
$$A = -\partial_x((1 + a\chi_{[\gamma,\pi]})\partial_x)$$

with $\gamma = 2.2$. The parameter γ determines the contact of two materials with a different diffusivity coefficient. The initial control $u = y(0)$ (left), the computed solution at time $t = T/2$ compared with the desired trajectory ω (middle), and the optimal final state compared with the target y^* (right) for three different values of the tolerance ε.

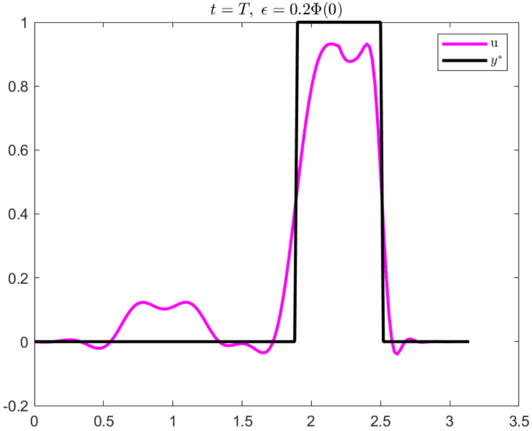
Diffusion in an in-homogeneous material in 1D II



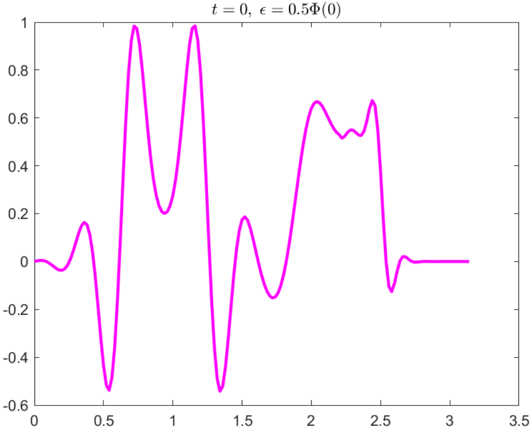
Diffusion in an in-homogeneous material in 1D III



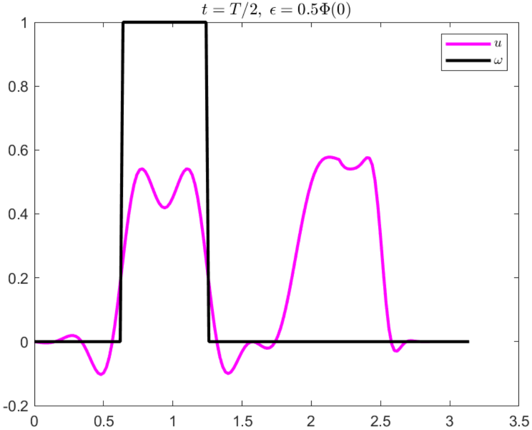
Diffusion in an in-homogeneous material in 1D IV



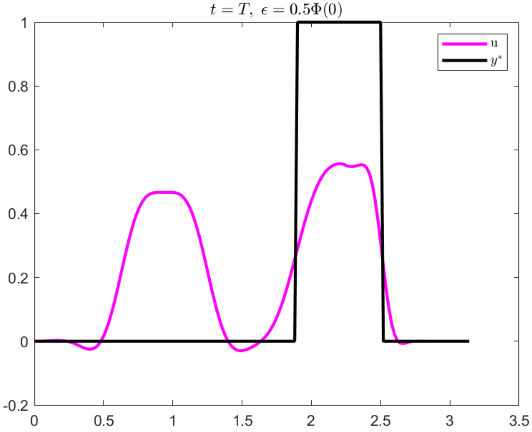
Diffusion in an in-homogeneous material in 1D V



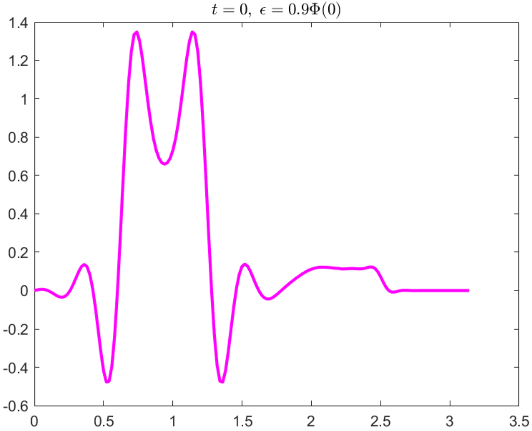
Diffusion in an in-homogeneous material in 1D VI



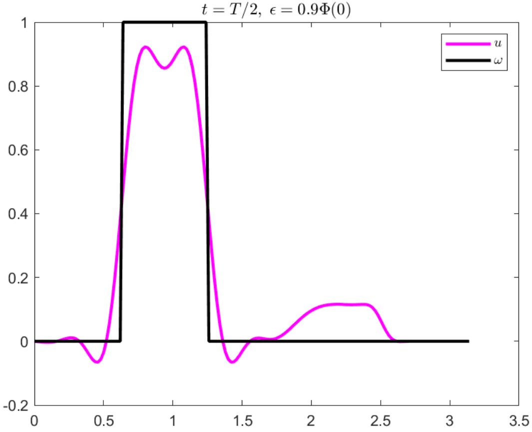
Diffusion in an in-homogeneous material in 1D VII



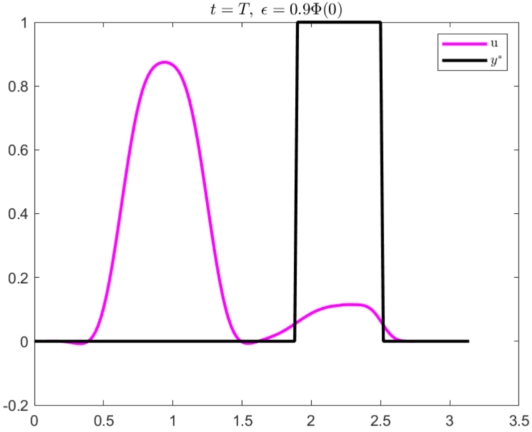
Diffusion in an in-homogeneous material in 1D VIII



Diffusion in an in-homogeneous material in 1D IX



Diffusion in an in-homogeneous material in 1D X

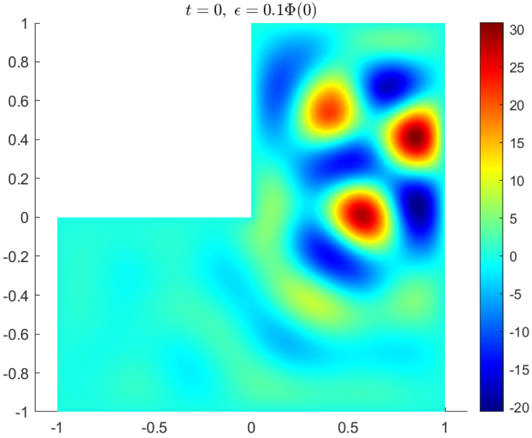


Difussion in 2D I

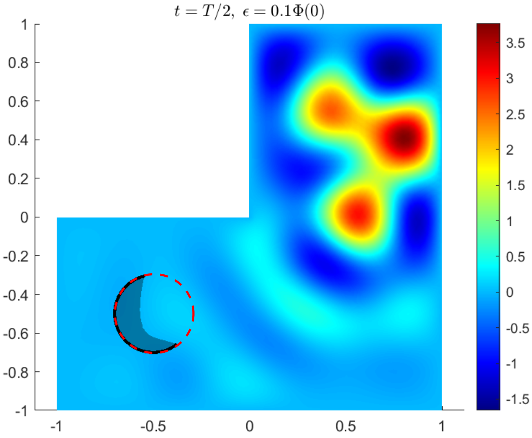
L-shaped domain

Take $A = \triangle$. The initial control $u = y(0)$ (left), the computed solution at time $t = T/2$ compared with the desired trajectory ω (middle), and the optimal final state (right) at $t = T$ for three different values of the tolerance ε. The red dashed circle marks the constraint ω on the trajectory.

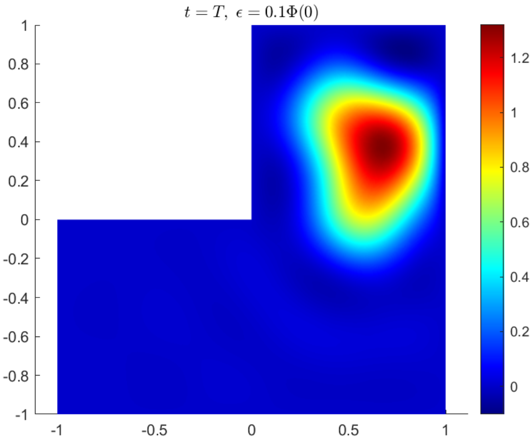
Difussion in 2D II



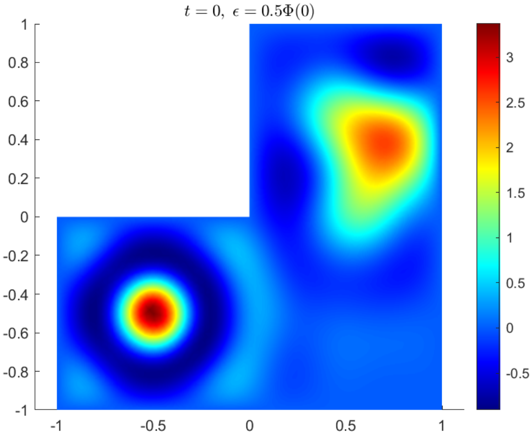
Difussion in 2D III



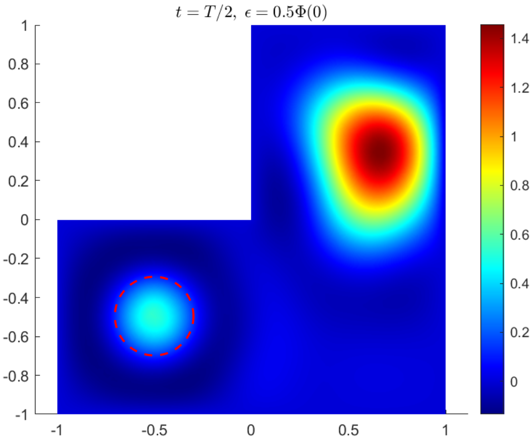
Difusion in 2D IV



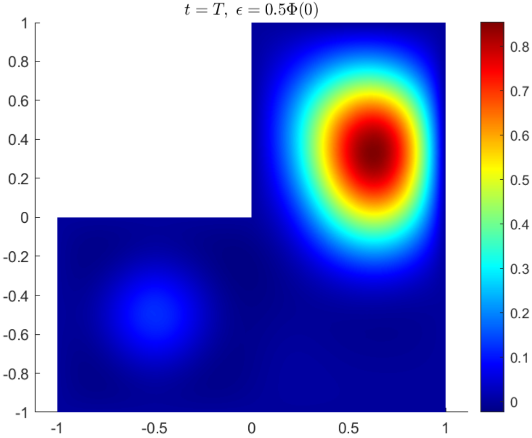
Difussion in 2D V



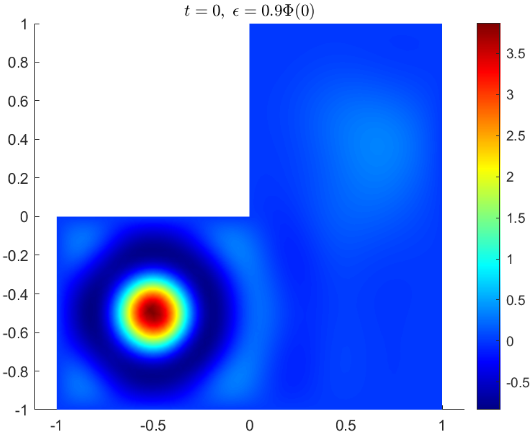
Difussion in 2D VI



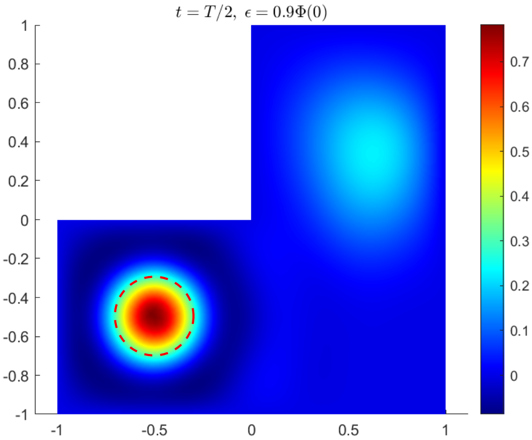
Difussion in 2D VII



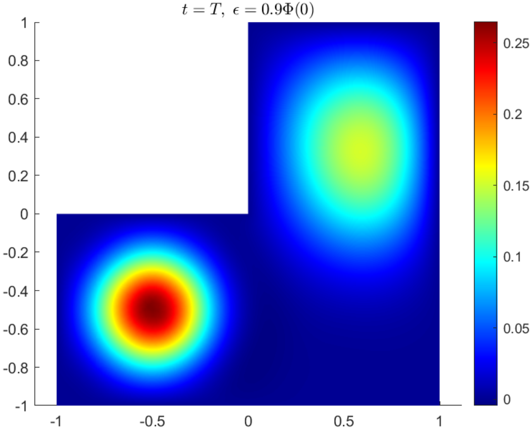
Difussion in 2D VIII



Difussion in 2D IX



Difussion in 2D X



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