Domain decomposition and applications to PDE-constrained optimization problems

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Lund

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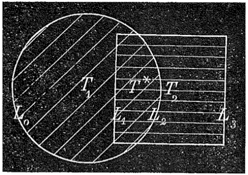
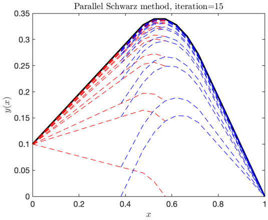
Domain decomposition

- Historical review
- Development
- Example
- Current research

PDE-constrained Optimization

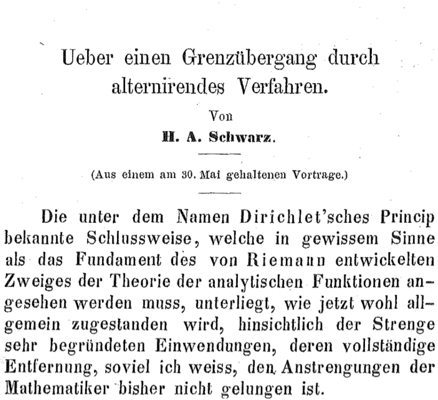
- Description and motivation
- Two frameworks
- Analysis
- Numerical tests





Historical review

The **alternating Schwarz method** is the earliest domain decomposition method invented by **H.A. Schwarz** in 1870 (About a border crossing through an alternating procedure).



Ueber einen Grenzübergang durch alternirendes Verfahren.

Von

H. A. Schwarz.

(Aus einem am 30. Mai gehaltenen Vortrage.)

Die unter dem Namen Dirichlet'sches Princip bekannte Schlussweise, welche in gewissem Sinne als das Fundament des von Riemann entwickelten Zweiges der Theorie der analytischen Funktionen angesehen werden muss, unterliegt, wie jetzt wohl allgemein zugestanden wird, hinsichtlich der Strenge sehr begründeten Einwendungen, deren vollständige Entfernung, soviel ich weiss, den Anstrengungen der Mathematiker bisher nicht gelungen ist.

Historical review

Problem: Show existence of harmonic functions

$$\Delta y = 0 \text{ in } \Omega, \quad y = g \text{ on } \partial\Omega.$$

Available tools: **Fourier (1807)** for rectangular domain and **Poisson (1815)** for circular domain.

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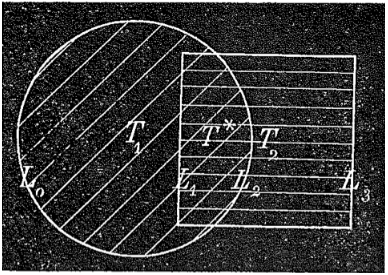
A *door handle* type domain Ω



Prove convergence of a iterative process with maximum principle.

Interpretation and illustration

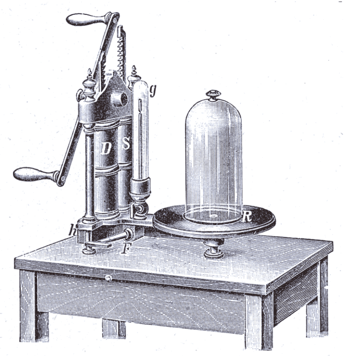
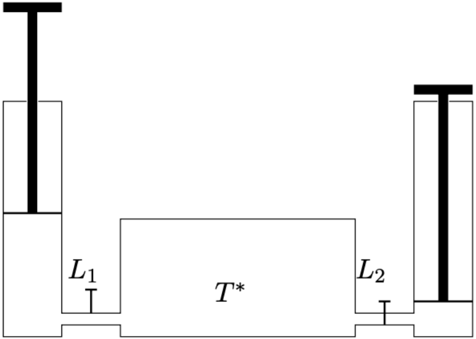


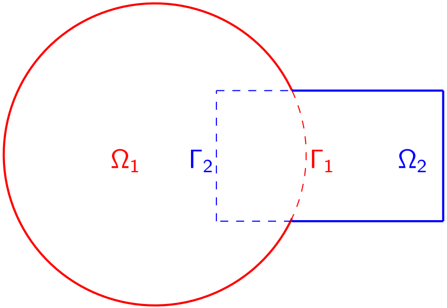
Fig. 103. Zweiſtiefelige Hahnluftpumpe



Interpretation and illustration

Domain: $\Omega = \Omega_1 \cup \Omega_2$

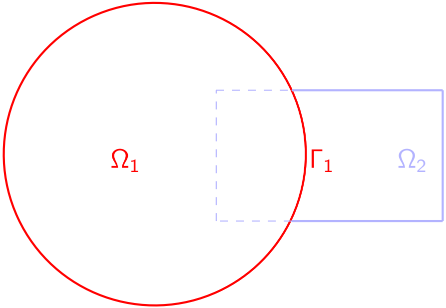
$$\begin{aligned} \Delta y &= 0 \quad \text{in } \Omega, \\ y &= g \quad \text{on } \partial\Omega. \end{aligned}$$



Interpretation and illustration

Subdomain: Ω_1 and a given y_2^0

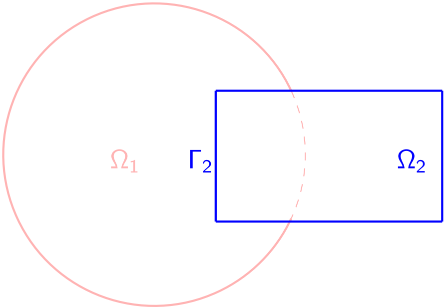
$$\begin{aligned} \Delta y_1^1 &= 0 && \text{in } \Omega_1, \\ y_1^1 &= g && \text{on } \partial\Omega \cap \bar{\Omega}_1, \\ y_1^1 &= y_2^0 && \text{on } \Gamma_1. \end{aligned}$$



Interpretation and illustration

Subdomain: Ω_2

$$\begin{aligned} \Delta y_2^1 &= 0 && \text{in } \Omega_2, \\ y_2^1 &= g && \text{on } \partial\Omega \cap \bar{\Omega}_2, \\ y_2^1 &= y_1^1 && \text{on } \Gamma_2 \end{aligned}$$



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\Delta y_1^\ell &= 0 && \text{in } \Omega_1,\\
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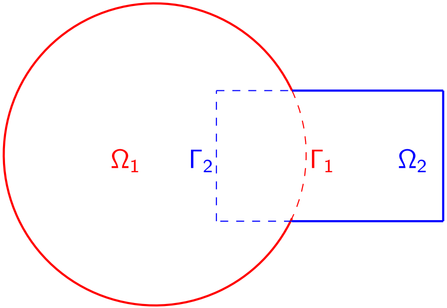

Towards a computational tool

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- **Gander (2025)**: Seven things I would have liked to know when starting to work on Domain Decomposition.

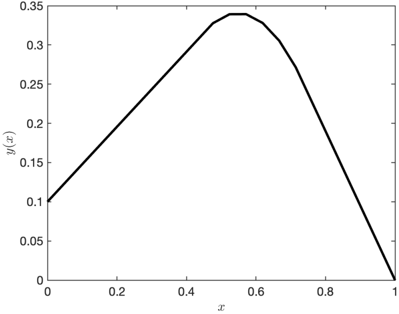
Alternating Schwarz method

Model problem:

$$\begin{aligned} -\partial_{xx} y &= f \quad \text{in } \Omega = (0,1), \\ y(0) &= 0.1, \\ y(1) &= 0, \end{aligned}$$

with

$$f = \begin{cases} 5 & \text{if } 0.4 < x < 0.7, \\ 0 & \text{else.} \end{cases}$$



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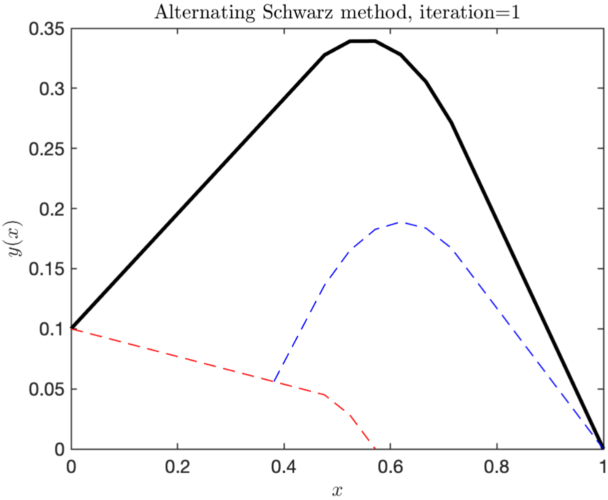
Subdomains: $\Omega_1 = (0, 0.57)$ and $\Omega_2 = (0.38, 1)$, a **given** $y_2^0(0.57) = 0$.



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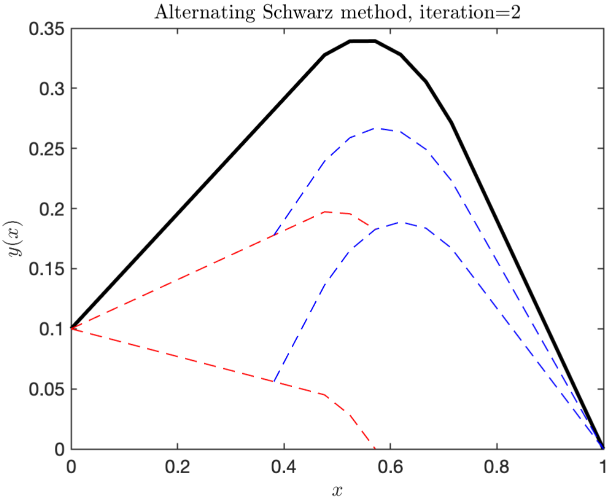

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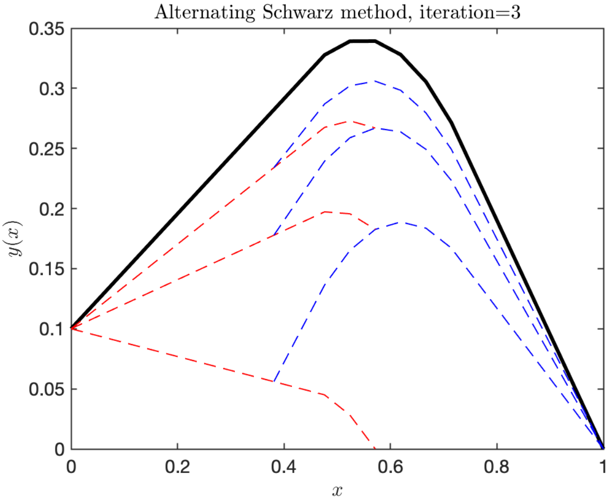

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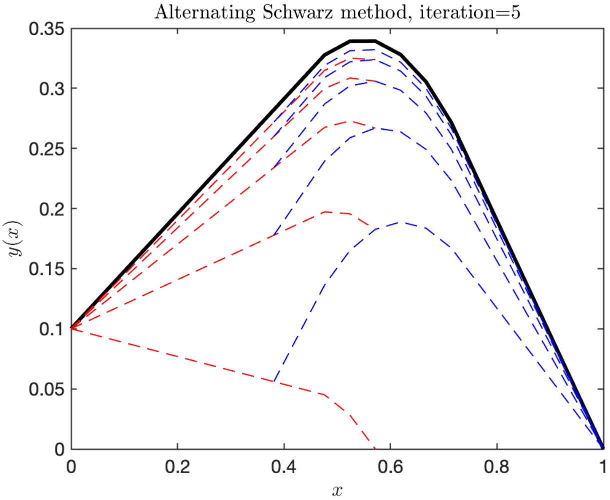

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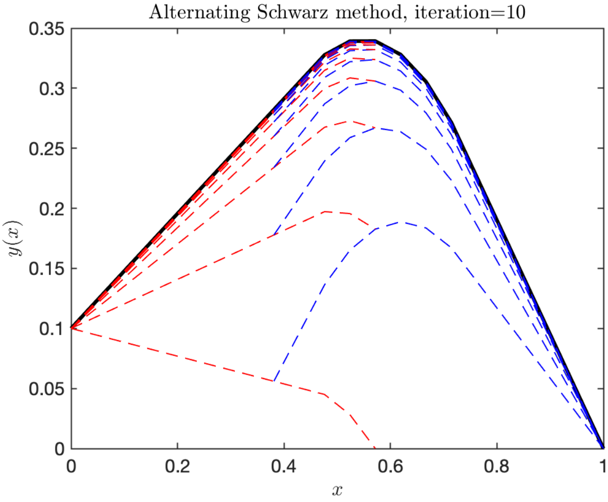

Convergence analysis

Model problem:

$$-\partial_{xx} y = f \quad \text{in } \Omega = (0,1), \quad y(0) = g_l, \quad y(1) = g_r.$$

Subdomains: $\Omega_1 = (0,b)$ and $\Omega_2 = (a,1)$ with $b > a$.

Given y_2^0, we solve

$$\begin{aligned} -\partial_{xx} y_1^\ell &= f \quad \text{in } \Omega_1, & -\partial_{xx} y_2^\ell &= f \quad \text{in } \Omega_2, \\ y_1^\ell(0) &= g_l, & y_2^\ell(1) &= g_r, \\ y_1^\ell(b) &= y_2^{\ell-1}(b), & y_2^\ell(a) &= y_1^\ell(a). \end{aligned}$$

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Evaluate C_1^ℓ and C_2^ℓ:

$$C_1^\ell = \frac{e_2^{\ell-1}(b)}{b}, \qquad C_2^\ell = \frac{e_1^\ell(a)}{a-1} = e_2^{\ell-1}(b)\frac{1}{a-1}\frac{a}{b}.$$

The convergence factor

$$e_2^\ell(b) = \rho(a,b) e_2^{\ell-1}(b), \quad \rho(a,b) := \frac{1-b}{1-a}\frac{a}{b}.$$

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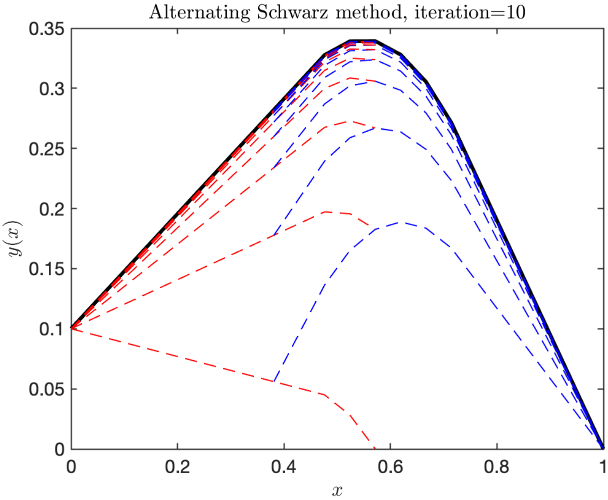
(i) The alternating Schwarz method always converges when $b > a$.
(ii) The larger the overlap size $b-a$, the better the convergence.
(iii) The alternating Schwarz method **does not converge** when $a = b$!

Parallel Schwarz method

Subdomains: $\Omega_1 = (0, 0.57)$ and $\Omega_2 = (0.38, 1)$, a **given** $y_2^0(0.57) = 0$.



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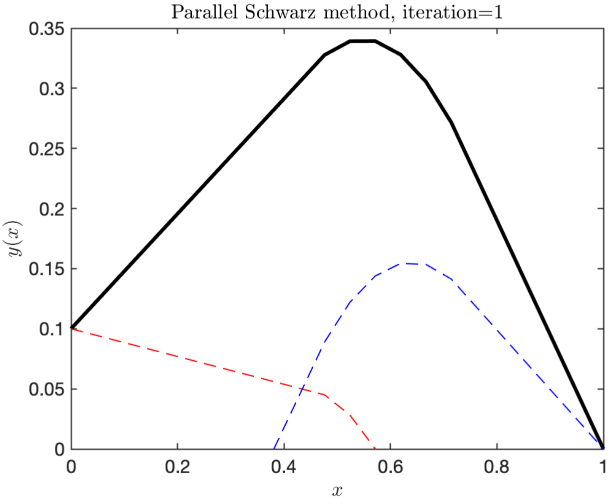

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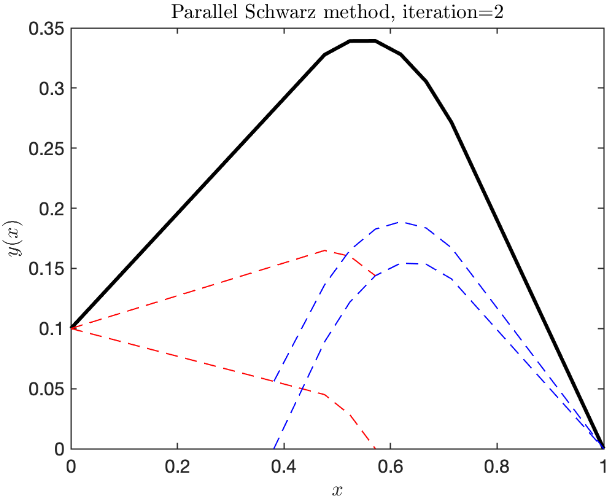

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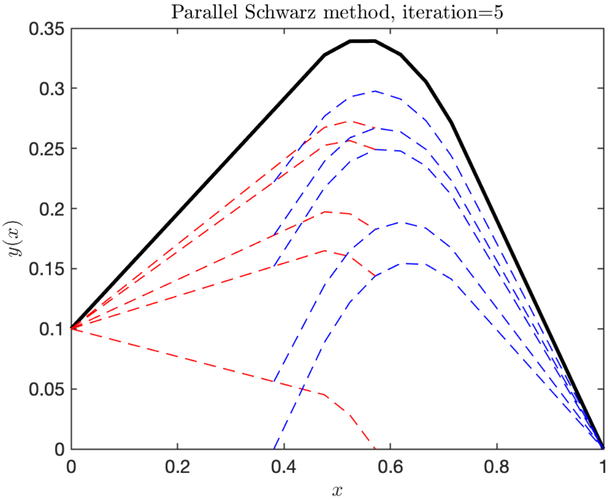

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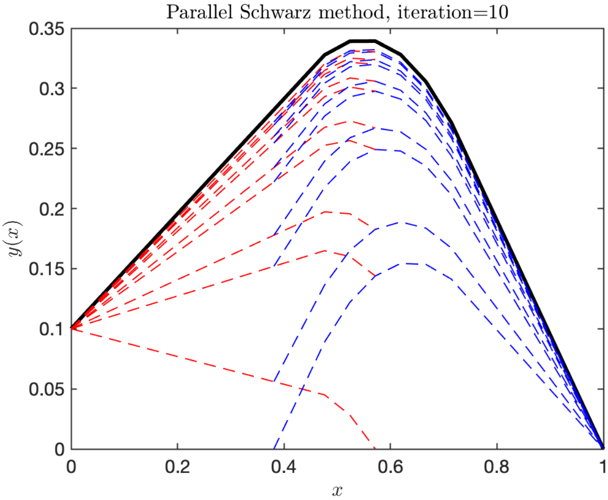

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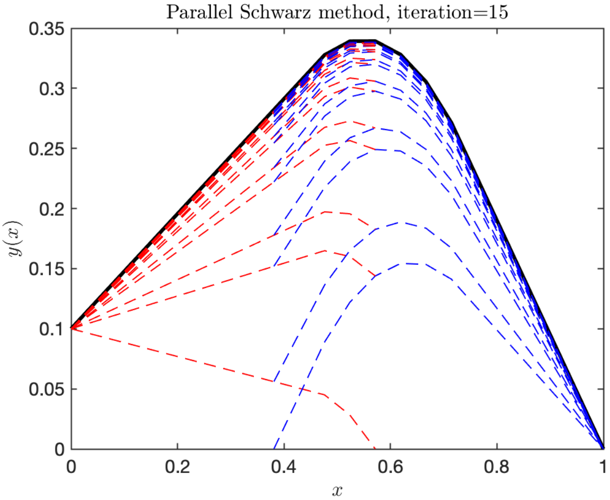

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The convergence factor is now

$$e_2^{\ell+1}(b) = \frac{1-b}{1-a}\frac{a}{b}\, e_2^{\ell-1}(b).$$

Research directions

- **Transmission conditions:** Dirichlet, Neumann, Robin, Ventcell, . . .

  Some methods: alternating Schwarz, parallel Schwarz, optimized Schwarz, Dirichlet-Neumann, Neumann-Neumann (BDD), FETI (Dirichlet-Dirichlet), . . .

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- **Preconditioning:** always use DD as preconditioners !

$$M\boldsymbol{y}^{\ell} = N\boldsymbol{y}^{\ell-1} + \boldsymbol{f} \quad \Leftrightarrow \quad \boldsymbol{y}^{\ell} = \boldsymbol{y}^{\ell-1} + M^{-1}(\boldsymbol{f} - A\boldsymbol{y}^{\ell-1}) \quad \Rightarrow \quad M^{-1}A\boldsymbol{y} = M^{-1}\boldsymbol{f}.$$

- **Time parallel time integration:** waveform relaxation, MGRIT, PFASST, . . .

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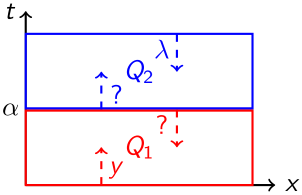

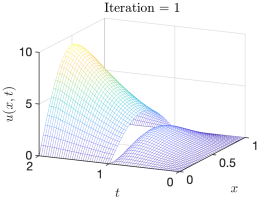

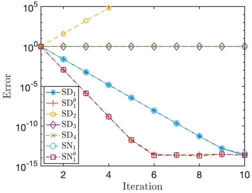

PDE-constrained optimization problems

General description: optimize a functional $J(y, u)$ subject to evolution PDEs $\mathcal{L}y = u$.

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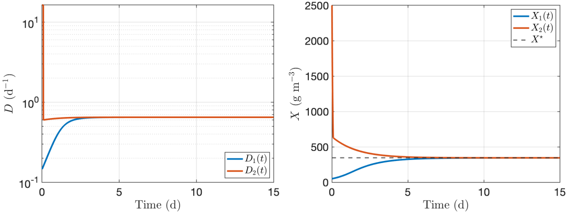
Example: maximize average biomass productivity:

$$J(y,u) = \frac{1}{T}\int_0^T \mu y \,\mathrm{d}t \quad \text{and} \quad \mathcal{L}y = \partial_t y + c\cdot\nabla y - \eta\Delta y + Dy;$$



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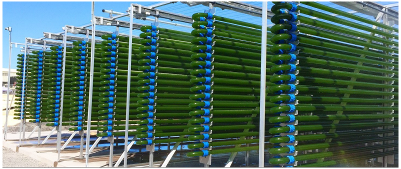
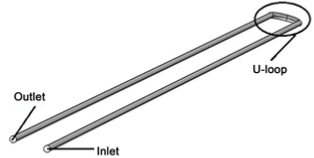
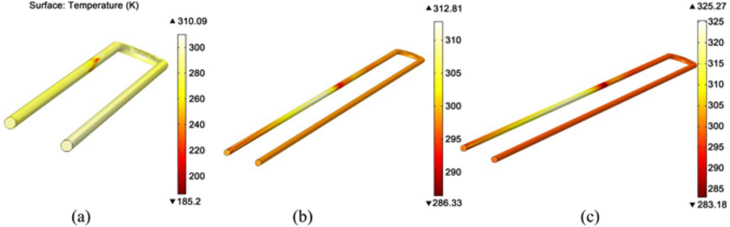
Example: control heat distribution w.r.t. target $\hat{y}$:

$$J(y, u) = \frac{1}{2}\|y - \hat{y}\|^2 + \frac{\nu}{2}\|u\|^2 \quad \text{and} \quad \mathcal{L}y = \partial_t y - \Delta y;$$







PDE-constrained optimization problems

General description: optimize a functional $J(y,u)$ subject to evolution PDEs $\mathcal{L}y = u$.

Example:

- maximize average biomass productivity:

$$J(y,u) = \frac{1}{T}\int_0^T \mu y \,\mathrm{d}t \quad \text{and} \quad \mathcal{L}y = \partial_t y + c \cdot \nabla y - \eta \Delta y + Dy;$$

- control heat distribution w.r.t. target $\hat{y}$ in photobioreactors:

$$J(y,u) = \frac{1}{2}\|y - \hat{y}\|^2 + \frac{\nu}{2}\|u\|^2 \quad \text{and} \quad \mathcal{L}y = \partial_t y - \Delta y;$$

- optimal control, mean field games, ...

Challenge: Time consuming for complex systems and/or high dimension.

Model problem

For $\hat{y} \in L^2(Q)$, $\gamma \geq 0$ and $\nu > 0$, minimize the cost functional

$$J(y, u) := \frac{1}{2}\|y - \hat{y}\|^2_{L^2(Q)} + \frac{\nu}{2}\|u\|^2_{L^2(\Omega)},$$

subject to $\partial_t y - \Delta y = u$ in $Q := (0, T) \times \Omega$ with some initial and boundary conditions.

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Lagrange multipliers method $\rightarrow$ First-order optimality system:

$$\begin{aligned}
\partial_t y - \Delta y &= \nu^{-1}\lambda \quad && \text{in } Q, \qquad & \partial_t \lambda + \Delta\lambda &= y - \hat{y} \quad && \text{in } Q,\\
y &= 0 && \text{in } \Sigma, & \lambda &= 0 && \text{in } \Sigma,\\
y &= y_0 && \text{in } \Sigma_0, & \lambda &= 0 && \text{in } \Sigma_T.
\end{aligned}$$

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For $\hat{y} \in L^2(Q)$, $\gamma \geq 0$ and $\nu > 0$, minimize the cost functional

$$J(y,u) := \frac{1}{2}\|y-\hat{y}\|^2_{L^2(Q)} + \frac{\nu}{2}\|u\|^2_{L^2(\Omega)},$$

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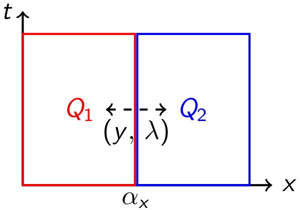
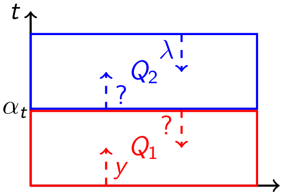
Lagrange multipliers method → First-order optimality system:

$$\begin{array}{rlrl} \partial_t y - \Delta y = \nu^{-1}\lambda & \text{in } Q, & \partial_t \lambda + \Delta\lambda = y - \hat{y} & \text{in } Q, \\ y = 0 & \text{in } \Sigma, & \lambda = 0 & \text{in } \Sigma, \\ y = y_0 & \text{in } \Sigma_0, & \lambda = 0 & \text{in } \Sigma_T. \end{array}$$

No classical time stepping method → domain decomposition !

space decomposition

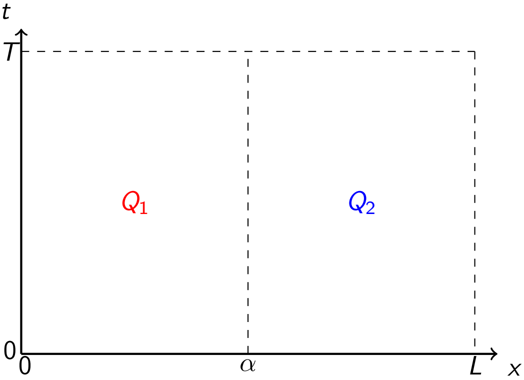




time decomposition

Alternating Schwarz waveform

Example: Control heat distribution w.r.t. a target $\hat{y}$.

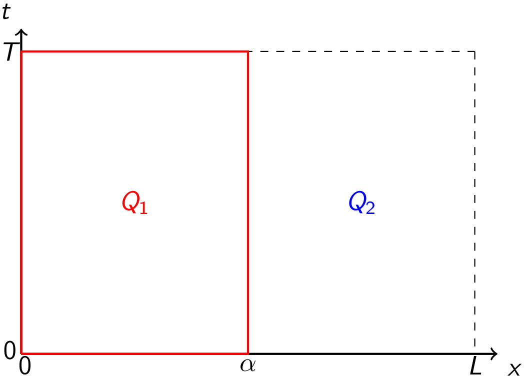


Subdomains: $Q_1 = (0, \alpha) \times (0, T)$ and $Q_2 = (\alpha, L) \times (0, T)$

$$\begin{aligned} \partial_t y - \partial_{xx} y &= \nu^{-1}\lambda, & \partial_t \lambda + \partial_{xx}\lambda &= y - \hat{y}, \\ y(0,t) &= 0, & \lambda(0,t) &= 0, \\ y(L,t) &= 0, & \lambda(L,t) &= 0, \\ y(x,0) &= y_0(x), & \lambda(x,T) &= 0. \end{aligned}$$

Alternating Schwarz waveform

Example: Control heat distribution w.r.t. a target $\hat{y}$.

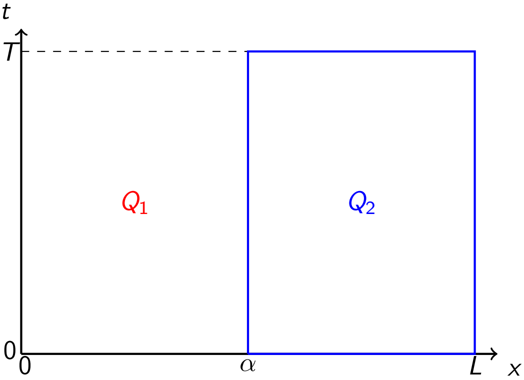


Subdomain: $Q_1 = (0, \alpha) \times (0, T)$

$$\begin{aligned} \partial_t y_1^\ell - \partial_{xx} y_1^\ell &= \nu^{-1}\lambda_1^\ell, & \partial_t \lambda_1^\ell + \partial_{xx}\lambda_1^\ell &= y_1^\ell - \hat{y}_1, \\ y_1^\ell(0,t) &= 0, & \lambda_1^\ell(0,t) &= 0, \\ y_1^\ell(\alpha,t) &= y_2^{\ell-1}(\alpha,t), & \lambda_1^\ell(\alpha,t) &= \lambda_2^{\ell-1}(\alpha,t), \\ y_1^\ell(x,0) &= y_{1,0}(x), & \lambda_1^\ell(x,T) &= 0. \end{aligned}$$

Alternating Schwarz waveform

Example: Control heat distribution w.r.t. a target $\hat{y}$.

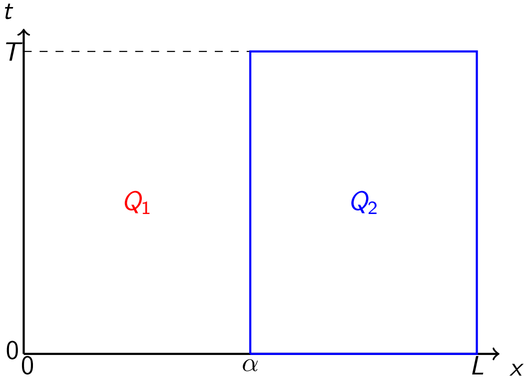


Subdomains: $Q_2 = (\alpha, 1) \times (0, T)$

$$\begin{aligned}
\partial_t y_2^\ell - \partial_{xx} y_2^\ell &= \nu^{-1}\lambda_2^\ell, & \partial_t \lambda_2^\ell + \partial_{xx}\lambda_2^\ell &= y_2^\ell - \hat{y}_2,\\
y_2^\ell(\alpha, t) &= y_1^\ell(\alpha, t), & \lambda_2^\ell(\alpha, t) &= \lambda_1^\ell(\alpha, t),\\
y_2^\ell(L, t) &= 0, & \lambda_2^\ell(L, t) &= 0,\\
y_2^\ell(x, 0) &= y_{2,0}(x), & \lambda_2^\ell(x, T) &= 0.
\end{aligned}$$

Alternating Schwarz waveform

Example: Control heat distribution w.r.t. a target $\hat{y}$.



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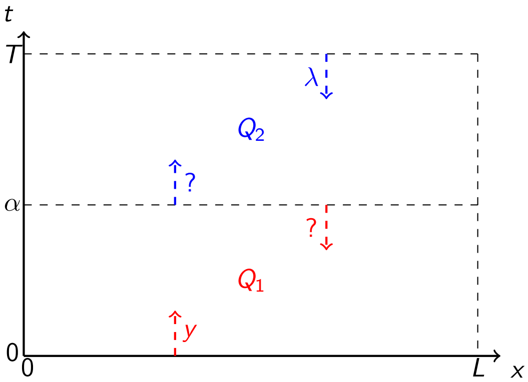
The algorithm **does not converge** without overlap !

Idea of time decomposition

Example: Control heat distribution w.r.t. a target $\hat{y}$.



Subdomains: $Q_1 = (0, L) \times (0, \alpha)$ and $Q_2 = (0, L) \times (\alpha, T)$

$$\begin{aligned} \partial_t y - \partial_{xx} y &= \nu^{-1}\lambda, & \partial_t \lambda + \partial_{xx}\lambda &= y - \hat{y}, \\ y(0,t) &= 0, & \lambda(0,t) &= 0, \\ y(L,t) &= 0, & \lambda(L,t) &= 0, \\ y(x,0) &= y_0(x), & \lambda(x,T) &= 0. \end{aligned}$$

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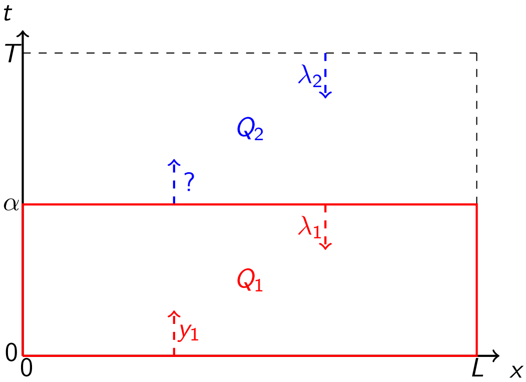
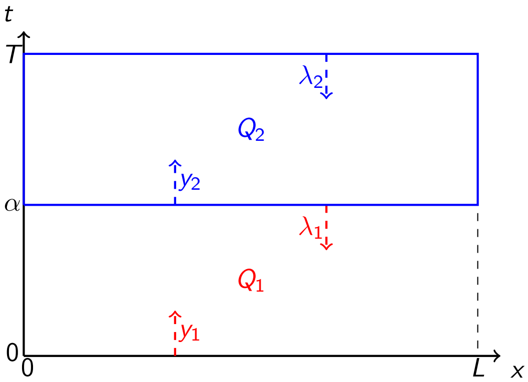


Subdomain: $Q_1 = (0, L) \times (0, \alpha)$

$$
\begin{aligned}
\partial_t y_1^\ell - \partial_{xx} y_1^\ell &= \nu^{-1} \lambda_1^\ell, & \partial_t \lambda_1^\ell + \partial_{xx} \lambda_1^\ell &= y_1^\ell - \hat{y}_1, \\
y_1^\ell(0, t) &= 0, & \lambda_1^\ell(0, t) &= 0, \\
y_1^\ell(L, t) &= 0, & \lambda_1^\ell(L, t) &= 0, \\
y_1^\ell(x, 0) &= y_0(x), & \lambda_1^\ell(x, \alpha) &= \lambda_2^{\ell-1}(x, \alpha).
\end{aligned}
$$

Idea of time decomposition

Example: Control heat distribution w.r.t. a target $\hat{y}$.



Subdomain: $Q_2 = (0, L) \times (\alpha, T)$

$$\begin{aligned}
\partial_t y_2^\ell - \partial_{xx} y_2^\ell &= \nu^{-1}\lambda_2^\ell, & \partial_t \lambda_2^\ell + \partial_{xx}\lambda_2^\ell &= y_2^\ell - \hat{y}_2,\\
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Idea of time decomposition

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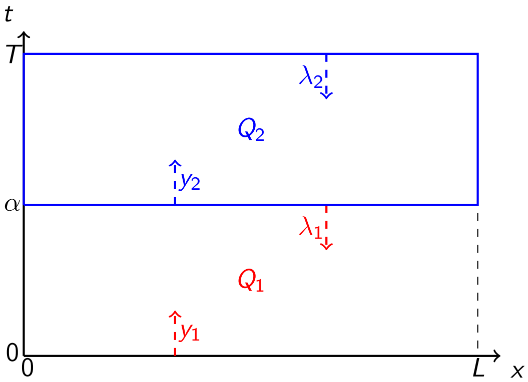

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The algorithm **does converge** without overlap !

Observations

First-order optimality system:

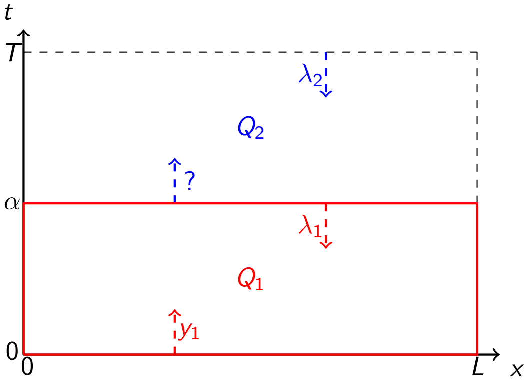
$$\begin{aligned} \partial_t y - \partial_{xx} y &= \nu^{-1}\lambda && \text{in } Q, & \partial_t \lambda + \partial_{xx}\lambda &= y - \hat{y} && \text{in } Q,\\ y &= 0 && \text{in } \Sigma, & \lambda &= 0 && \text{in } \Sigma,\\ y &= y_0 && \text{in } \Sigma_0, & \lambda &= 0 && \text{in } \Sigma_T. \end{aligned}$$

Relation between y and λ:

$$\begin{aligned} \partial_t y - \partial_{xx} y = \nu^{-1}\lambda \quad &\to \quad \lambda = \nu(\partial_t y - \partial_{xx} y),\\ \partial_t \lambda + \partial_{xx}\lambda = y - \hat{y} \quad &\to \quad y = \partial_t\lambda + \partial_{xx}\lambda + \hat{y}. \end{aligned}$$

Observations

Two relations $\lambda = \nu(\partial_t y - \partial_{xx} y)$ and $y = \partial_t \lambda + \partial_{xx} \lambda + \hat{y}$.



Subdomain: $Q_1 = (0, L) \times (0, \alpha)$

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\partial_t y_1^\ell - \partial_{xx} y_1^\ell &= \nu^{-1} \lambda_1^\ell, \\
y_1^\ell(0, t) &= 0, \\
y_1^\ell(L, t) &= 0, \\
y_1^\ell(x, 0) &= y_0(x), \\
\partial_t \lambda_1^\ell + \partial_{xx} \lambda_1^\ell &= y_1^\ell - \hat{y}_1, \\
\lambda_1^\ell(0, t) &= 0, \\
\lambda_1^\ell(L, t) &= 0, \\
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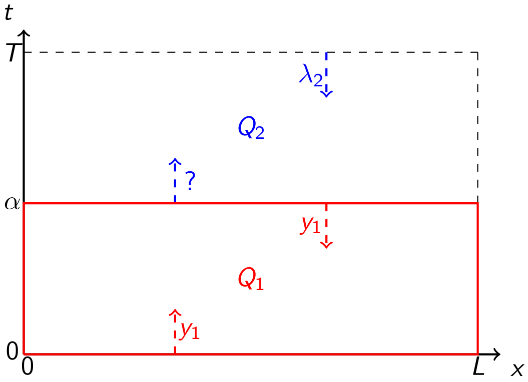

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y_1^\ell(x, 0) &= y_0(x), \\
(\partial_t - \partial_{xx}) y_1^\ell(x, \alpha) &= (\partial_t - \partial_{xx}) y_2^{\ell-1}(x, \alpha), \\
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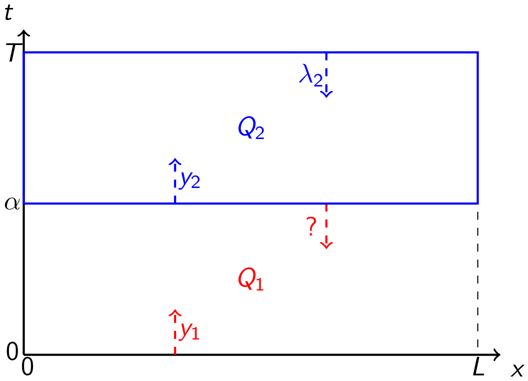

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$$
\begin{aligned}
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y_2^\ell(x, \alpha) &= y_1^\ell(x, \alpha), \\
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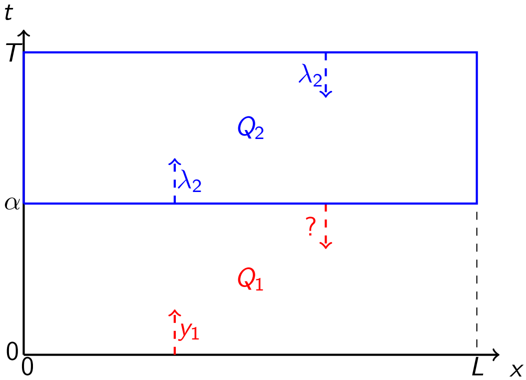

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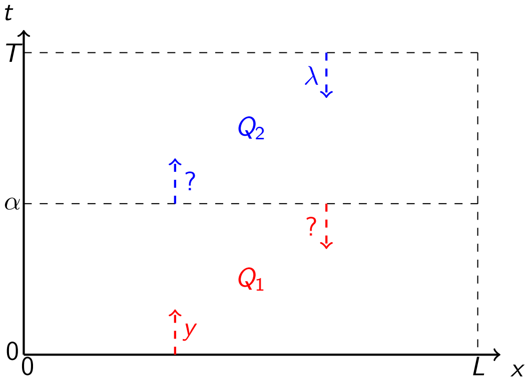
\lambda_2^\ell(0, t) &= 0,\\
\lambda_2^\ell(L, t) &= 0,\\
(\partial_t + \partial_{xx})\lambda_2^\ell(x, \alpha) &= (\partial_t + \partial_{xx})\lambda_1^\ell(x, \alpha),\\
\lambda_2^\ell(x, T) &= 0.
\end{aligned}$$

Observations



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(i) **Dirichlet** condition transform to **Robin** type condition !

(ii) Forward-backward **might be** less important ?

Variants and convergence

Dirichlet type transmission condition:

name	SD_1	SD_2	SD_3	SD_4
Q_1	λ	y	y	λ
Q_2	y	λ	y	λ

Variants and convergence

Dirichlet type transmission condition:

name	SD_1	SD_2	SD_3	SD_4
Q_1	λ	y	y	λ
Q_2	y	λ	y	λ

Analysis: Fourier transform or semi-discretization in space:

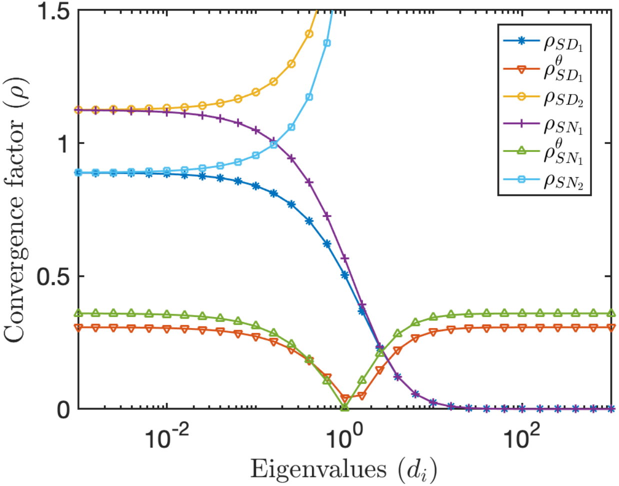
$$\begin{aligned}
\rho_{\mathrm{SD}_1} &= \max_{d_i \in D} \left| \frac{1+\gamma(\sigma_i \coth(b_i) - d_i)}{\nu(\sigma_i \coth(a_i) + d_i)(\sigma_i \coth(b_i) + d_i + \gamma\nu^{-1})} \right|, \\
\rho_{\mathrm{SD}_2} &= \max_{d_i \in D} \left| \frac{\nu(\sigma_i \coth(a_i) + d_i)(\sigma_i \coth(b_i) + d_i + \gamma\nu^{-1})}{1+\gamma(\sigma_i \coth(b_i) - d_i)} \right|, \\
\rho_{\mathrm{SD}_3} &= 1, \\
\rho_{\mathrm{SD}_4} &= 1.
\end{aligned}$$

Relaxation:

$$f^{\ell+1}(x) = (1-\theta) f^{\ell}(x) + \theta \lambda_2^{\ell}(x,\alpha), \qquad \theta \in (0,1).$$

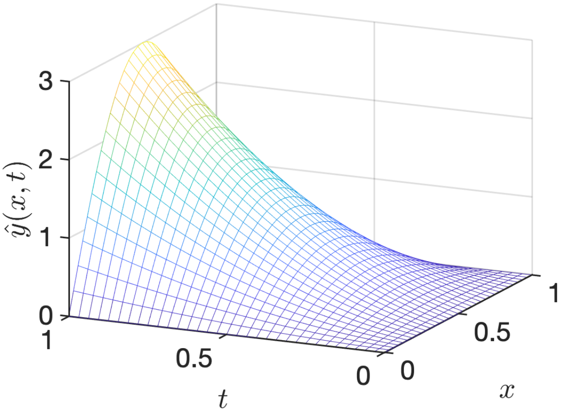
Variants and convergence

Convergence factors



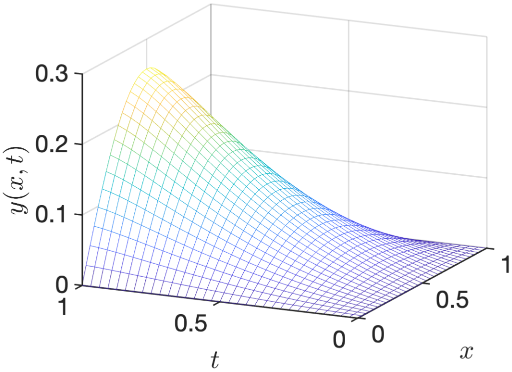
Numerical experiments

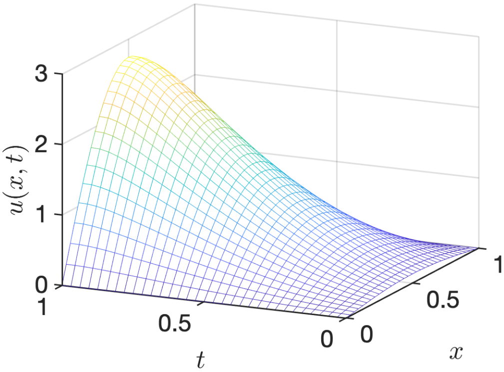
Test case: consider the target function $\hat{y}(x,t) = \sin(\pi x)(2t^2+2)$.



Numerical experiments

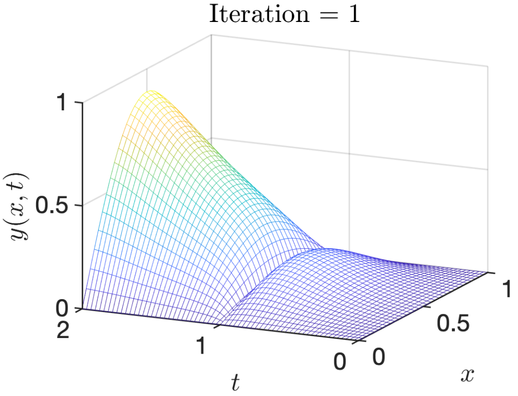
Numerical solutions: Crank-Nicolson with mesh size $h_t = h_x = \frac{1}{32}$ and penalization parameters: $\nu = 0.1$, $\gamma = 0.1$.

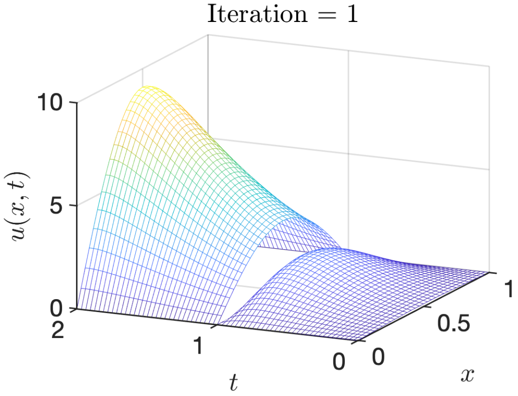




Numerical experiments

SD$_1$





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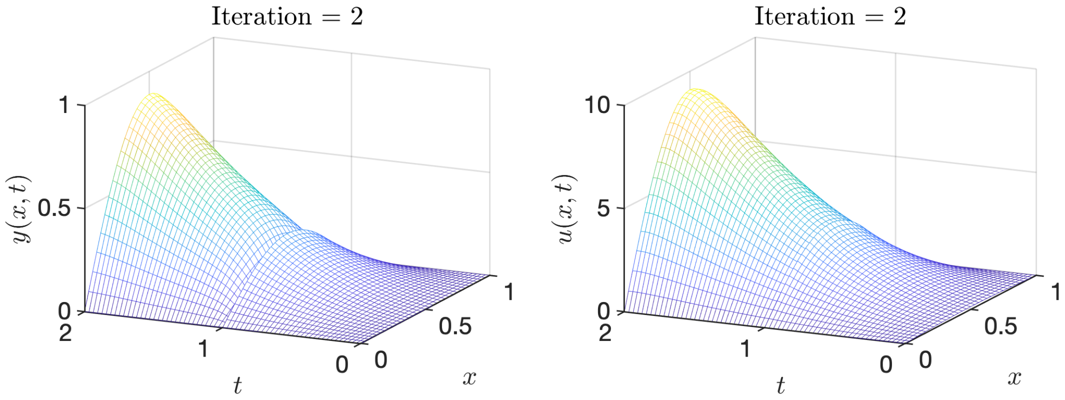
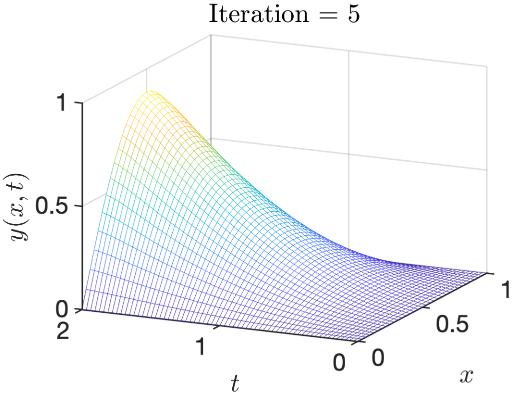
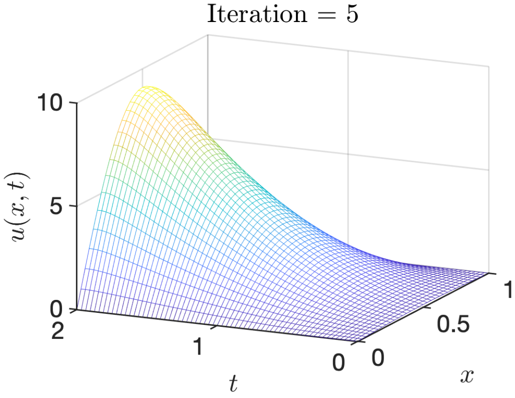


Numerical experiments

SD$_1$



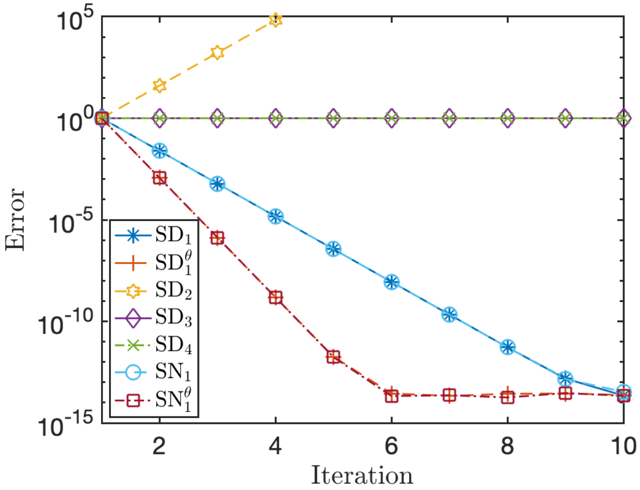
Iteration $= 5$



Iteration $= 5$

Numerical experiments

Convergence behavior



Conclusion and perspective

Some observations:

- Time decomposition is **different** from space decomposition
- Forward-backward structure is **very important** for alternating Schwarz
- Relaxation is **not necessary** for convergence
- Same analysis for higher dimension in space

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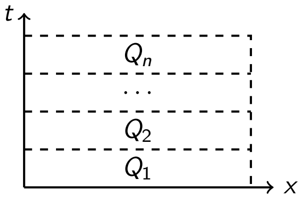
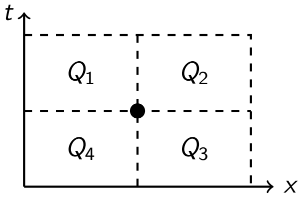


Future work:

- Scalability: **weak** ? strong ? corse correction ?
- Space-time decomposition: **cross point** ?
- Extension to other PDE constraints: advection-diffusion ? **Stokes** ?



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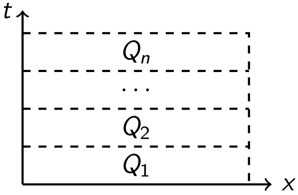
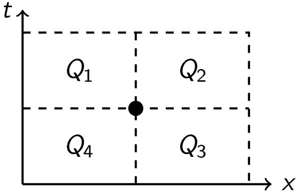
Some observations:

- Time decomposition is **different** from space decomposition
- Forward-backward structure is **very important** for alternating Schwarz
- Relaxation is **not necessary** for convergence
- Same analysis for higher dimension in space



Future work:

- Scalability: **weak** ? strong ? corse correction ?
- Space-time decomposition: **cross point** ?
- Extension to other PDE constraints: advection-diffusion ? **Stokes** ?



Thank you for your attention !