Substructuring-based Methods for Elliptic and Parabolic Optimal Control Problems

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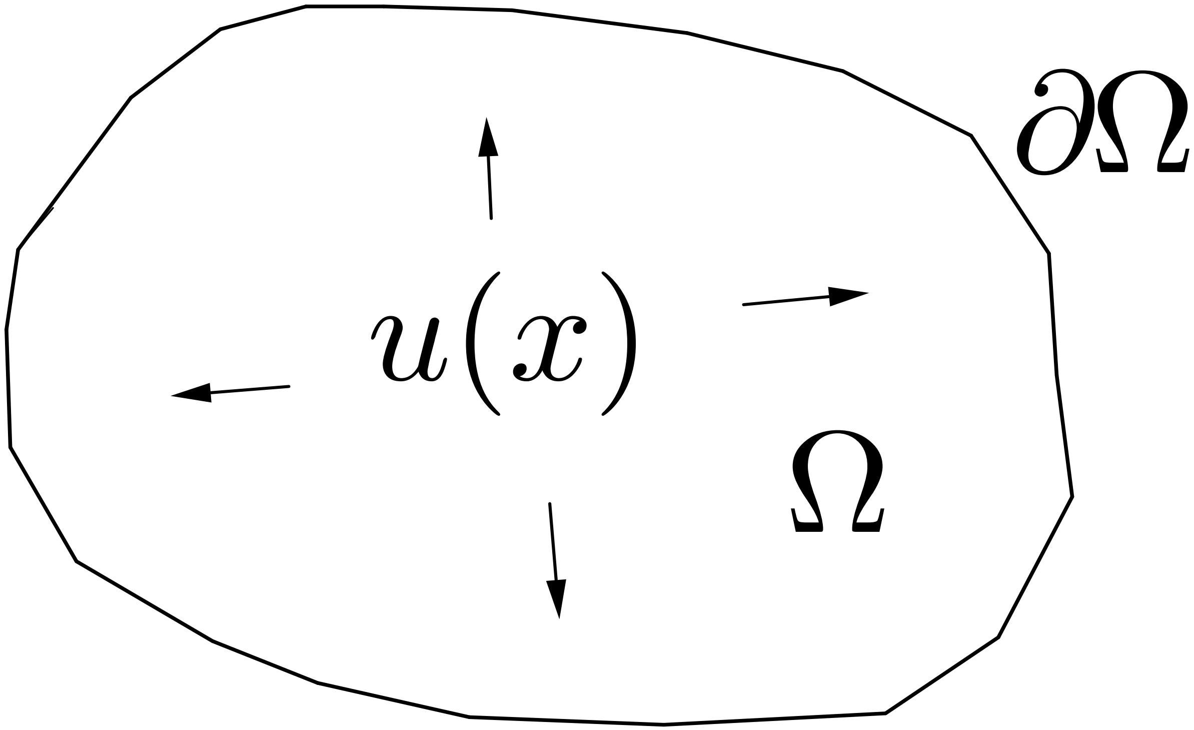
Example 1: Stationary optimal heating problem.

- Heating of a body Ω by a controlled heat source u (example: electromagnetic induction or microwaves) to reach the target $\hat{y}$.



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- Heating of a body Ω by a controlled heat source u (example: electromagnetic induction or microwaves) to reach the target $\hat{y}$.

$$\text{Minimize } J(y,u) = \frac{1}{2}\int_{\Omega} (y(x) - \hat{y}(x))^2 \, dx + \frac{\lambda}{2}\int_{\Omega} u^2(x) dx,$$

$$\text{subject to } \begin{cases} -\mathrm{div}\,(\kappa \nabla y(x)) = u(x), & x \in \Omega, \\ y(x) = 0, & x \in \partial\Omega. \end{cases}$$

λ is a regularization parameter.

Example 2: Cooling of the wire of the Rope-balance.

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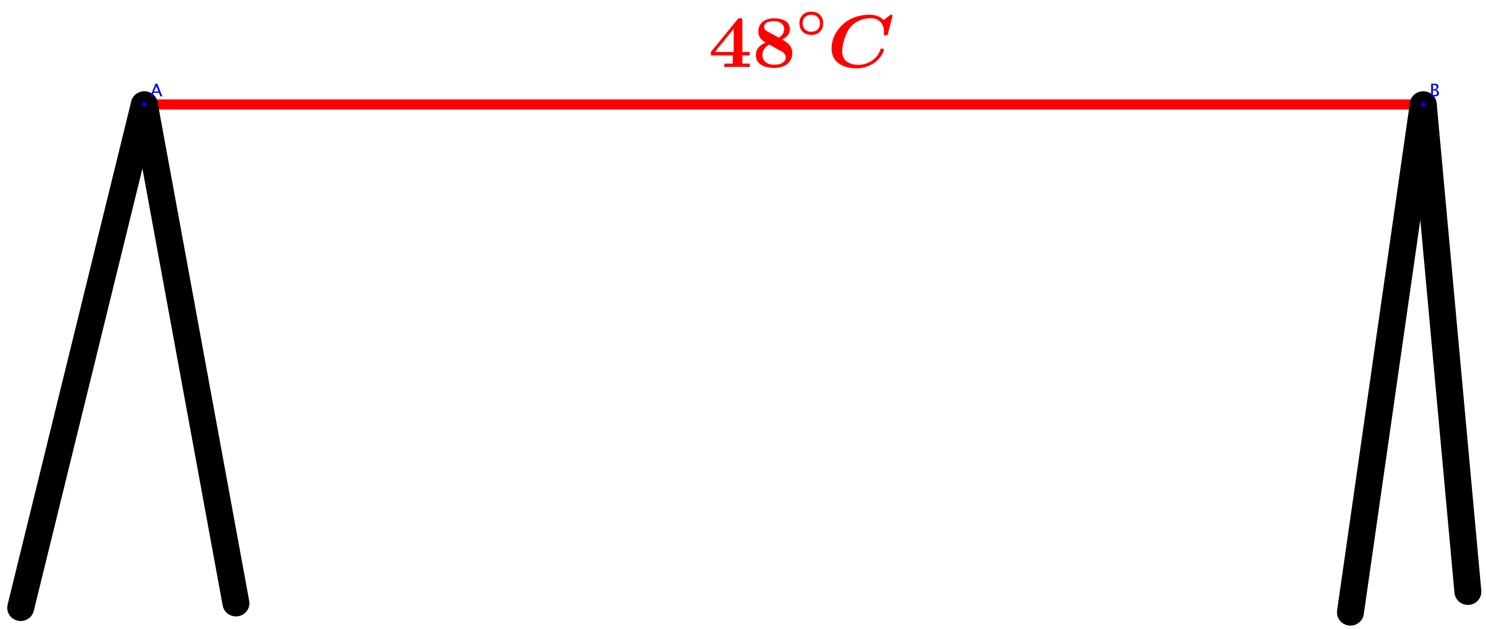

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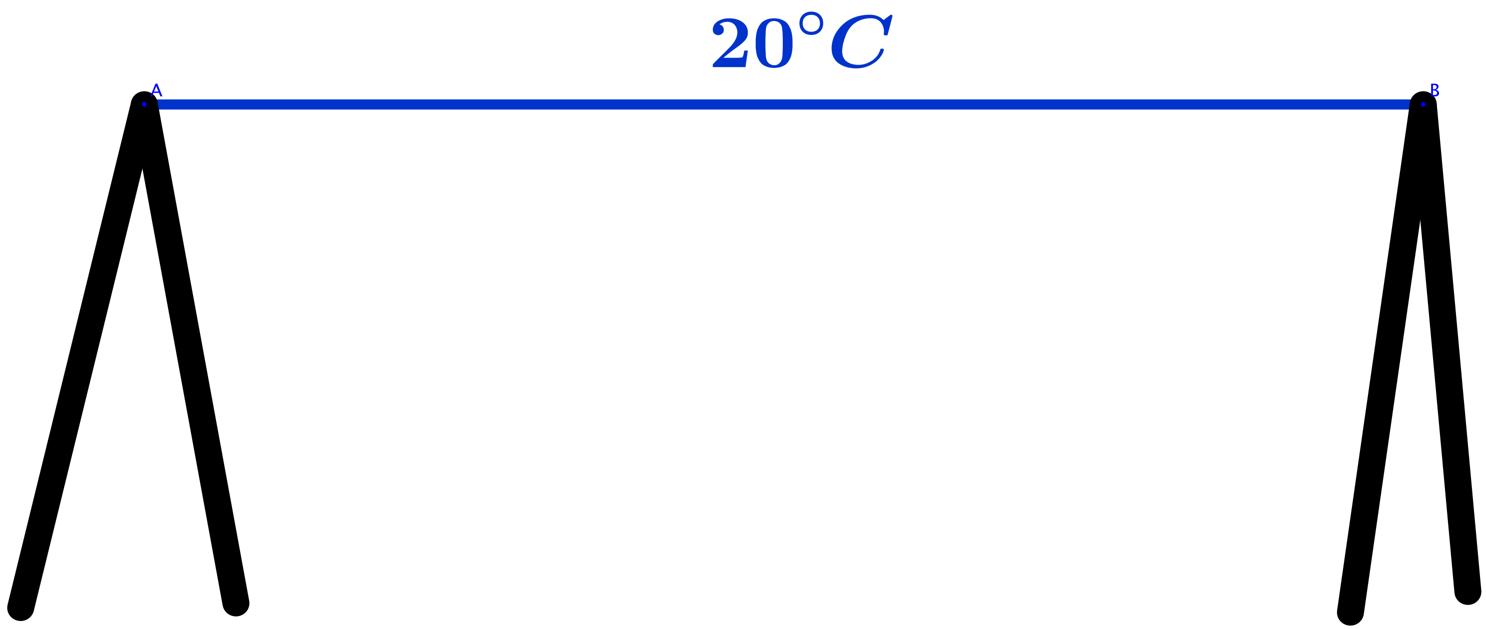

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- To cool down the temperature $y(x,t)$ of the wire by putting ice (external source $u(x,t)$) so as to achieve a final temperature target $\hat{y}(x)$.

y satisfies:

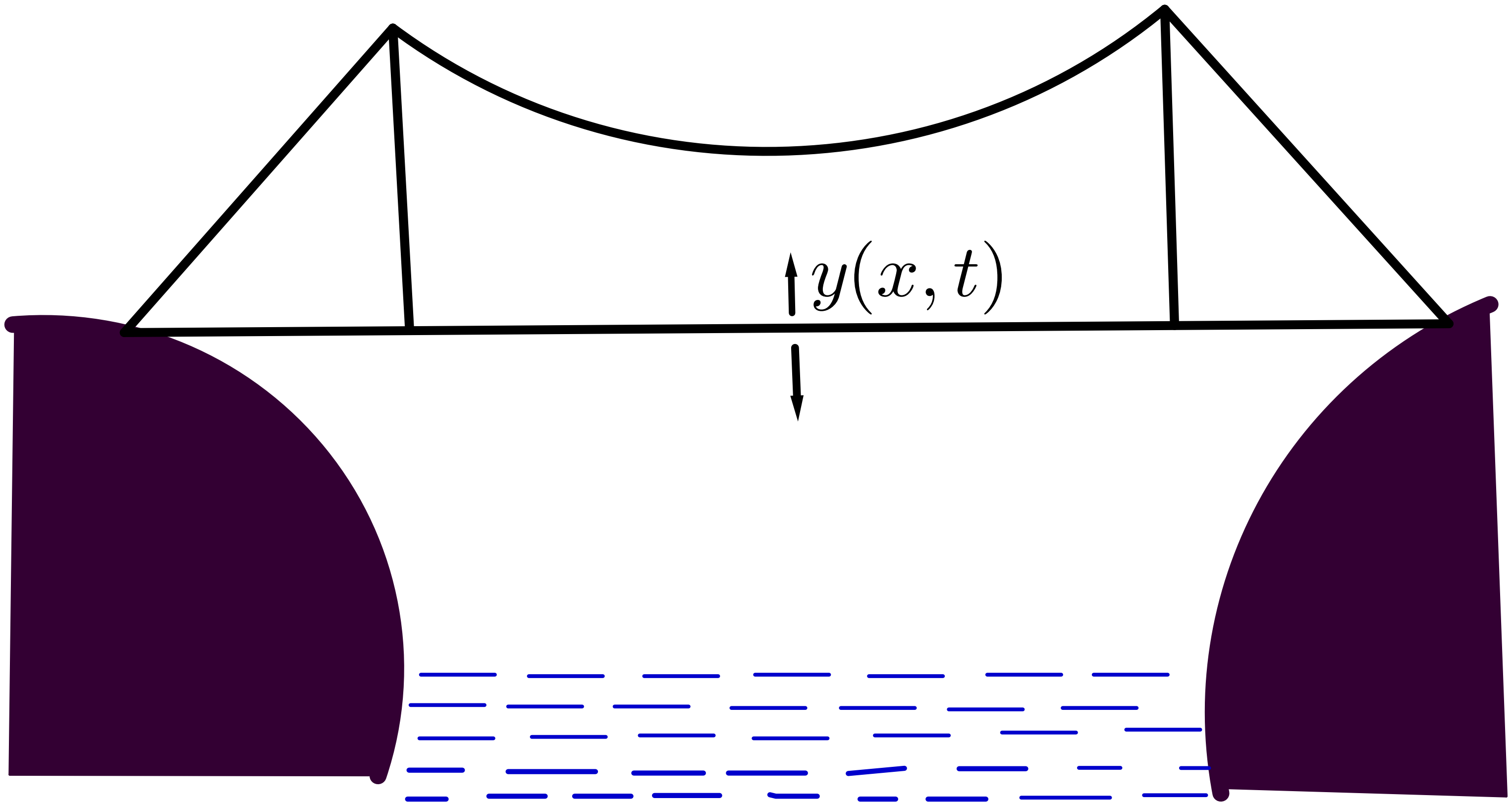
$$\begin{cases} \partial_t y - \mathrm{div}\,(\nu \nabla y) = u, & x \in \Omega, t \in (0,T), \\ y(x,0) = y_0(x), & x \in \Omega, \\ y(x,t) = g(x,t), & x \in \partial\Omega \times (0,T). \end{cases}$$

The goal is to approximate the desired temperature $\hat{y}$ at the final time T

$$\frac{1}{2}\int_\Omega (y(x,T) - \hat{y}(x))^2\, dx + \frac{\lambda}{2}\int_0^T \int_\Omega u^2(x,t) dx dt.$$

Example 3: Optimal vibration problem.

- Suppose a group of students are jumping on a river bridge while crossing. $y(x,t)$ is the transversal displacement of the bridge and $u(x,t)$ is the vertical force acting on it.



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To minimize

$$\frac{1}{2}\int_0^T \int_\Omega (y(x,t)-\hat{y}(x,t))^2\, dxdt + \frac{\lambda}{2}\int_0^T \int_\Omega u^2(x,t)dxdt.$$

subject to

$$\begin{cases} \partial_{tt} y - \Delta y = u, & x \in \Omega, t \in (0,T), \\ y(x,0) = y_0(x), & x \in \Omega, \\ \partial_t y(x,0) = \bar{y}_0(x), & x \in \Omega, \\ y(x,t) = g(x,t), & x \in \partial\Omega \times (0,T). \end{cases}$$

Formulation of PDE-constrained optimization problem

- F. Tröltzsch: *Optimal Control of Partial Differential Equations - Theory, Methods and Applications*, 2010.

Optimality system: For state equation $E(y,u) = 0$, the Lagrangian is:

$$L(y,u,p) := J(y,u) + \int_\Omega E(y,u)p,$$

with $\nabla_p L(y,u,p) = 0, \nabla_y L(y,u,p) = 0, \nabla_u L(y,u,p) = 0.$

$$\begin{cases} -\kappa\Delta y = u, \\ y|_{\partial\Omega} = 0, \end{cases} \qquad \begin{cases} -\kappa\Delta p = y - \hat{y}, \\ p|_{\partial\Omega} = 0, \end{cases}$$

$$p(x) + \lambda u(x) = 0.$$

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$$\boxed{\begin{array}{c} \begin{cases} \partial_t y - \nu\Delta y = u, \\ y(x,0) = y_0(x), \\ y|_{\partial\Omega} = g, \end{cases} \qquad \begin{cases} -\partial_t p - \nu\Delta p = y - \hat{y}, \\ p(x,T) = 0, \\ p|_{\partial\Omega} = 0, \end{cases} \\ \\ p(x,t) + \lambda u(x,t) = 0. \end{array}}$$

▶ Need fast and robust numerical methods to solve the PDEs.

Domain Decomposition Methods as solution tool

- Heinkenschloss and Herty: *A spatial domain decomposition method for parabolic optimal control problems*, J. Comp. Appl. Math., 2007.

  1. The optimality conditions are decomposed using a spatial domain decomposition.
  2. The subdomain problems are coupled through Neumann transmission conditions.
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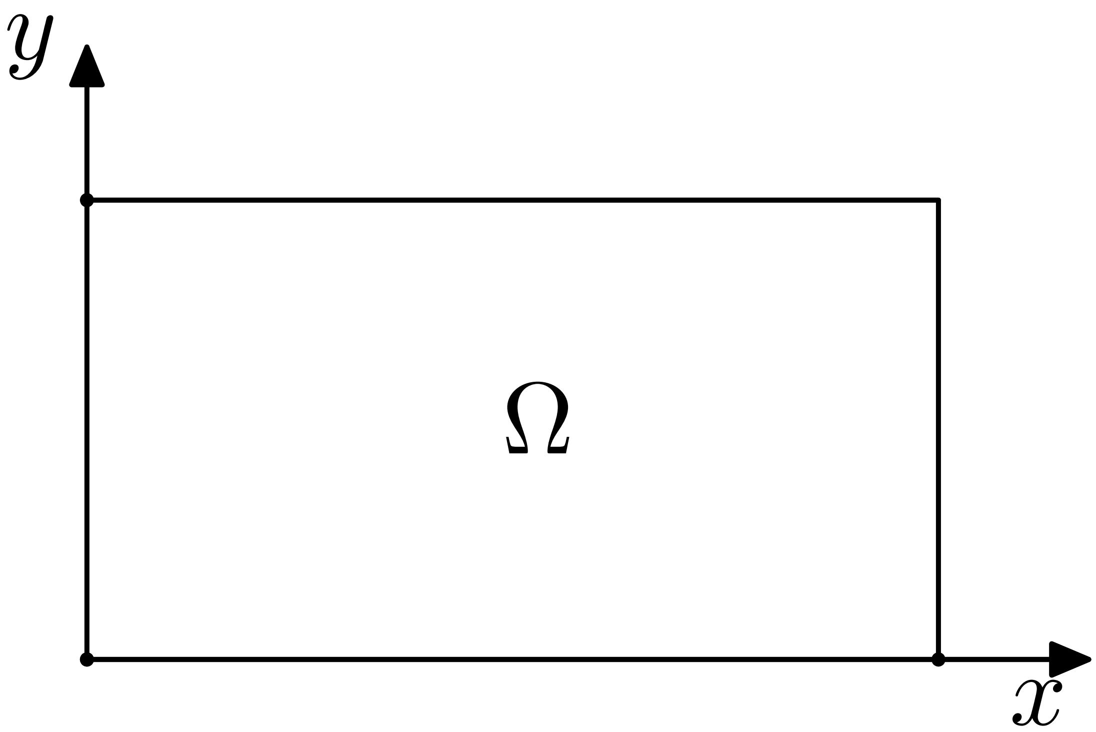
▶ No convergence analysis available!

1. SUBSTRUCTURING METHODS
   - Behavior for steady problems
   - Convergence for Optimal Control Problems
2. DIRICHLET-NEUMANN WAVEFORM RELAXATION
   - Linear PDEs
   - Non-linear PDEs
3. NEUMANN-NEUMANN WAVEFORM RELAXATION
   - Linear PDEs
   - Non-linear PDEs
4. APPLICATION TO OCP
   - Efficiency of DNWR and NNWR
   - Numerically optimum parameters for Control Problem

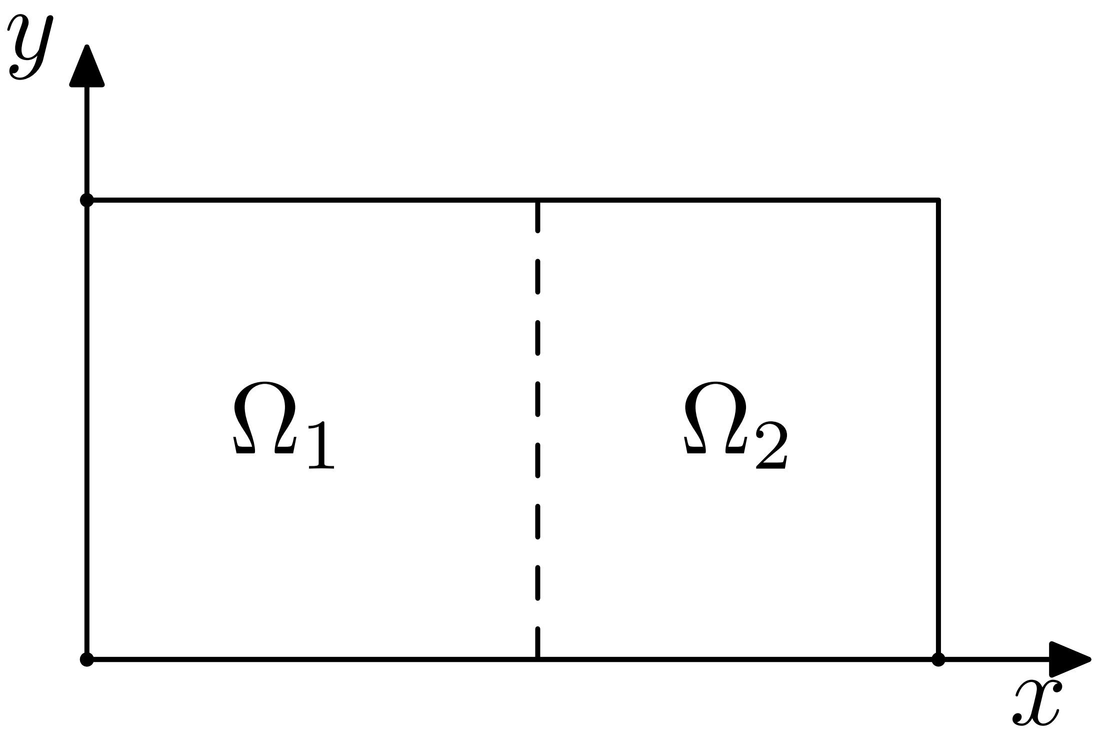
Dirichlet-Neumann Method



Poisson Equation

$$
\begin{aligned}
-\Delta u &= f, && \text{in } \Omega \\
u &= 0, && \text{on } \partial\Omega.
\end{aligned}
$$

Dirichlet-Neumann Method



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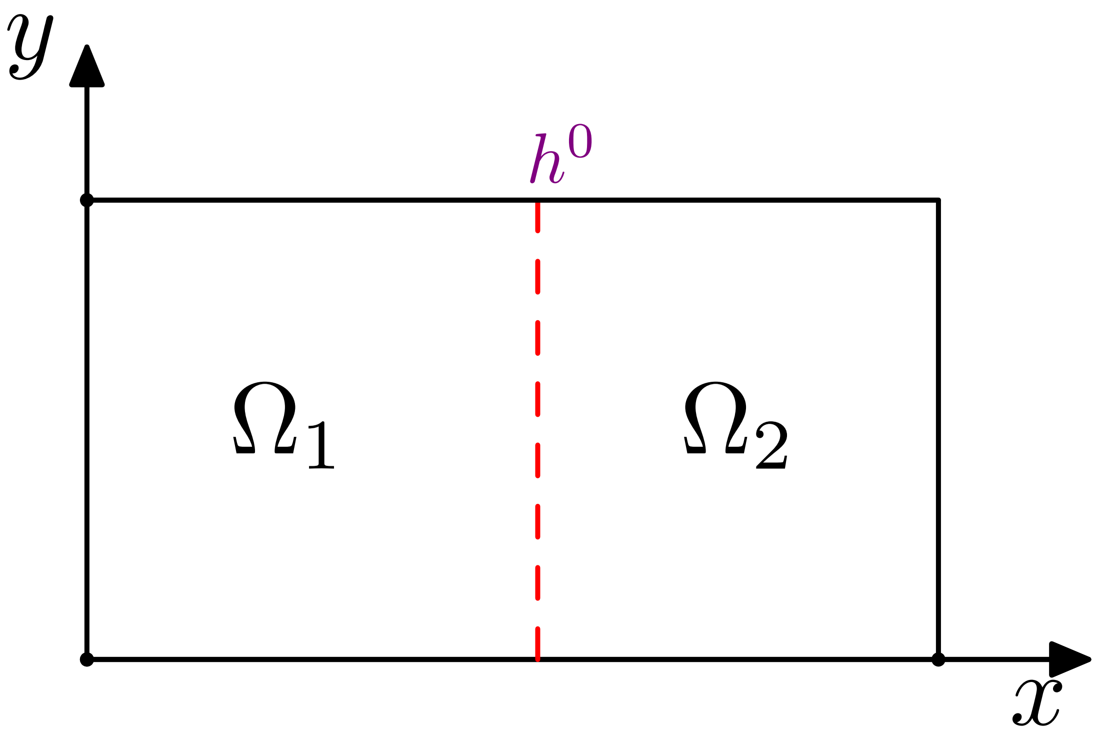
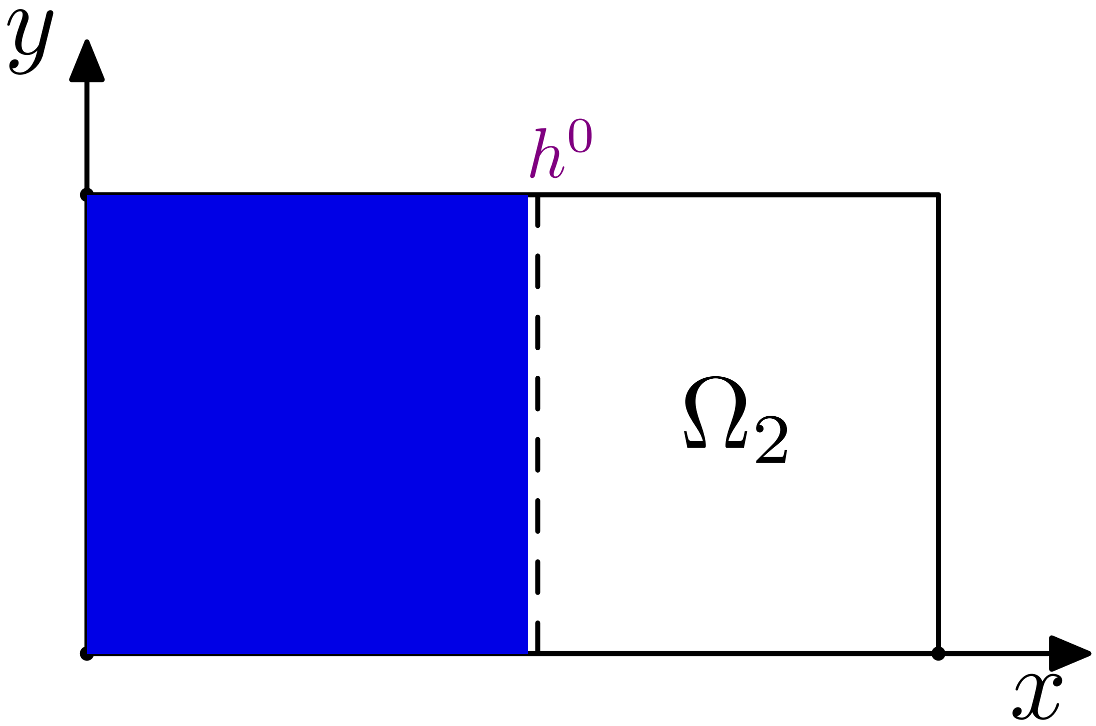


Dirichlet Trace $h^0(y)$ along the interface is given.

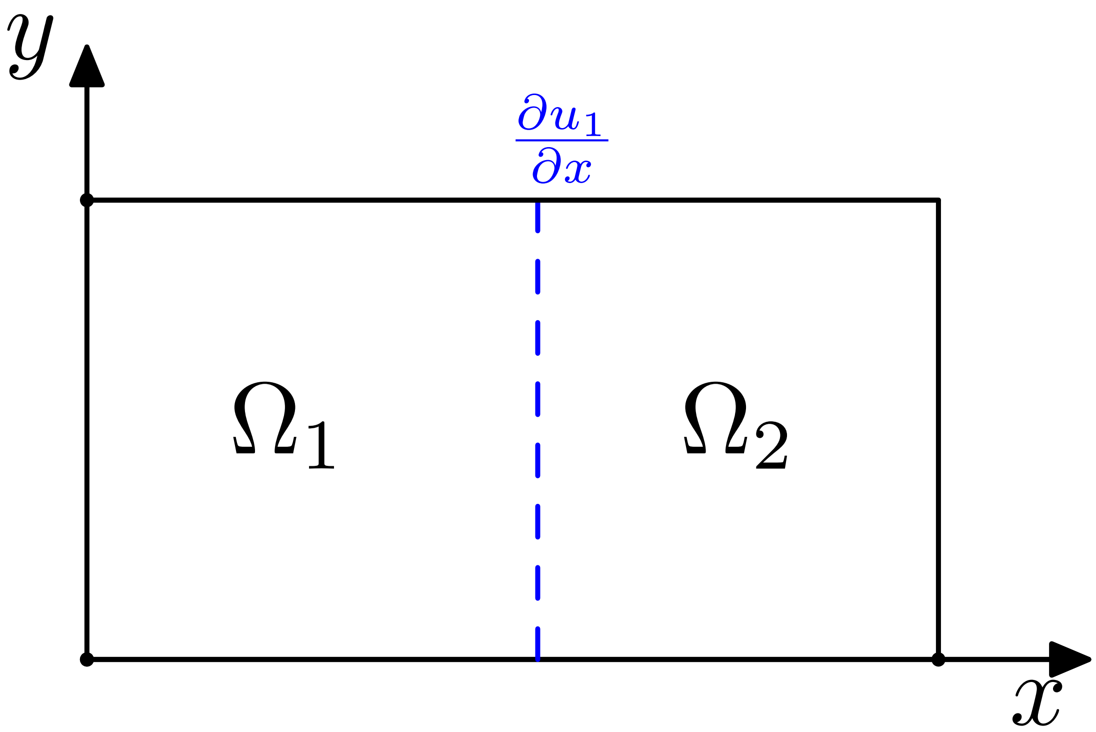
Dirichlet-Neumann Method



$$\begin{cases} -\triangle u_1^k & = f, \\ u_1^k(-a, y) & = 0, \\ u_1^k(0, y) & = h^{k-1}(y). \end{cases}$$

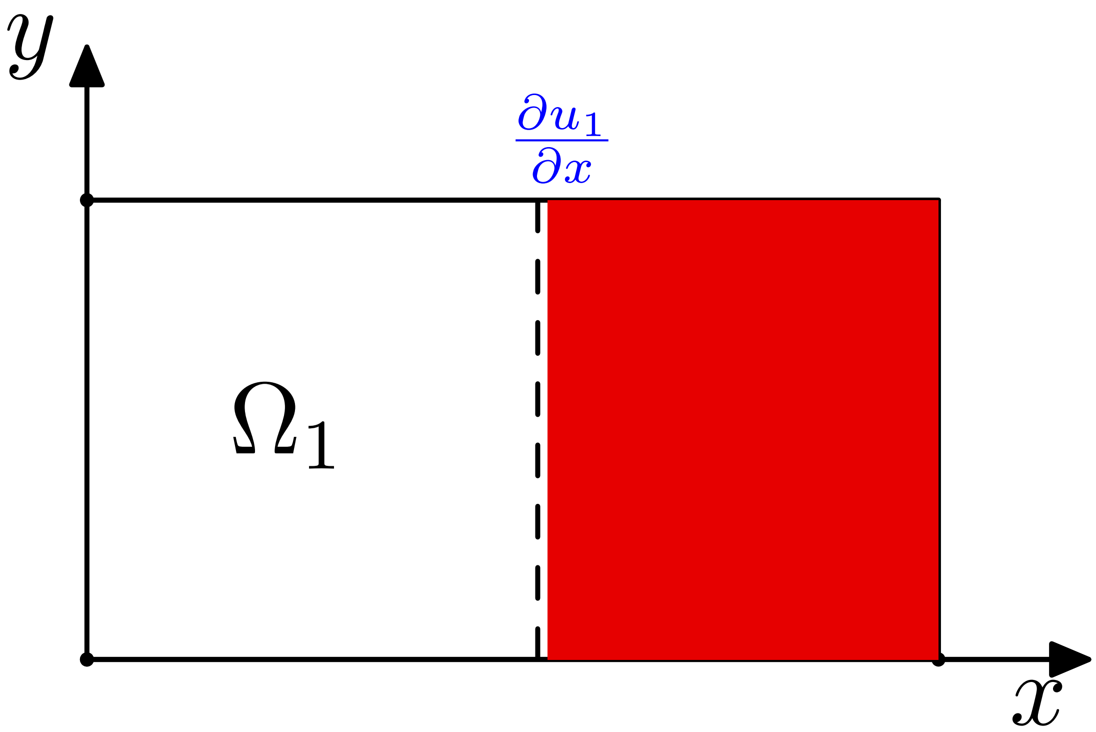
Dirichlet Subproblem

Dirichlet-Neumann Method



$$\begin{cases} -\triangle u_1^k & = f, \\ u_1^k(-a, y) & = 0, \\ u_1^k(0, y) & = h^{k-1}(y). \end{cases} \Longrightarrow \frac{\partial u_1^k}{\partial x}(0, y) \quad \underline{\text{Neumann Trace}}$$

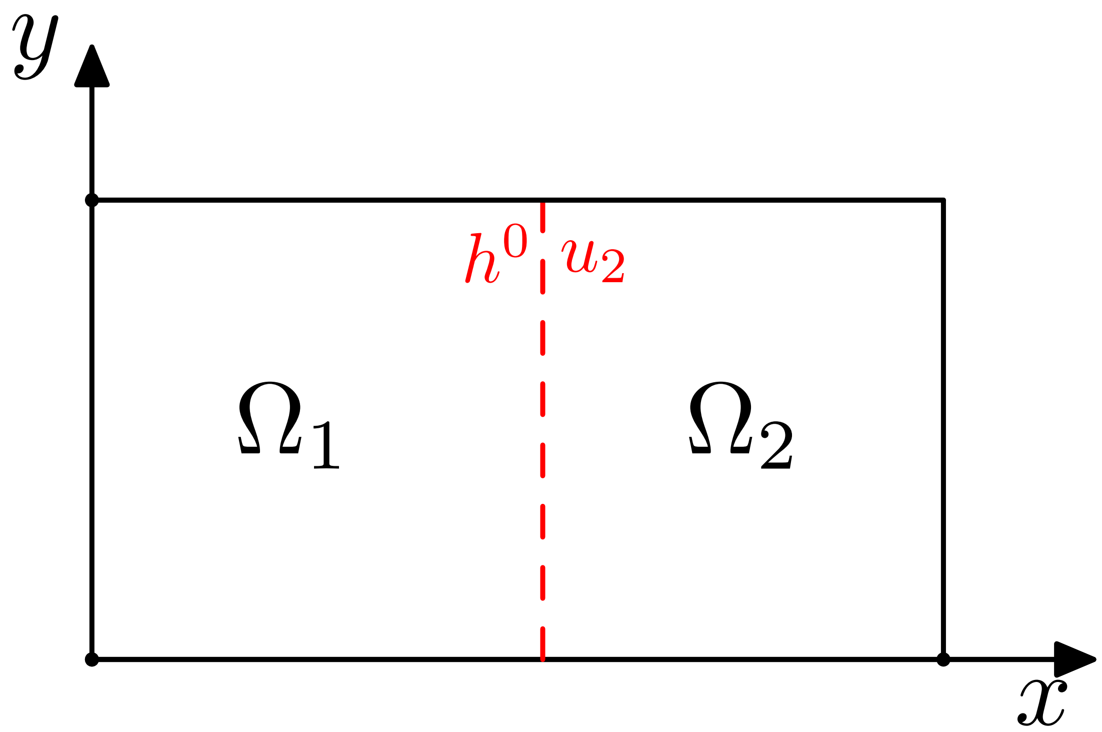
Dirichlet-Neumann Method



Neumann Subproblem

$$\begin{cases} -\triangle u_2^k & = f, \\ \partial_x u_2^k(0,y) & = \partial_x u_1^k(0,y), \\ u_2^k(b,y) & = 0. \end{cases}$$

Dirichlet-Neumann Method

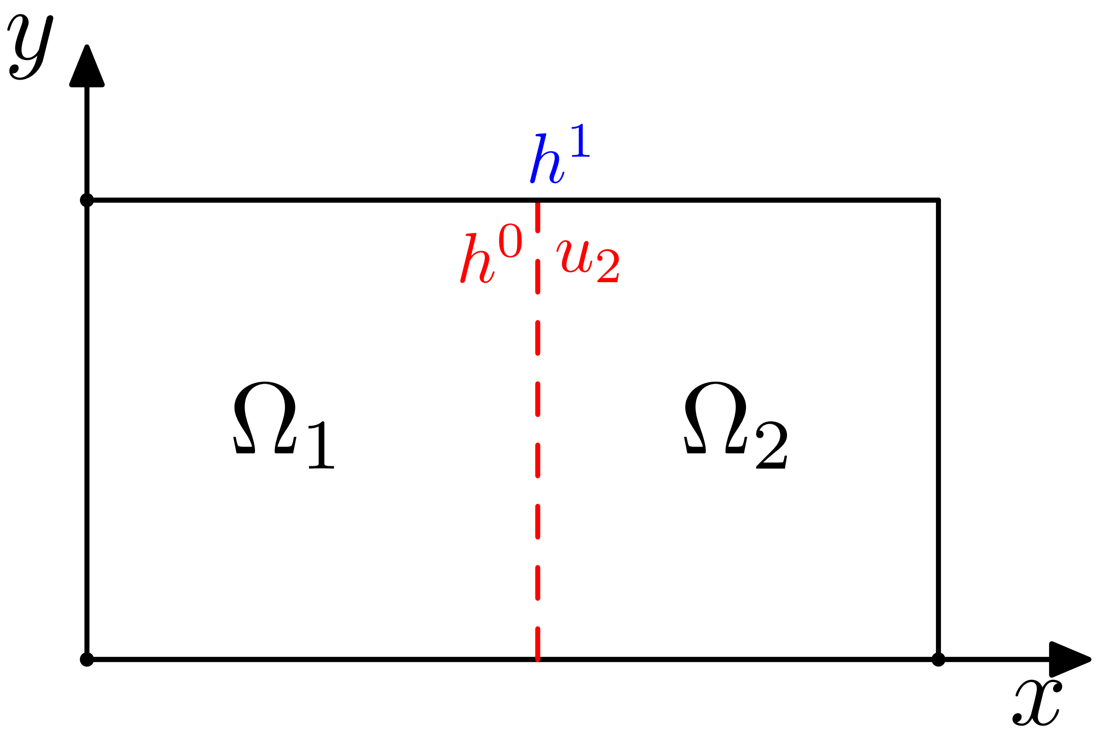


Update condition

$$h^k(y) = (1-\theta)h^{k-1}(y) + \theta u_2^k(0,y),$$

θ : positive relaxation parameter.

Dirichlet-Neumann Method



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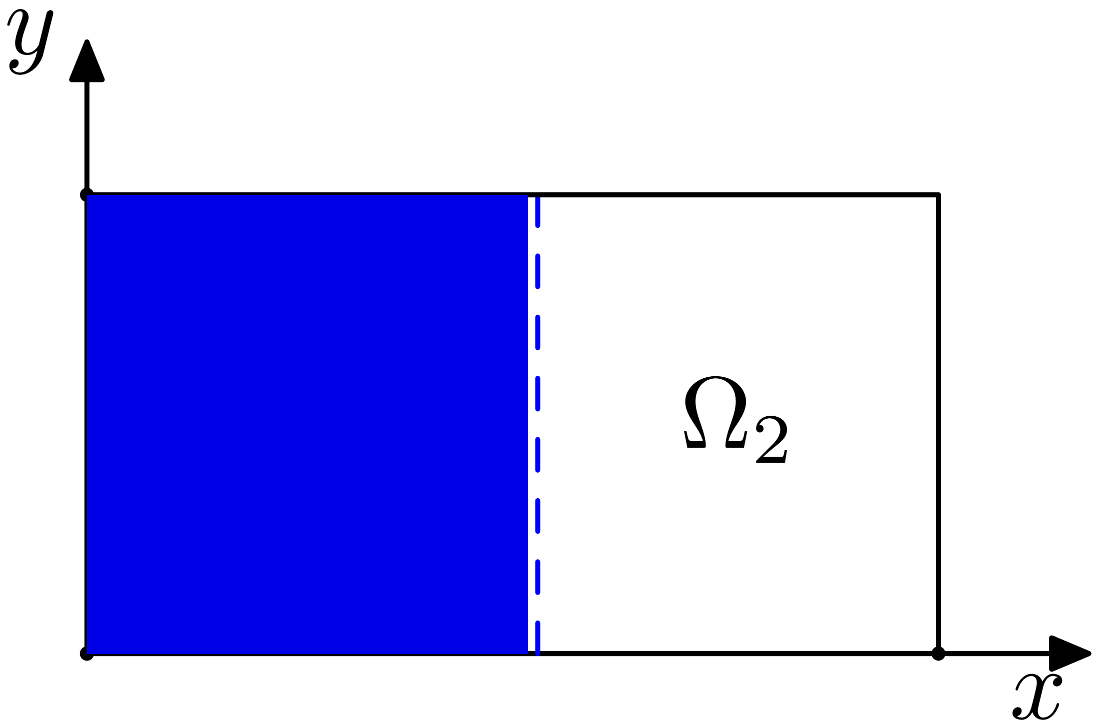

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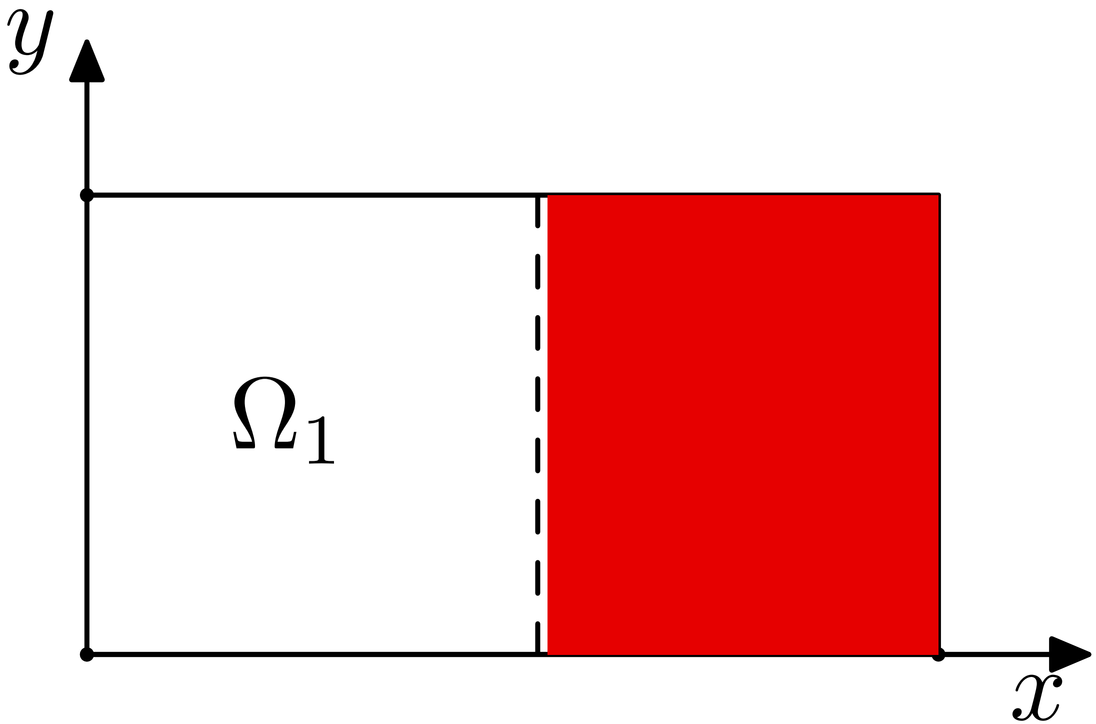

DN Method: Convergence Result

Given h^0 along the interface,

$$\begin{cases} -\triangle u_1^{[k]} & = 0, \\ u_1^{[k]}(-a) & = 0, \\ u_1^{[k]}(0) & = h^{[k-1]}, \end{cases} \qquad \begin{cases} -\triangle u_2^{[k]} & = 0, \\ \partial_x u_2^{[k]}(0) & = \partial_x u_1^{[k]}(0), \\ u_2^{[k]}(b) & = 0. \end{cases}$$

The update condition:

$$h^{[k]} = \left\{1 - \theta \frac{l(\Omega)}{l(\Omega_1)}\right\}^k h^{[0]}, \qquad k = 1, 2, 3, \ldots,$$

with θ being a relaxation parameter.

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$$h^{[k]} = \left\{1 - \theta \frac{l(\Omega)}{l(\Omega_1)}\right\}^k h^{[0]}, \qquad k = 1, 2, 3, \ldots,$$

with θ being a relaxation parameter.

- The convergence is linear for $\theta \neq \frac{l(\Omega_1)}{l(\Omega)}$.
- Two step convergence to the exact solution for $\theta = \frac{l(\Omega_1)}{l(\Omega)}$.

$$\begin{cases} -u'' = 0, & x \in \Omega = (-3, 2), \\ u(-3) = 0 = u(2). \end{cases}$$

$\Omega_1 = (-3, 0), \Omega_2 = (0, 2), h^0 = 10.$

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$l(\Omega_1) = 3, l(\Omega) = 5, \Longrightarrow \theta^* = \frac{l(\Omega_1)}{l(\Omega)} = \frac{3}{5}.$

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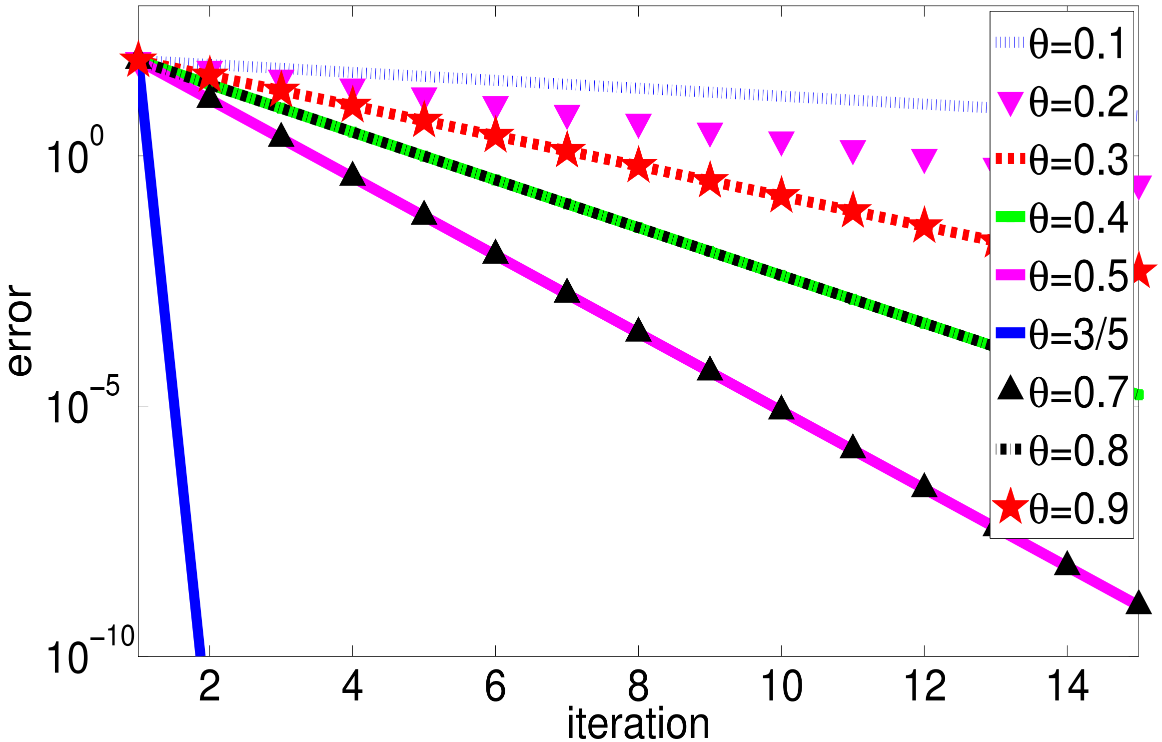


Optimal Control Problem: DN Method

$$\text{Minimize } J(y,u) = \frac{1}{2}\int_0^1 (y(x)-\hat{y}(x))^2\,dx + \frac{\lambda}{2}\int_0^1 u^2(x)dx,$$
$$\text{subject to } \begin{cases} -\Delta y(x) = u(x), & x \in \Omega, \\ y(x) = 0, & x \in \partial\Omega, \end{cases} \tag{1}$$

The adjoint equation is:

$$\begin{cases} -\Delta p(x) = y(x) - \hat{y}(x), & x \in \Omega, \\ p(x) = 0, & x \in \partial\Omega, \end{cases} \tag{2}$$

with the optimality condition

$$p(x) + \lambda u(x) = 0.$$

Given initial Dirichlet values $h_y^{[0]}$ and $h_p^{[0]}$ at $x = \alpha$

$$\begin{cases} -y_1'' = p_1/\lambda, & x \in \Omega_1, \\ y_1(0) = 0, \\ y_1(\alpha) = h_y \end{cases} \qquad \begin{cases} -p_1'' = y_1, & x \in \Omega_1, \\ p_1(0) = 0, \\ p_1(\alpha) = h_p \end{cases}$$

$$\begin{cases} -y_2'' = p_2/\lambda, & x \in \Omega_2, \\ \partial_x y_2(\alpha) = \partial_x y_1(\alpha), \\ y_2(1) = 0 \end{cases} \qquad \begin{cases} -p_2'' = y_2, & x \in \Omega_2, \\ \partial_x p_2(\alpha) = \partial_x p_1(\alpha), \\ p_2(1) = 0 \end{cases}$$

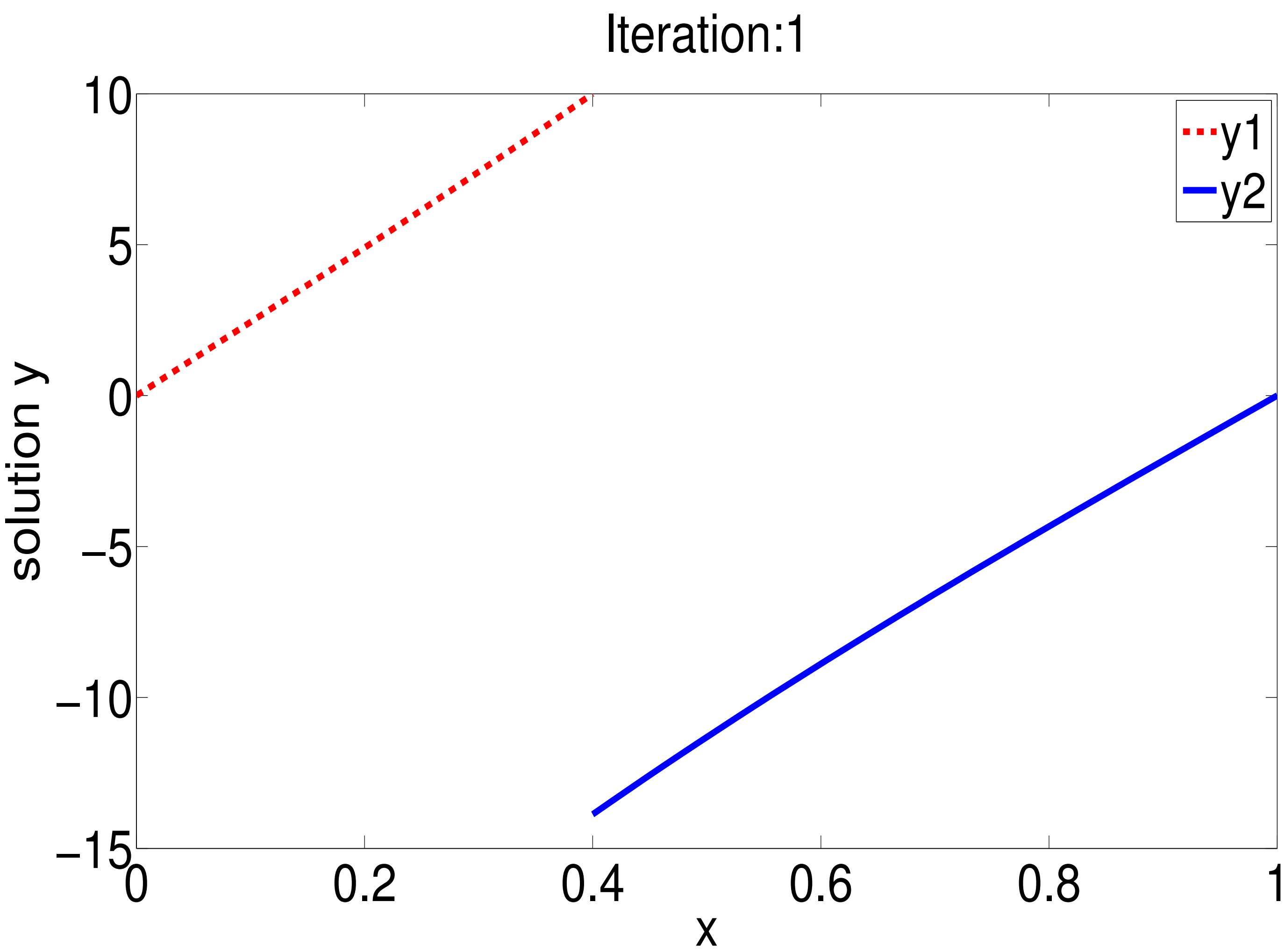
with the update conditions

$$\begin{aligned} h_y &= \theta_y y_2(\alpha) + (1-\theta_y) h_y, \\ h_p &= \theta_p p_2(\alpha) + (1-\theta_p) h_p. \end{aligned}$$

$\theta_y, \theta_p \in (0,1)$ being two relaxation parameters.

Optimal Control Problem: DN Method

Numerical experiment: $\alpha = 0.4, \lambda = 1$, $\theta_y = \theta_p = 0.6$. $h_y^0 = 10$.



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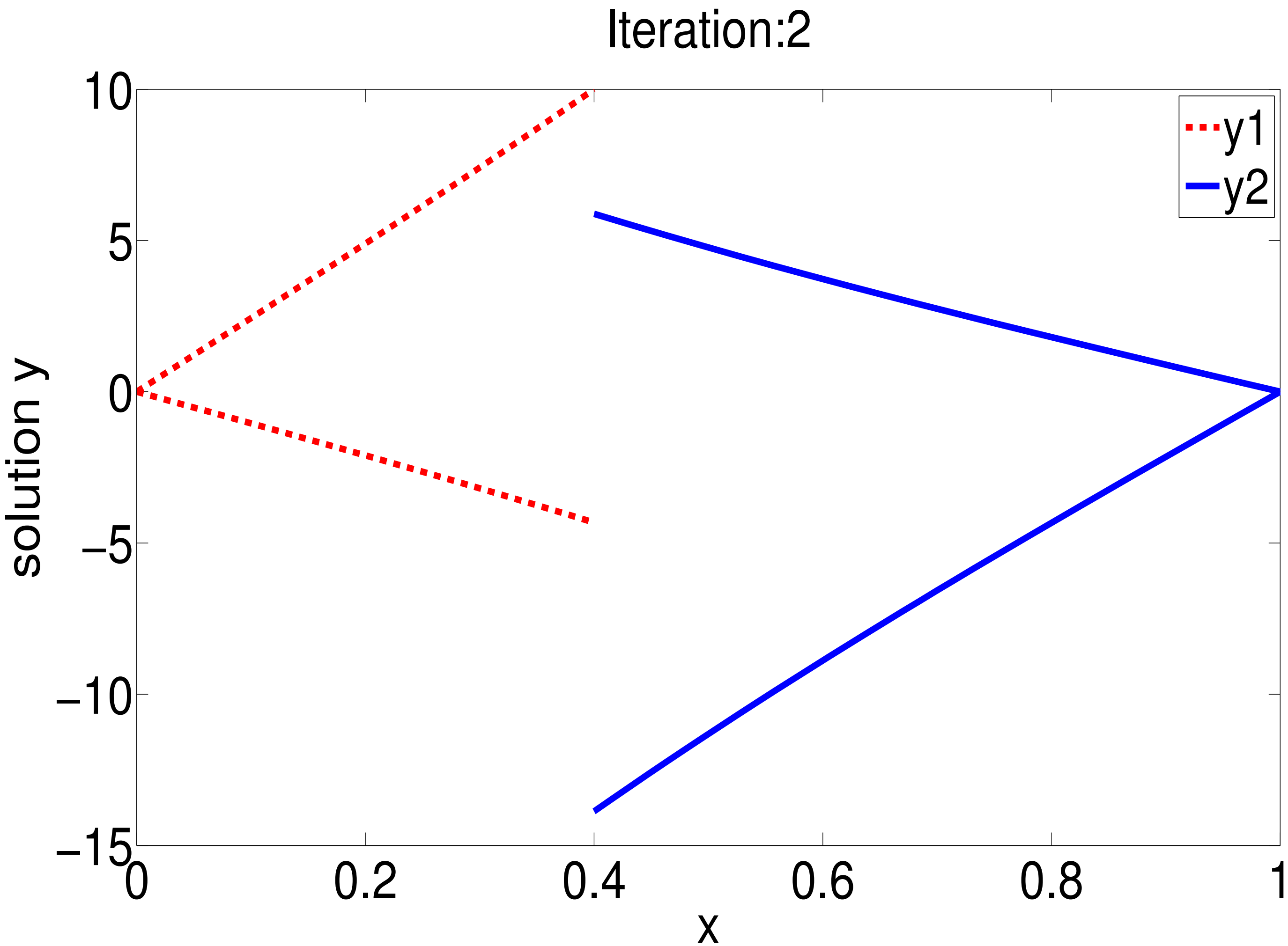

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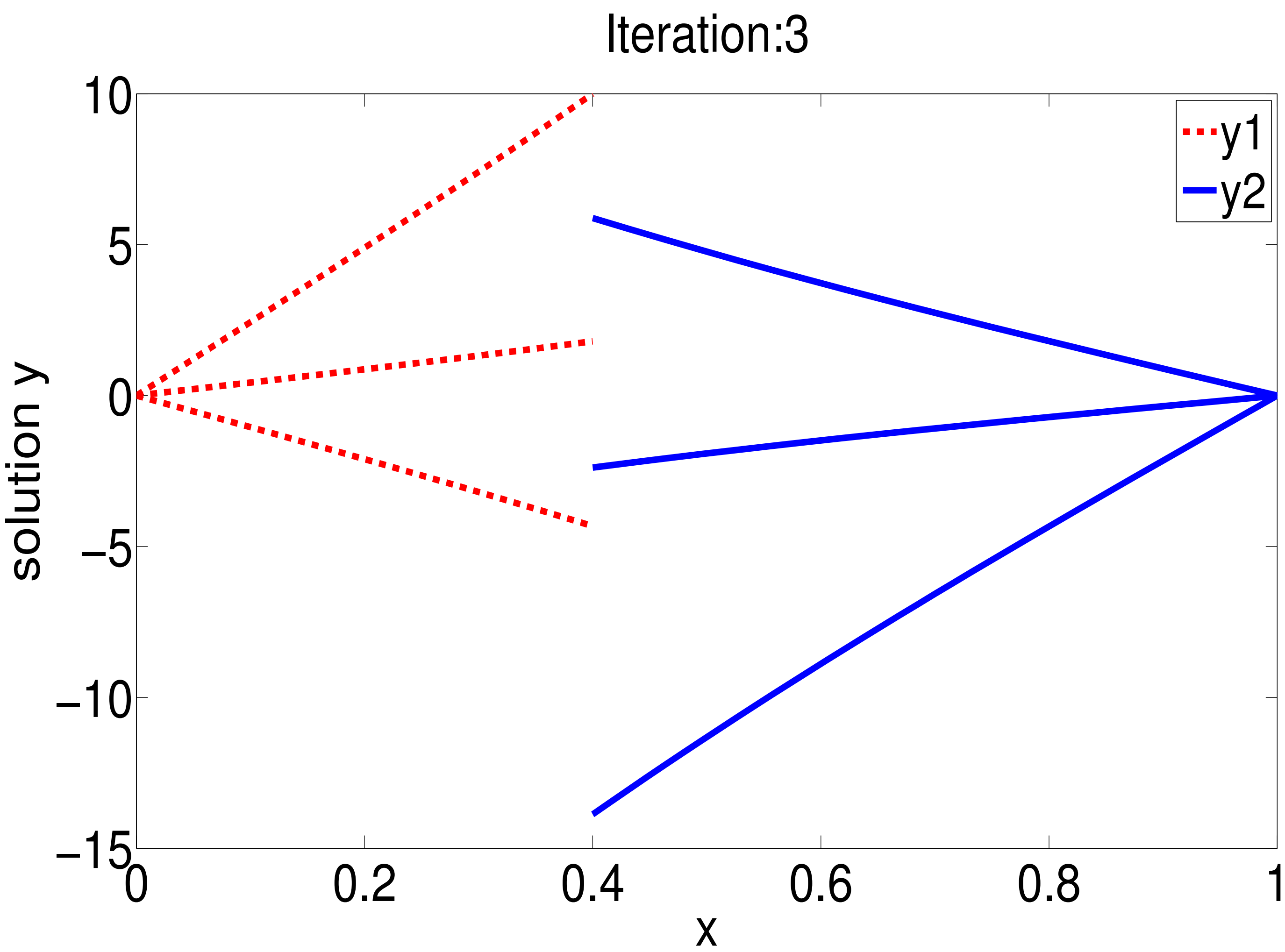

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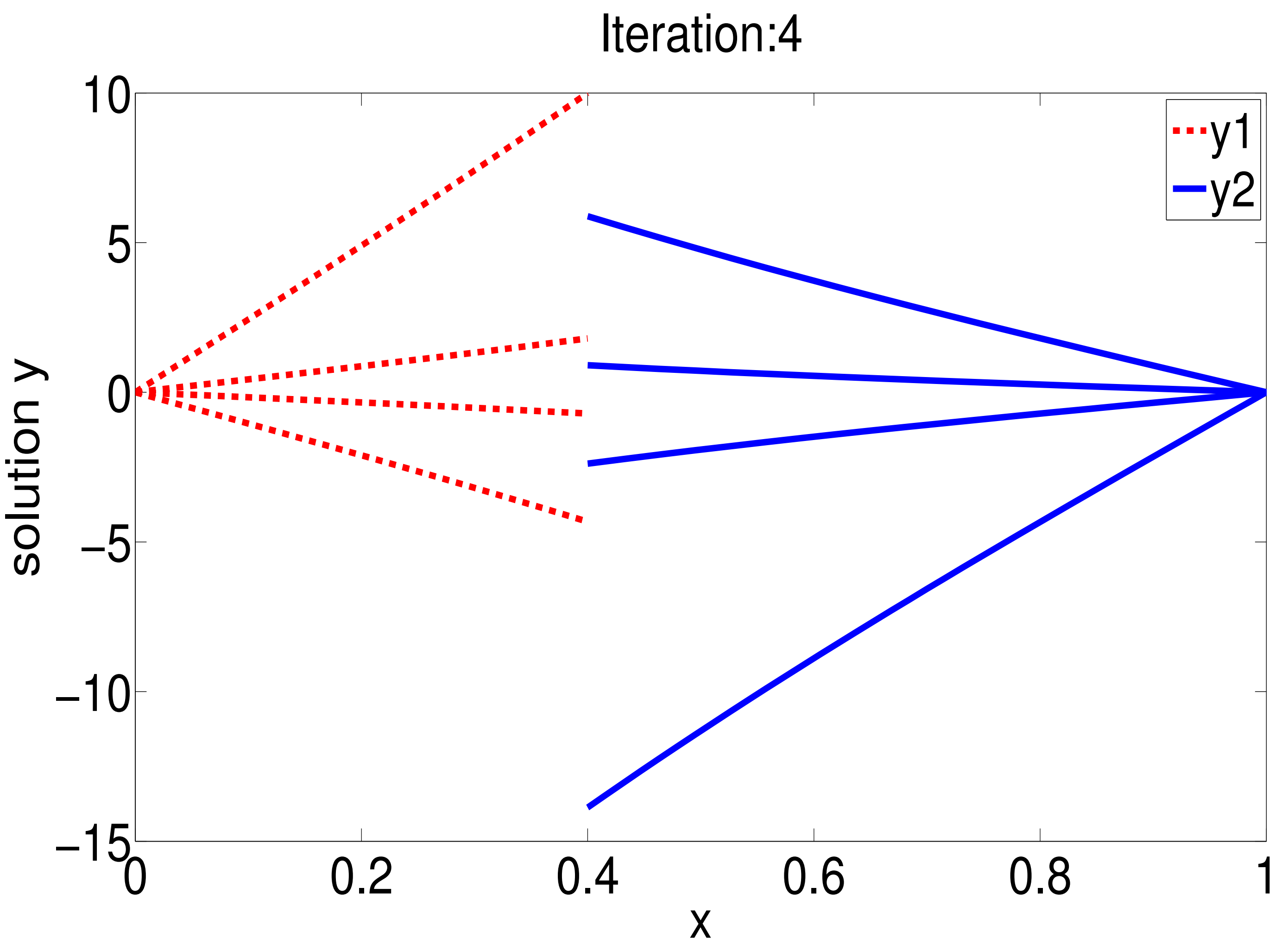

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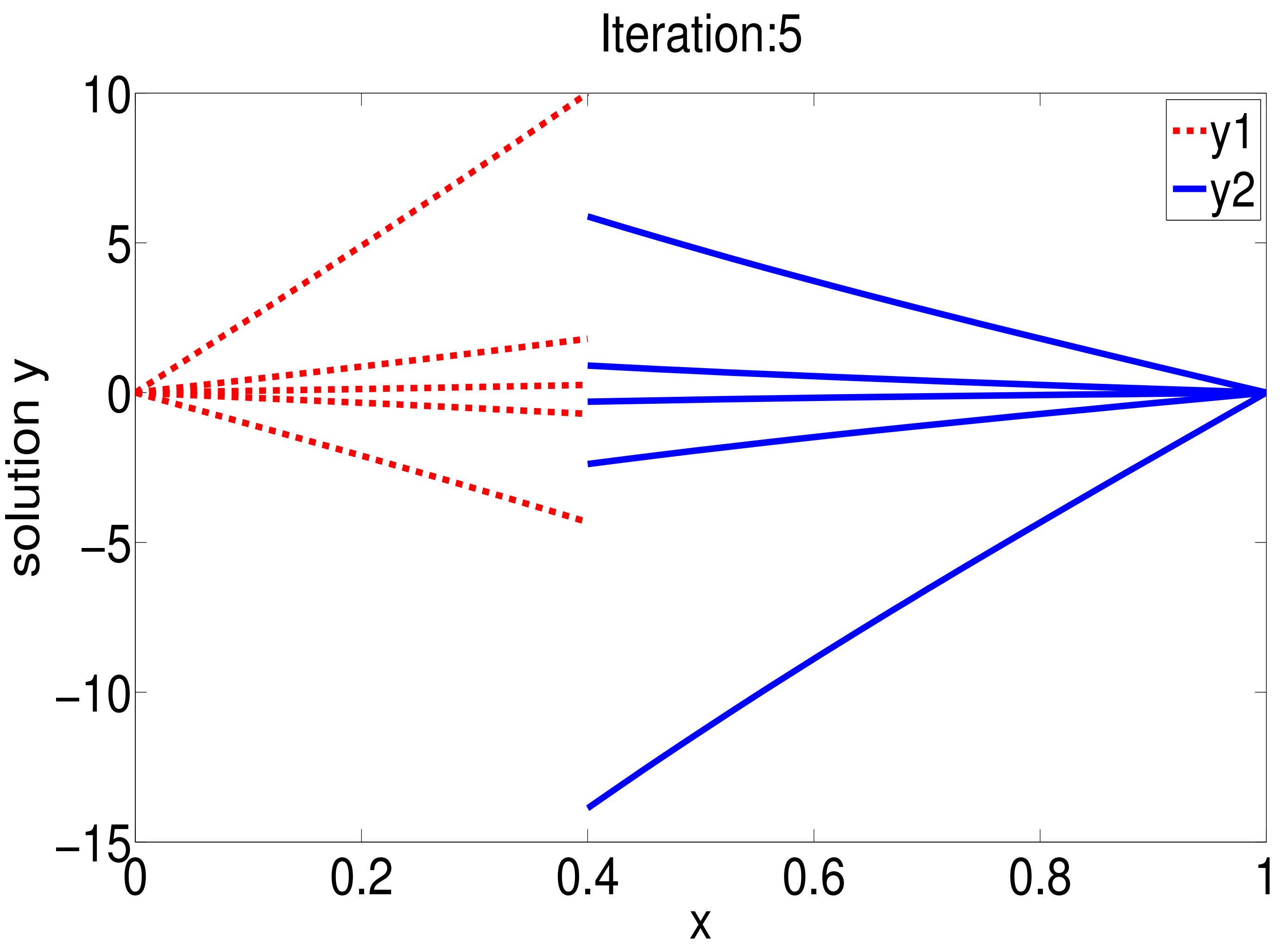

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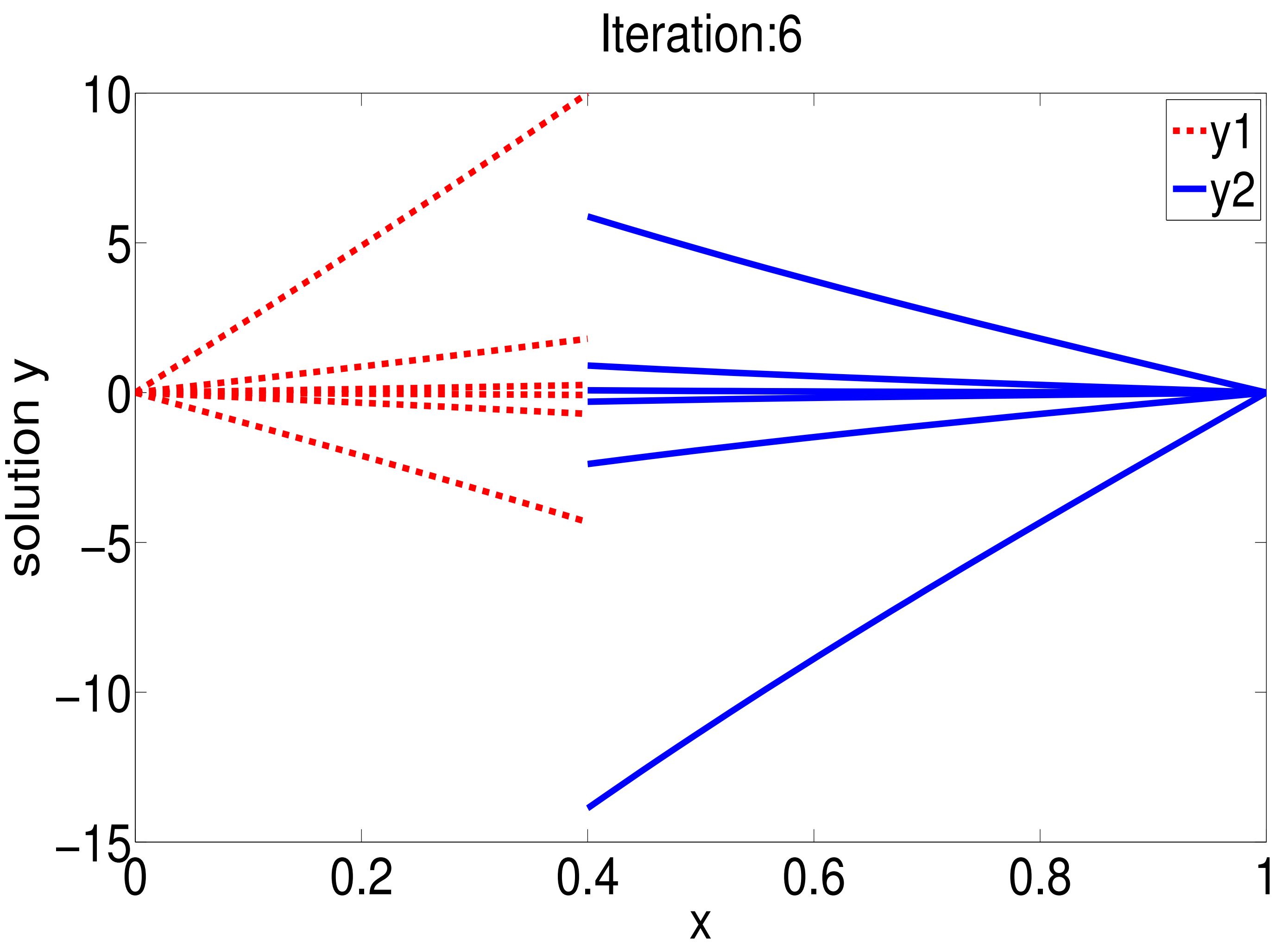

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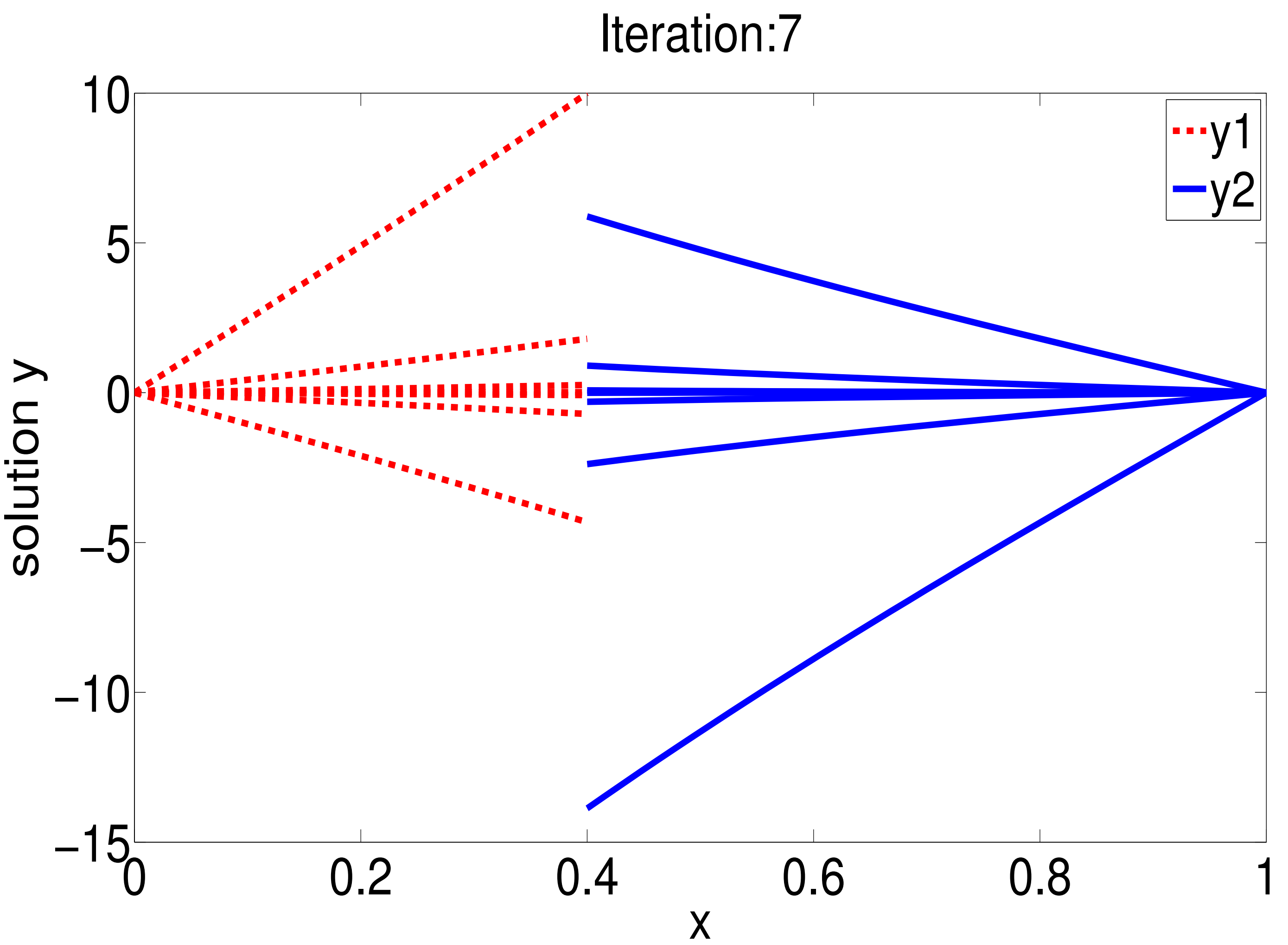

Optimal Control Problem: DN Method

- Can we optimize the convergence, like the DN method?

Optimal Control Problem: DN Method

The update conditions become:

$$\begin{pmatrix} h_y \\ h_p \end{pmatrix}^k = A^k \begin{pmatrix} h_y \\ h_p \end{pmatrix}^0, A = \begin{pmatrix} 1-\theta_y(1-v) & -\theta_y w \\ \theta_p w & 1-\theta_p(1-v) \end{pmatrix}$$

$\Rightarrow$ Convergence in $n+1$ iterations if $A^n = 0$.

$$w := \frac{\sinh\left(2\mu\alpha/\sqrt{2}\right)\sin\left(2\mu(1-\alpha)/\sqrt{2}\right) - \sin\left(2\mu\alpha/\sqrt{2}\right)\sinh\left(2\mu(1-\alpha)/\sqrt{2}\right)}{4\left(\left(\sinh\left(\frac{\mu\alpha}{\sqrt{2}}\right)\right)^2 + \left(\sin\left(\frac{\mu\alpha}{\sqrt{2}}\right)\right)^2\right)\left(\left(\cos\left(\frac{\mu(1-\alpha)}{\sqrt{2}}\right)\right)^2 + \left(\sinh\left(\frac{\mu(1-\alpha)}{\sqrt{2}}\right)\right)^2\right)},$$

$$v := -\frac{\sin\left(2\mu\alpha/\sqrt{2}\right)\sin\left(2\mu(1-\alpha)/\sqrt{2}\right) + \sinh\left(2\mu\alpha/\sqrt{2}\right)\sinh\left(2\mu(1-\alpha)/\sqrt{2}\right)}{4\left(\left(\sinh\left(\frac{\mu\alpha}{\sqrt{2}}\right)\right)^2 + \left(\sin\left(\frac{\mu\alpha}{\sqrt{2}}\right)\right)^2\right)\left(\left(\cos\left(\frac{\mu(1-\alpha)}{\sqrt{2}}\right)\right)^2 + \left(\sinh\left(\frac{\mu(1-\alpha)}{\sqrt{2}}\right)\right)2\right)}$$

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- $A \neq 0, A^2 = 0$, if θ_y, θ_p chosen carefully!

Optimal Control Problem: DN Method

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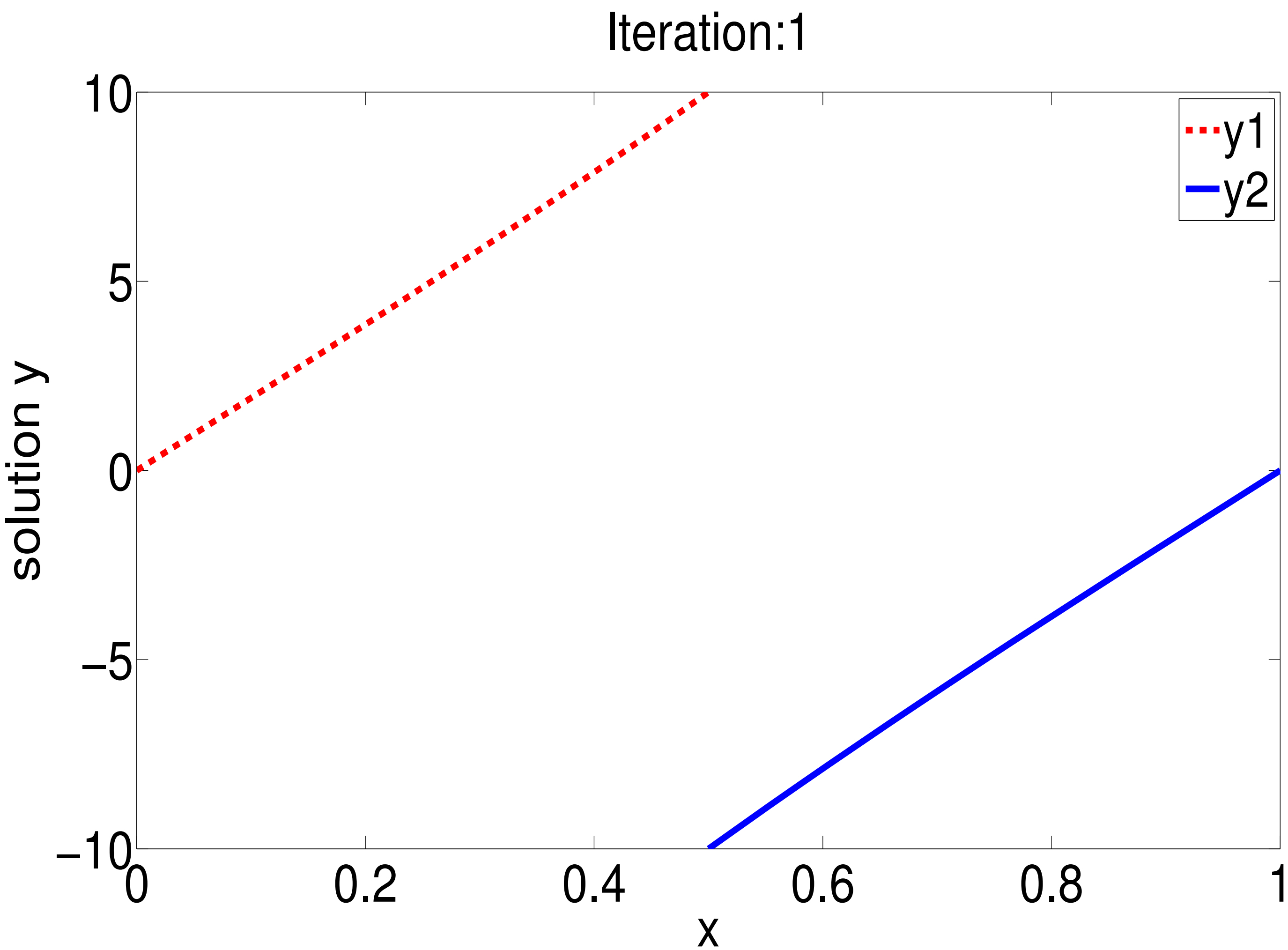
Theorem (*Convergence of DN) (Gander, Kwok, M. '18)*

The DN algorithm converges in at most 3 iterations, if the parameters (θ_y^*, θ_p^*) are given by

$$\theta_y^* = \frac{1}{(1-v)} + \frac{|w|}{(1-v)\sqrt{(1-v)^2+w^2}}, \theta_p^* = \frac{1}{(1-v)} - \frac{|w|}{(1-v)\sqrt{(1-v)^2+w^2}}.$$

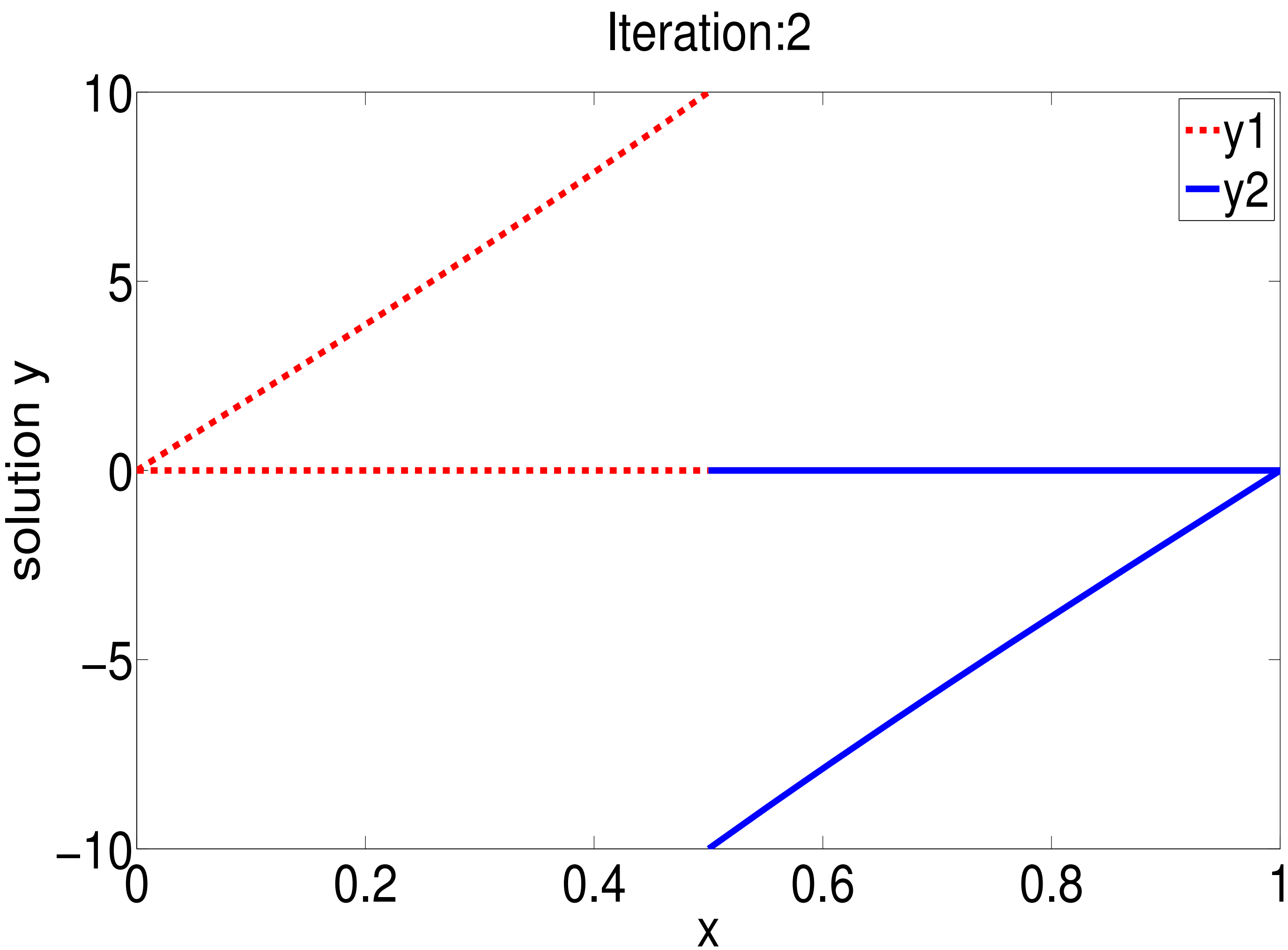
DN Method: Numerical test

1st experiment: $\alpha = 0.5, \lambda = 1,\ \theta_y^* = 1/2, \theta_p^* = 1/2.$



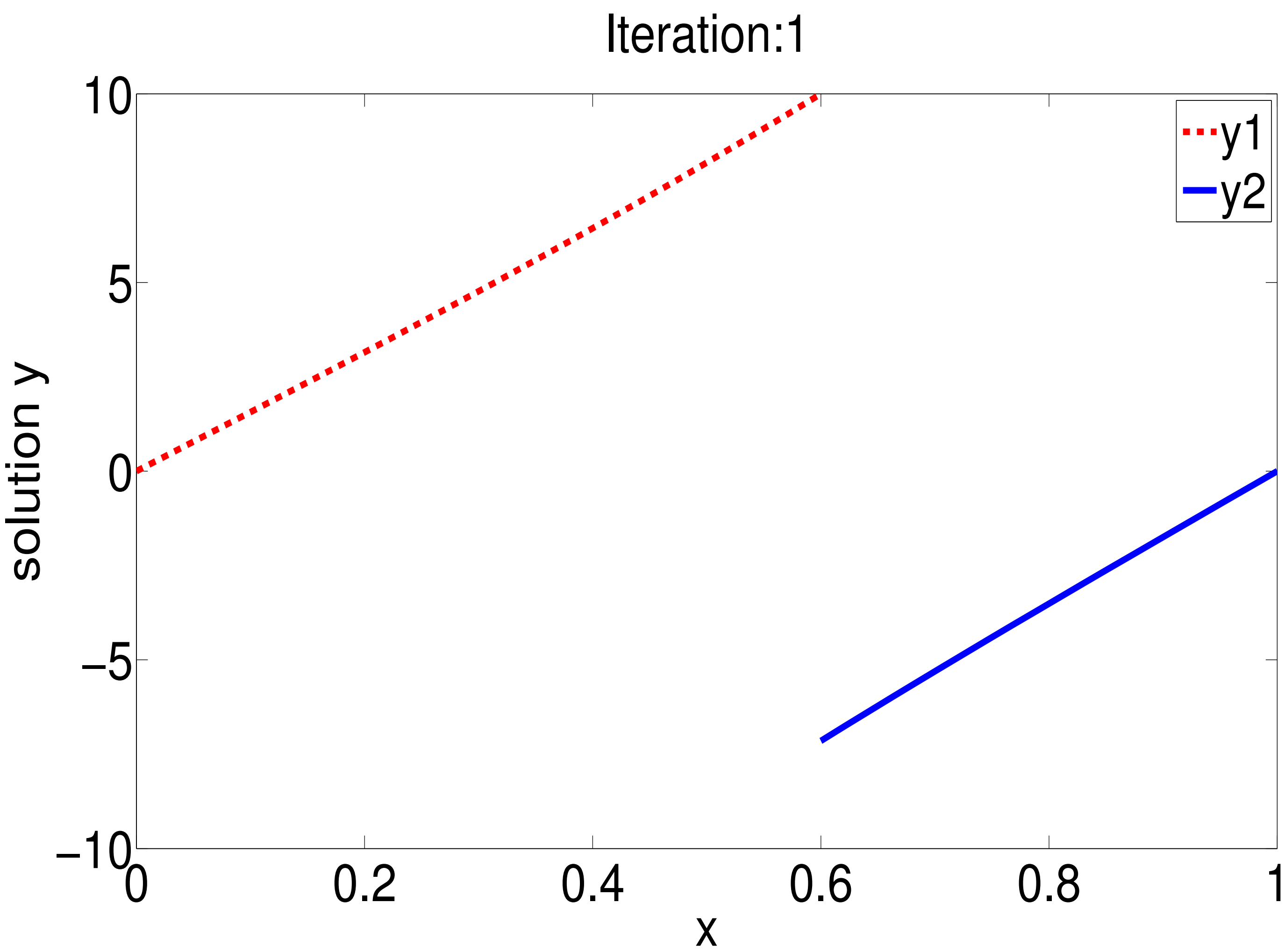
DN Method: Numerical test

1st experiment: $\alpha = 0.5, \lambda = 1,\ \theta_y^* = 1/2, \theta_p^* = 1/2.$



DN Method: Numerical test

2nd experiment: $\alpha = 0.6, \lambda = 1$, $\theta_y^* \approx 0.58, \theta_p^* \approx 0.61$.



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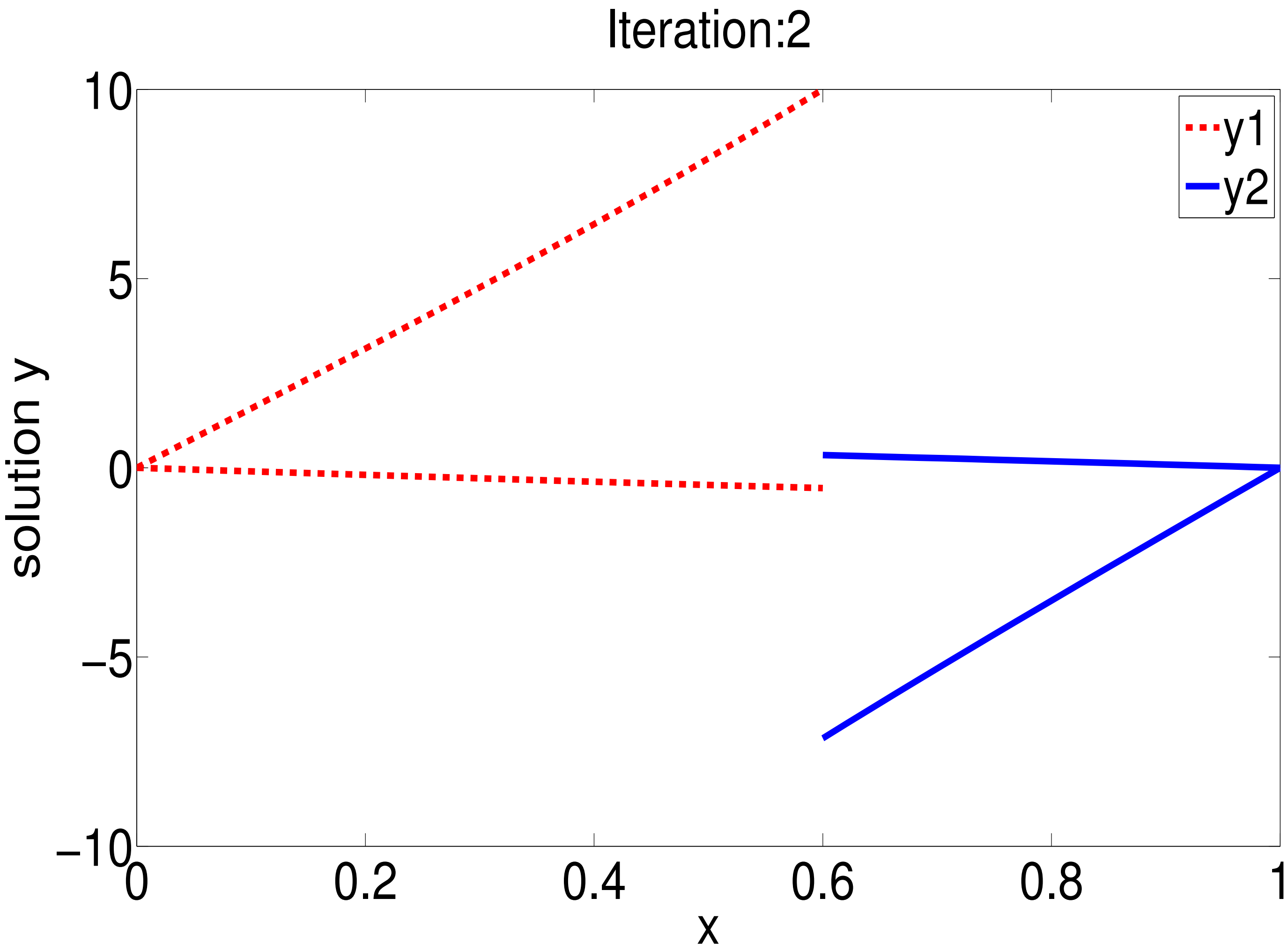

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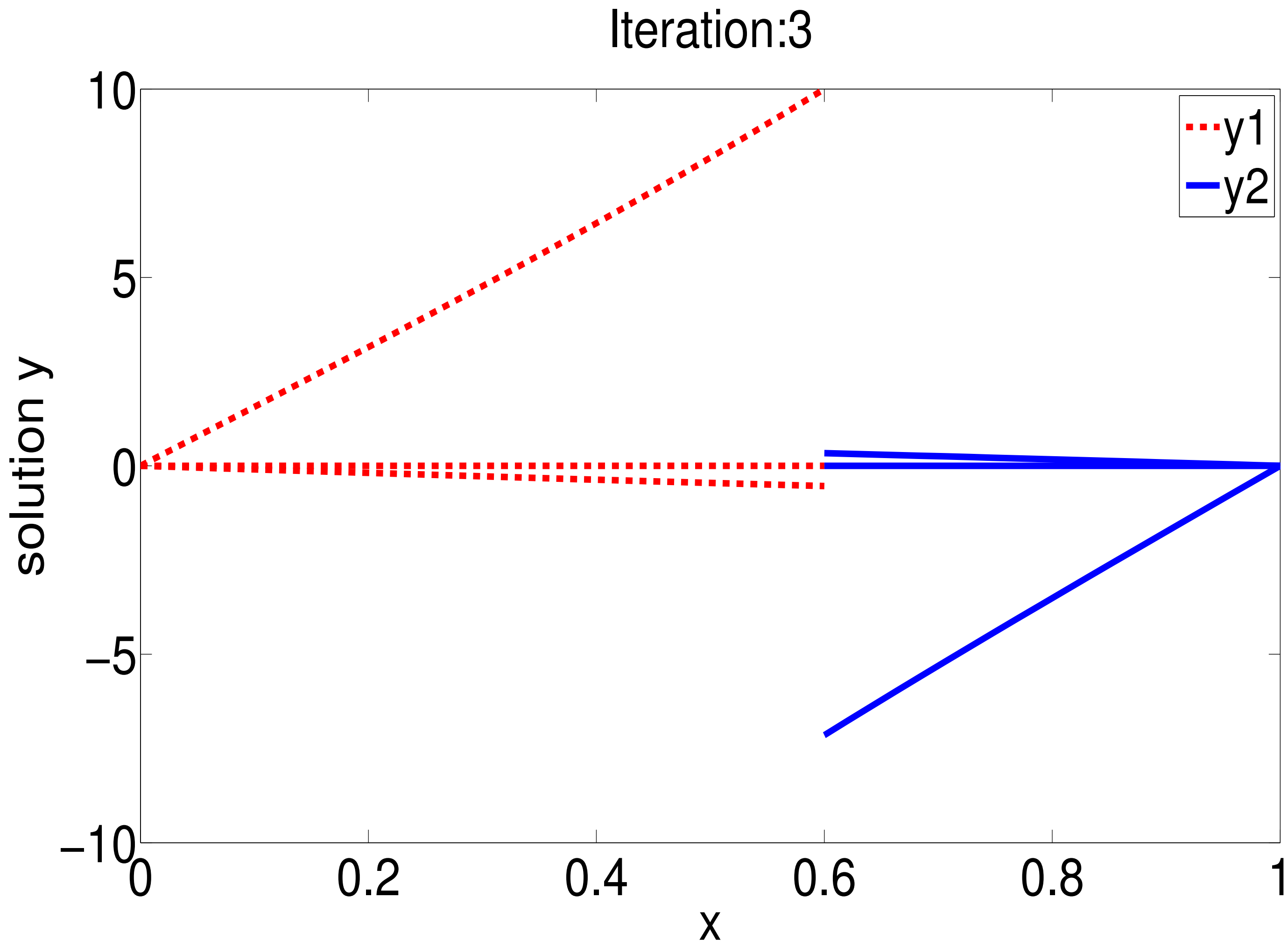
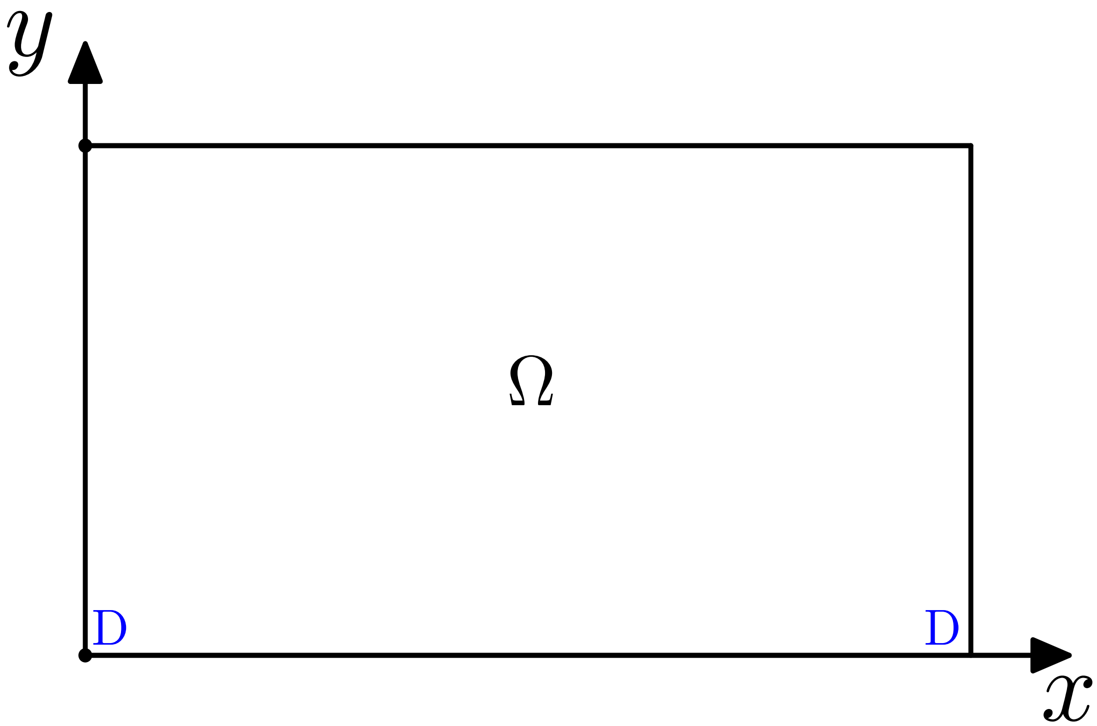


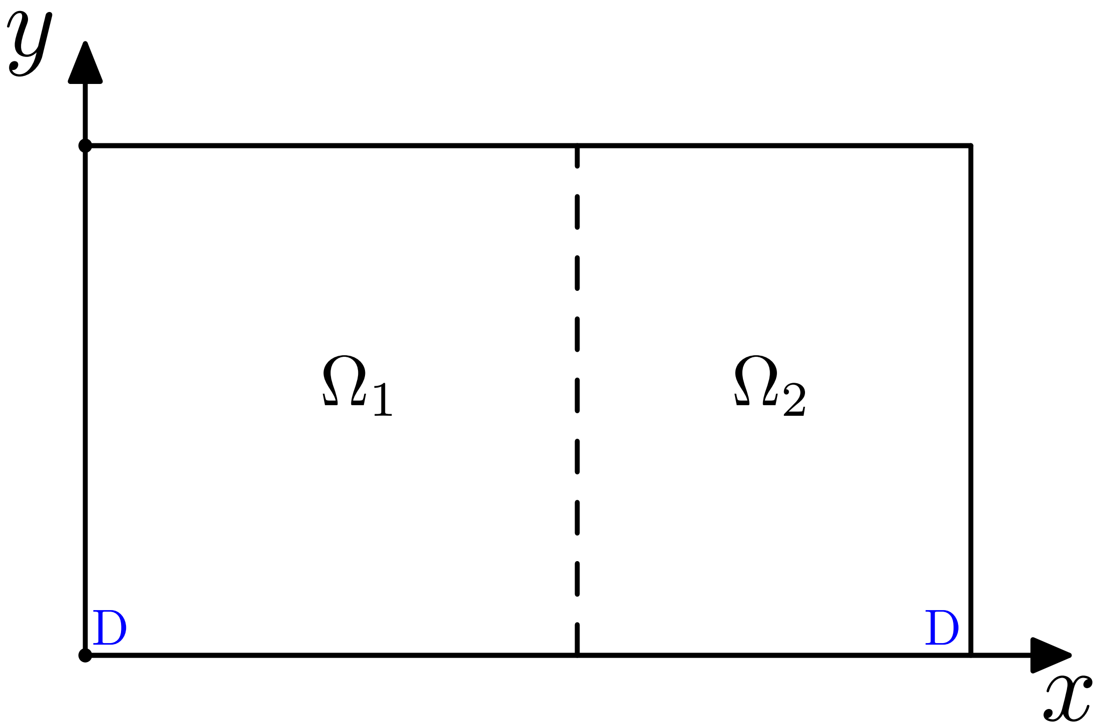
Neumann-Neumann Method



Poisson Equation

$$
\begin{aligned}
-\Delta u &= f, && \text{in } \Omega \\
u &= 0, && \text{on } \partial\Omega.
\end{aligned}
$$

Neumann-Neumann Method



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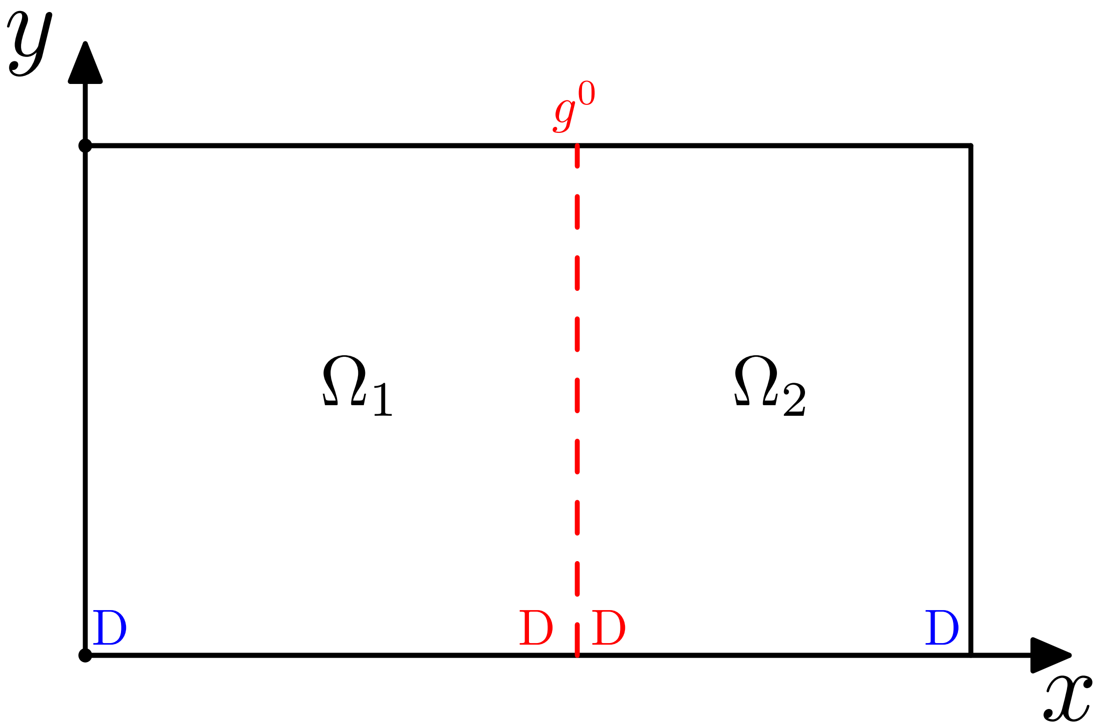
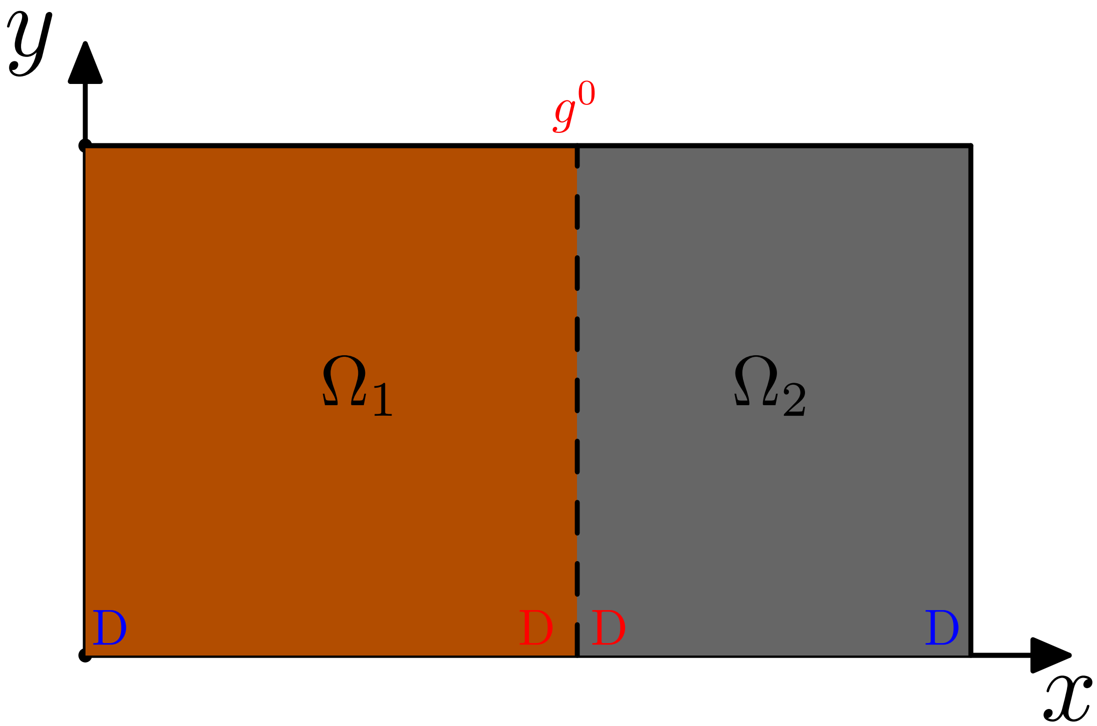
Neumann-Neumann Method



Given Dirichlet Trace g^0:

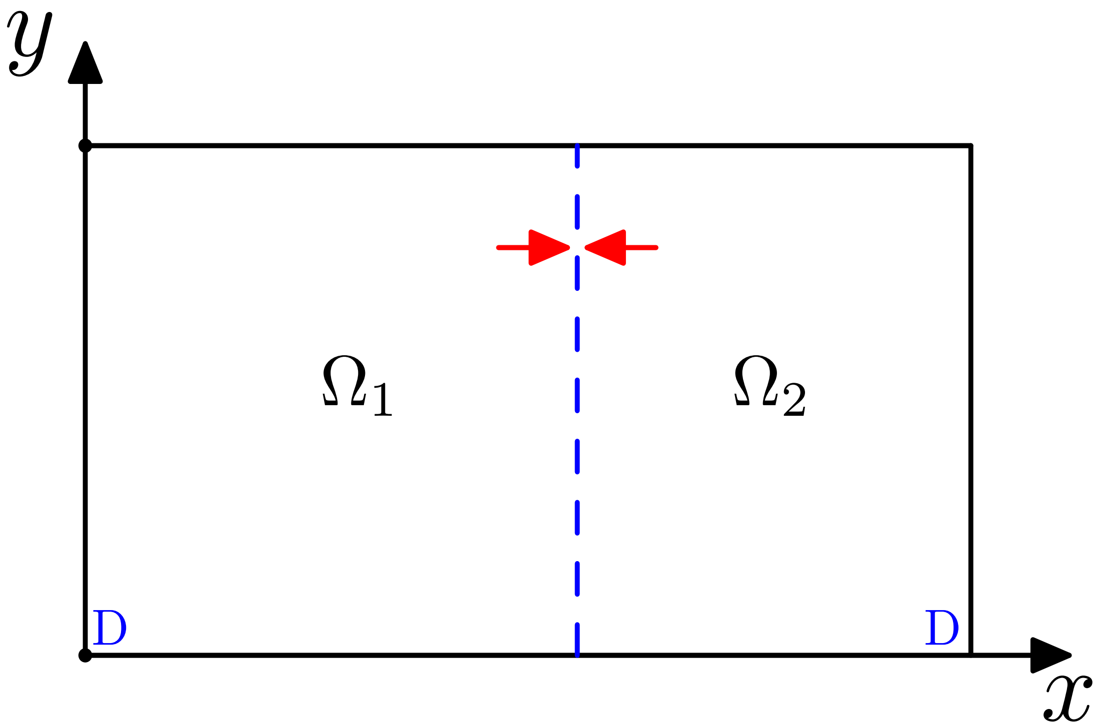
Neumann-Neumann Method



Given Dirichlet Trace g^0:

1. Solve Dirichlet Subproblems on Ω_1, Ω_2.

Neumann-Neumann Method



Given Dirichlet Trace g^0:

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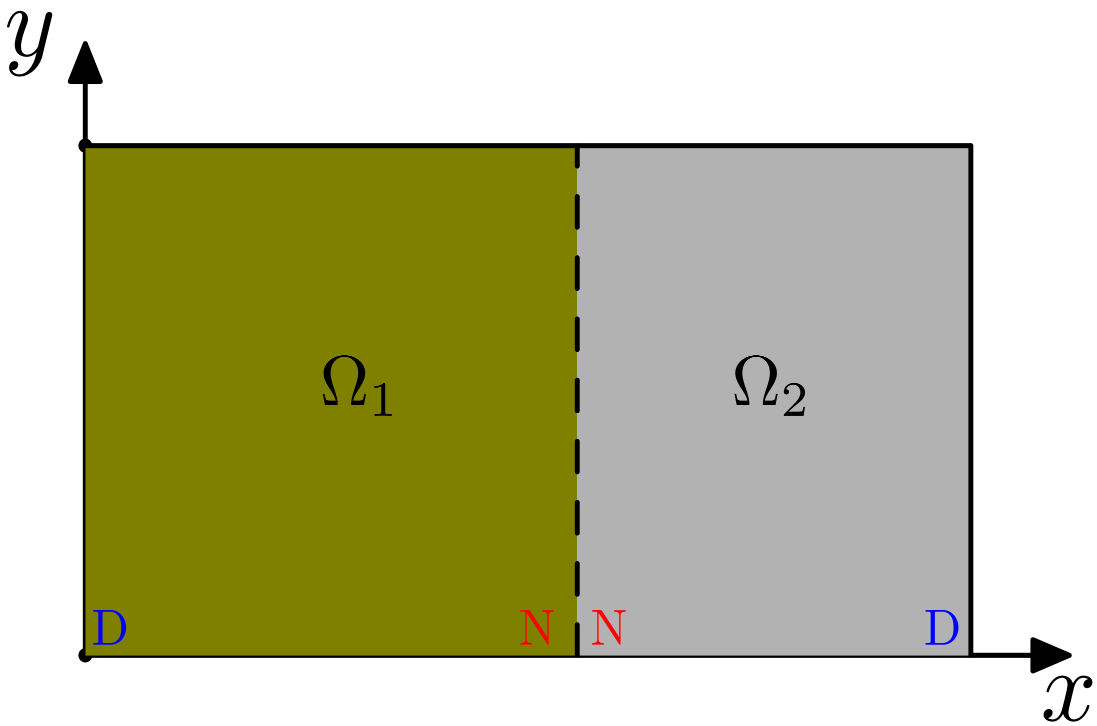
2. Calculate jump in Neumann trace.

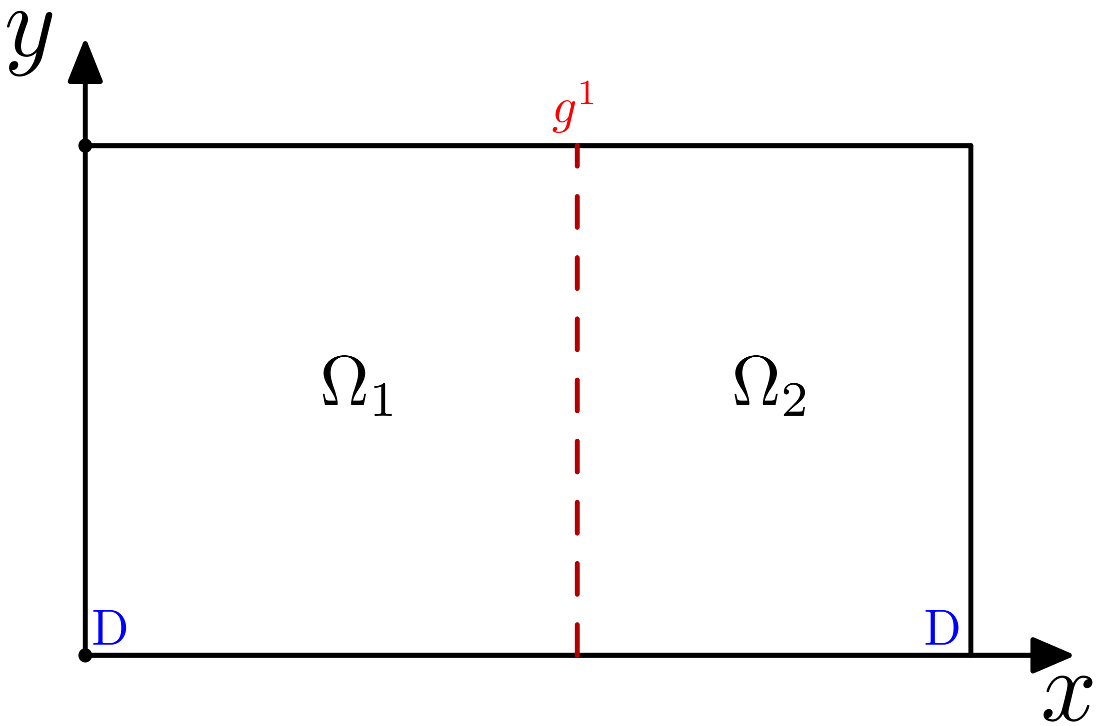
Neumann-Neumann Method



Given Dirichlet Trace g^0:

1. Solve Dirichlet Subproblems on Ω_1, Ω_2.
2. Calculate jump in Neumann trace.
3. Solve Neumann Subproblems on Ω_1, Ω_2.

Neumann-Neumann Method



Given Dirichlet Trace g^0:

1. Solve Dirichlet Subproblems on Ω_1, Ω_2.
2. Calculate jump in Neumann trace.
3. Solve Neumann Subproblems on Ω_1, Ω_2.
4. Update Dirichlet Trace: $g^k = g^{k-1} - \theta \left(\psi_1^k \mid_\Gamma + \psi_2^k \mid_\Gamma \right).$

Convergence: NN Method

$$\begin{cases} -u'' = 0, & x \in (-3, 2), \\ u(-3) = 0 = u(2). \end{cases}$$

$\Omega_1 = (-3, 0), \Omega_2 = (0, 2), g^0 = 10.$

Convergence: NN Method

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$\Omega_1 = (-3, 0), \Omega_2 = (0, 2), g^0 = 10.$

$l(\Omega_1) = 3, l(\Omega) = 5, \Longrightarrow \theta^* = \frac{l(\Omega_1)l(\Omega_2)}{l(\Omega)^2} = \frac{6}{25}.$

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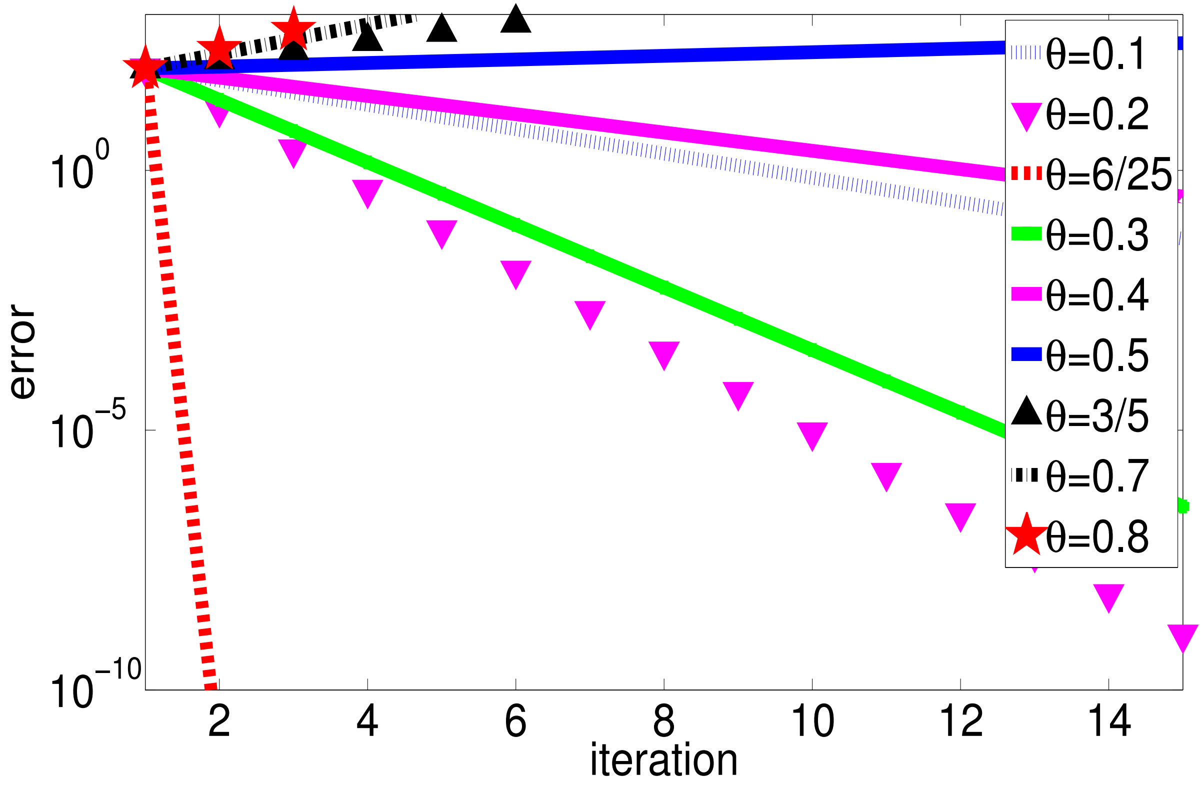


Optimal Control Problem: NN Method

Theorem (*Convergence of NN method*)

The NN algorithm converges in at most 3 iterations, if the parameters (θ_y^*, θ_p^*) are given by

$$\theta_y^* = \frac{1}{z_1} + \frac{|\, z_2 \,|}{z_1\sqrt{z_1^2 + z_2^2}}, \quad \theta_p^* = \frac{1}{z_1} - \frac{|\, z_2 \,|}{z_1\sqrt{z_1^2 + z_2^2}}.$$

Proof.

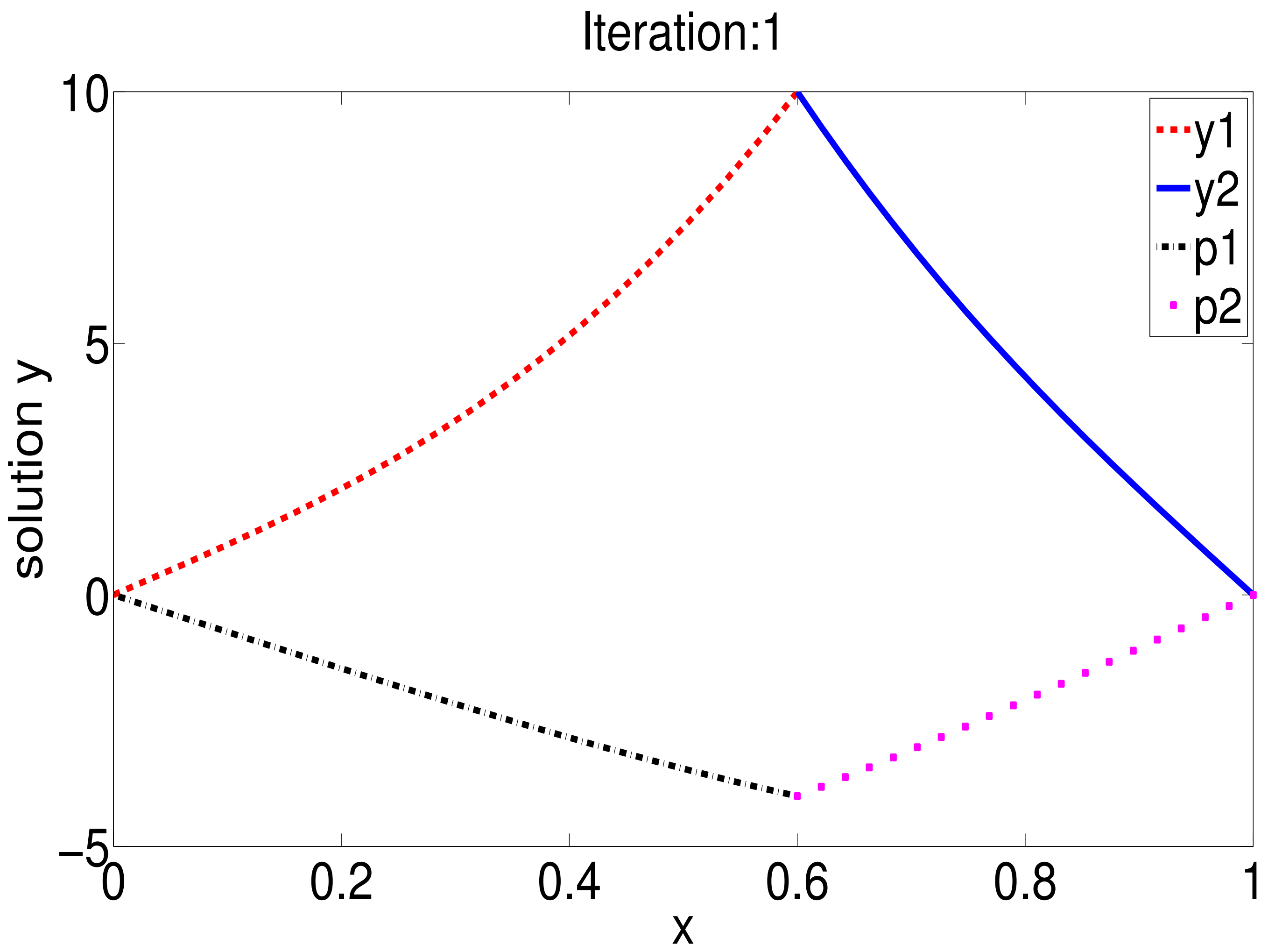
The updating matrix is:

$$A = \begin{pmatrix} 1 - \theta_y z_1 & -\theta_y z_2 \\ \theta_p z_2 & 1 - \theta_p z_1 \end{pmatrix}$$

where $z_1 = z_1(\alpha, \lambda), z_2 = z_2(\alpha, \lambda)$. $A \neq 0, A^2 = 0$, if θ_y, θ_p chosen carefully! □

NN Method: Numerical test

$\alpha = 0.6, \lambda = 1/2^4$, $\theta_y^* \approx 0.304, \theta_p^* \approx 0.165.$



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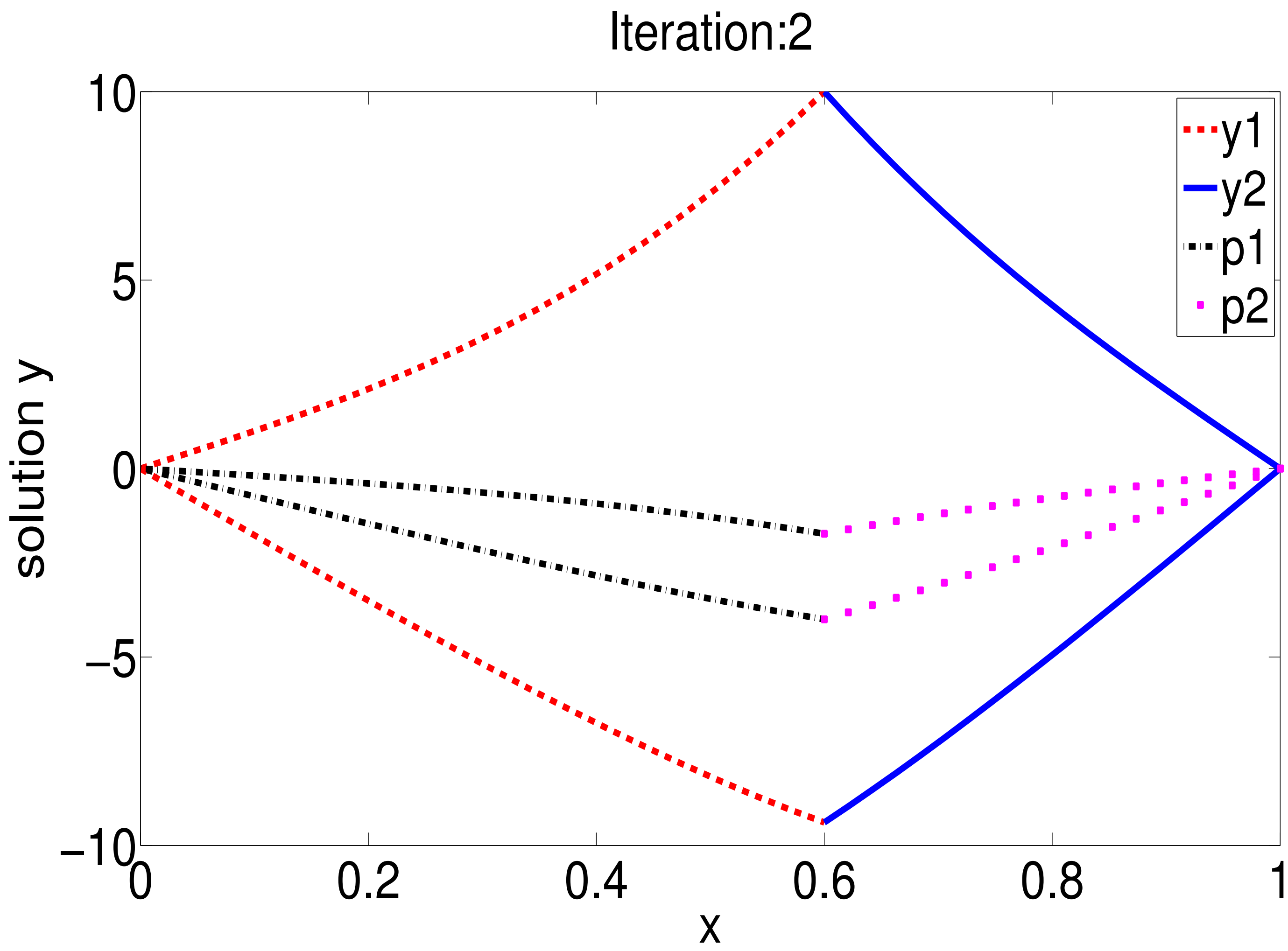

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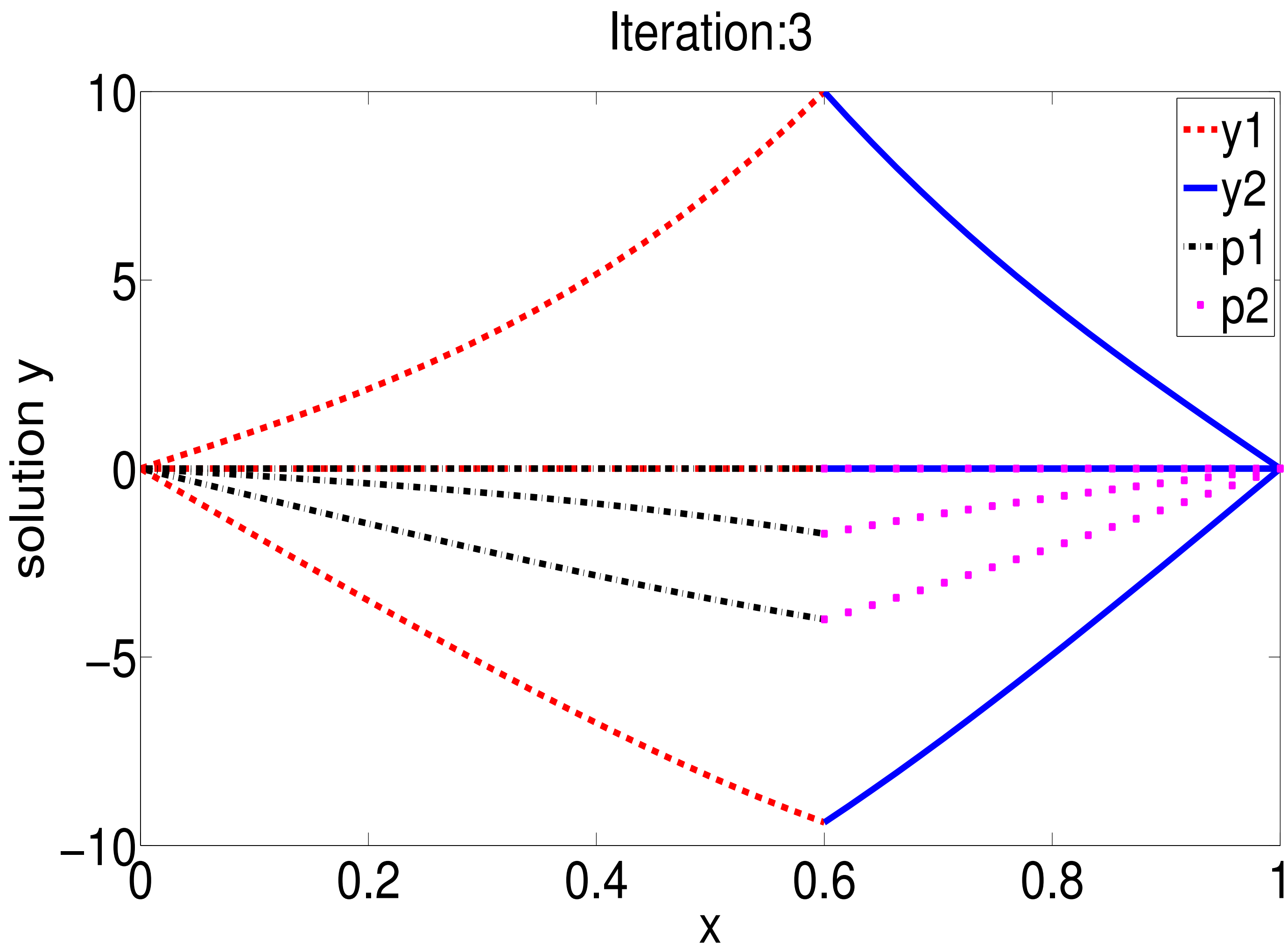


$$\text{Minimize } J(y,u) = \frac{1}{2}\int_0^T\int_0^1 (y-\hat{y})^2\,dxdt + \frac{\lambda}{2}\int_0^T\int_0^1 u^2 dxdt,$$

$$\text{subject to } \begin{cases} \partial_t y(x,t) - \nu\Delta y(x,t) = u(x,t), & x\in\Omega, t\in(0,T),\\ y(x,0) = y_0(x), & x\in\Omega,\\ y(x,t) = 0, & x\in\partial\Omega\times(0,T). \end{cases} \tag{3}$$

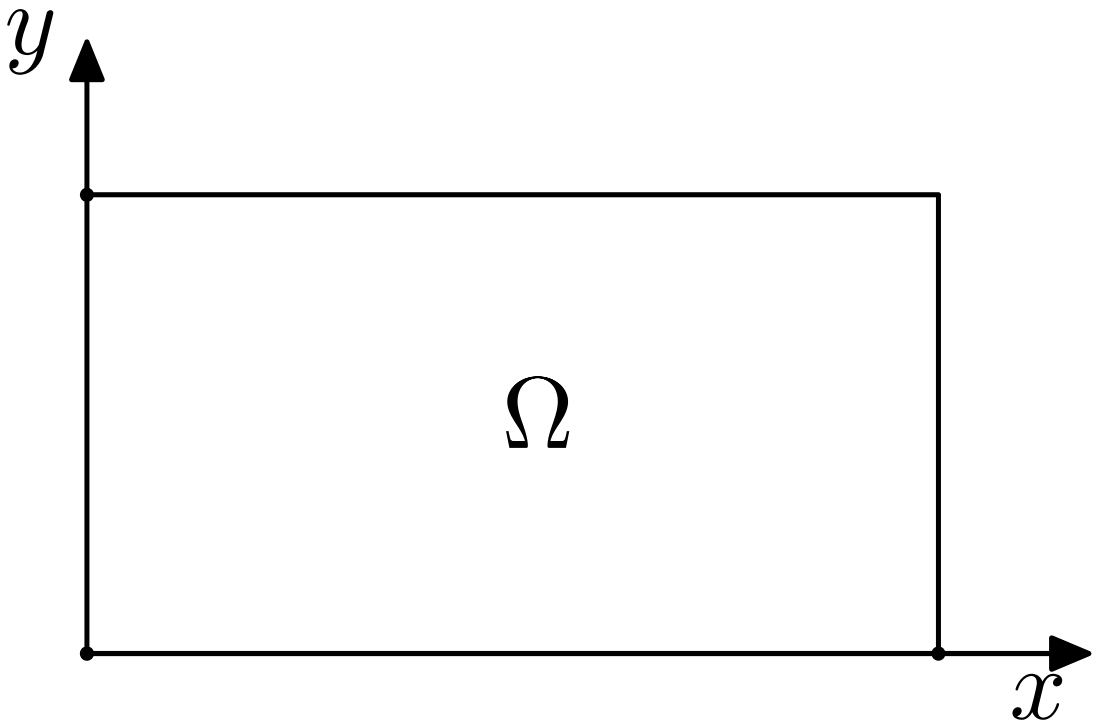
The adjoint equation would be:

$$\begin{cases} -\partial_t p(x,t) - \nu\Delta p(x,t) = y(x,t) - \hat{y}(x,t), & x\in\Omega, t\in(0,T),\\ p(x,T) = 0, & x\in\Omega,\\ p(x,t) = 0, & x\in\partial\Omega\times(0,T), \end{cases} \tag{4}$$

with the optimality condition:

$$p(x,t) + \lambda u(x,t) = 0.$$

Dirichlet-Neumann Waveform Relaxation



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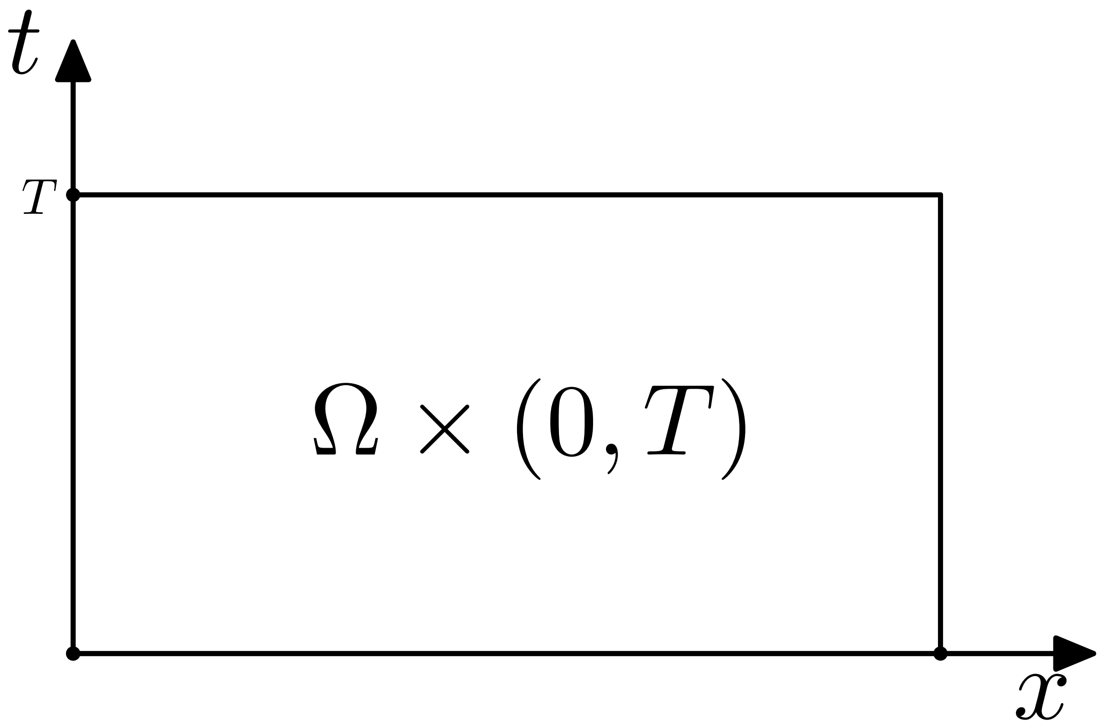
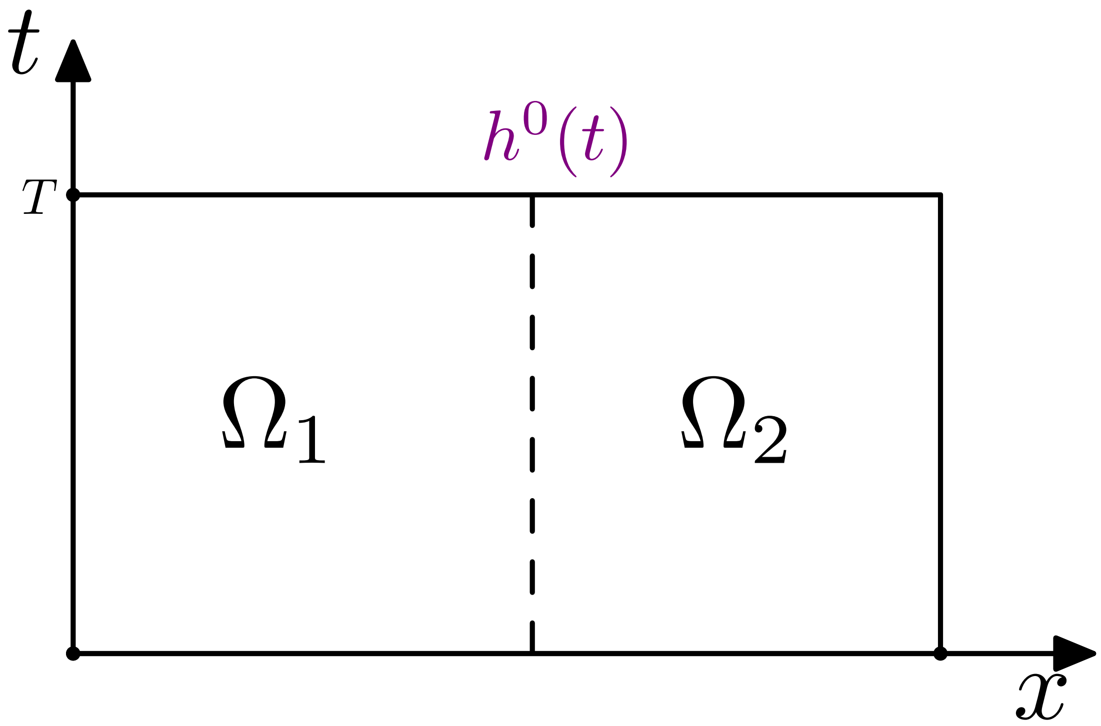
Dirichlet-Neumann Waveform Relaxation



Heat Equation

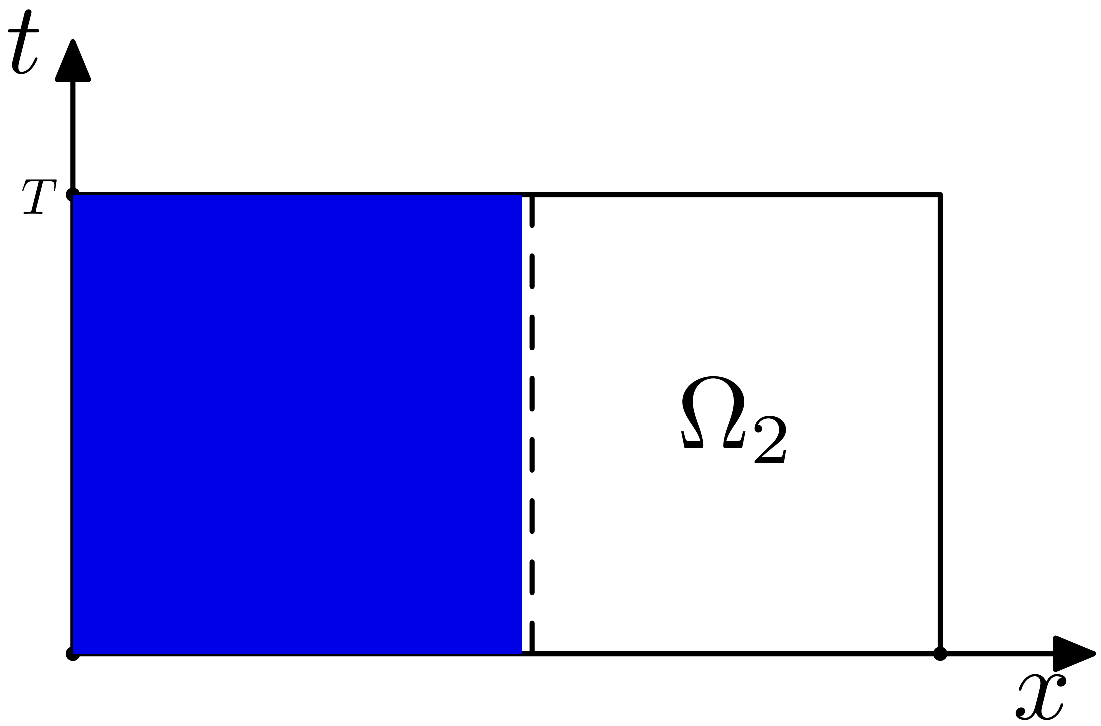
$$
\begin{aligned}
u_t - \nu u_{xx} &= f(x,t), \quad (x,t) \in \Omega \times (0,T) \\
u(x,0) &= u_0(x), \quad x \in \Omega. \\
u(x,t) &= g(x,t), \quad x \in \partial\Omega, 0 < t < T.
\end{aligned}
$$

Dirichlet-Neumann Waveform Relaxation



Dirichlet Trace $h^0(t)$ along the interface is given.

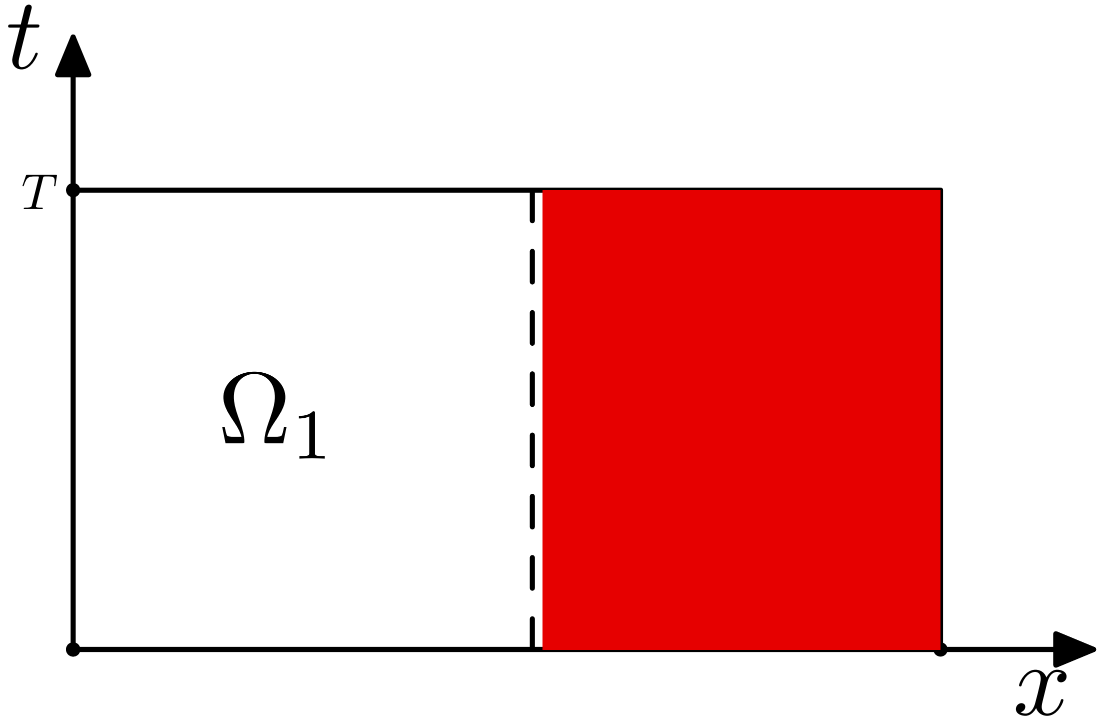
Dirichlet-Neumann Waveform Relaxation



$$\begin{cases} \partial_t u_1^k - \partial_{xx} u_1^k &= f, \\ u_1^k(x,0) &= u_0(x), \\ u_1^k(-a,t) &= g(-a,t), \\ u_1^k(0,t) &= h^{k-1}(t). \end{cases}$$

Dirichlet Subproblem

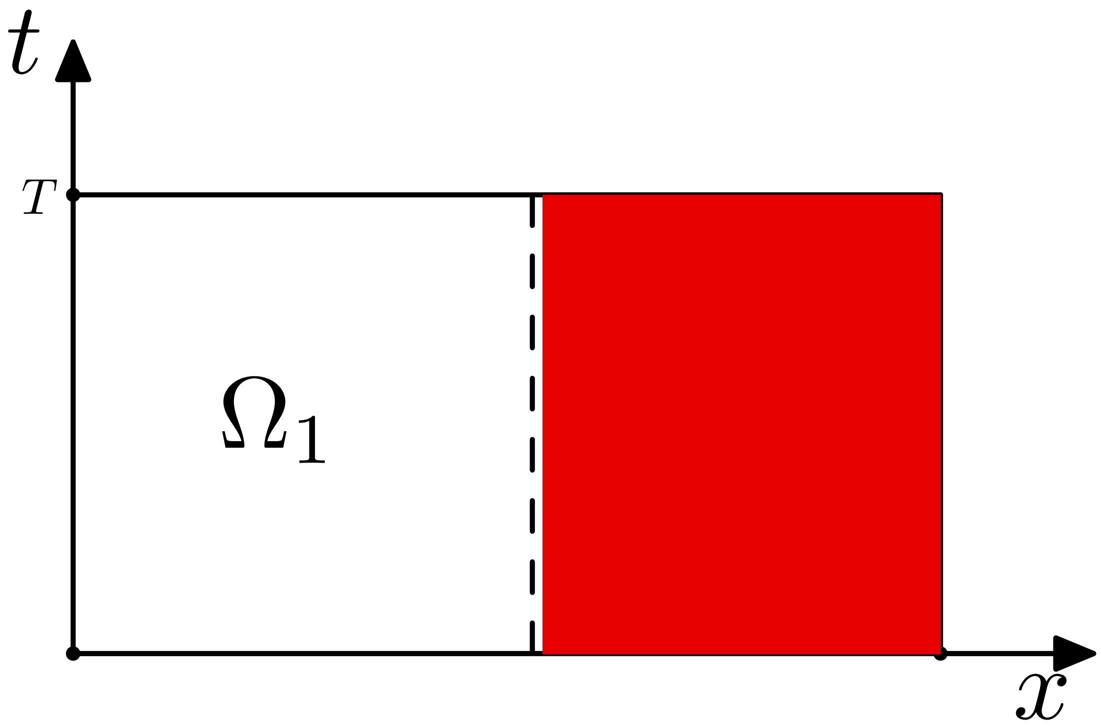
Dirichlet-Neumann Waveform Relaxation



Neumann Subproblem

$$\begin{cases} \partial_t u_2^k - \partial_{xx} u_2^k & = f, \\ u_2^k(x,0) & = u_0(x), \\ \partial_x u_2^k(0,t) & = \partial_x u_1^k(0,t), \\ u_2^k(b,t) & = g(b,t) \end{cases}$$

Dirichlet-Neumann Waveform Relaxation



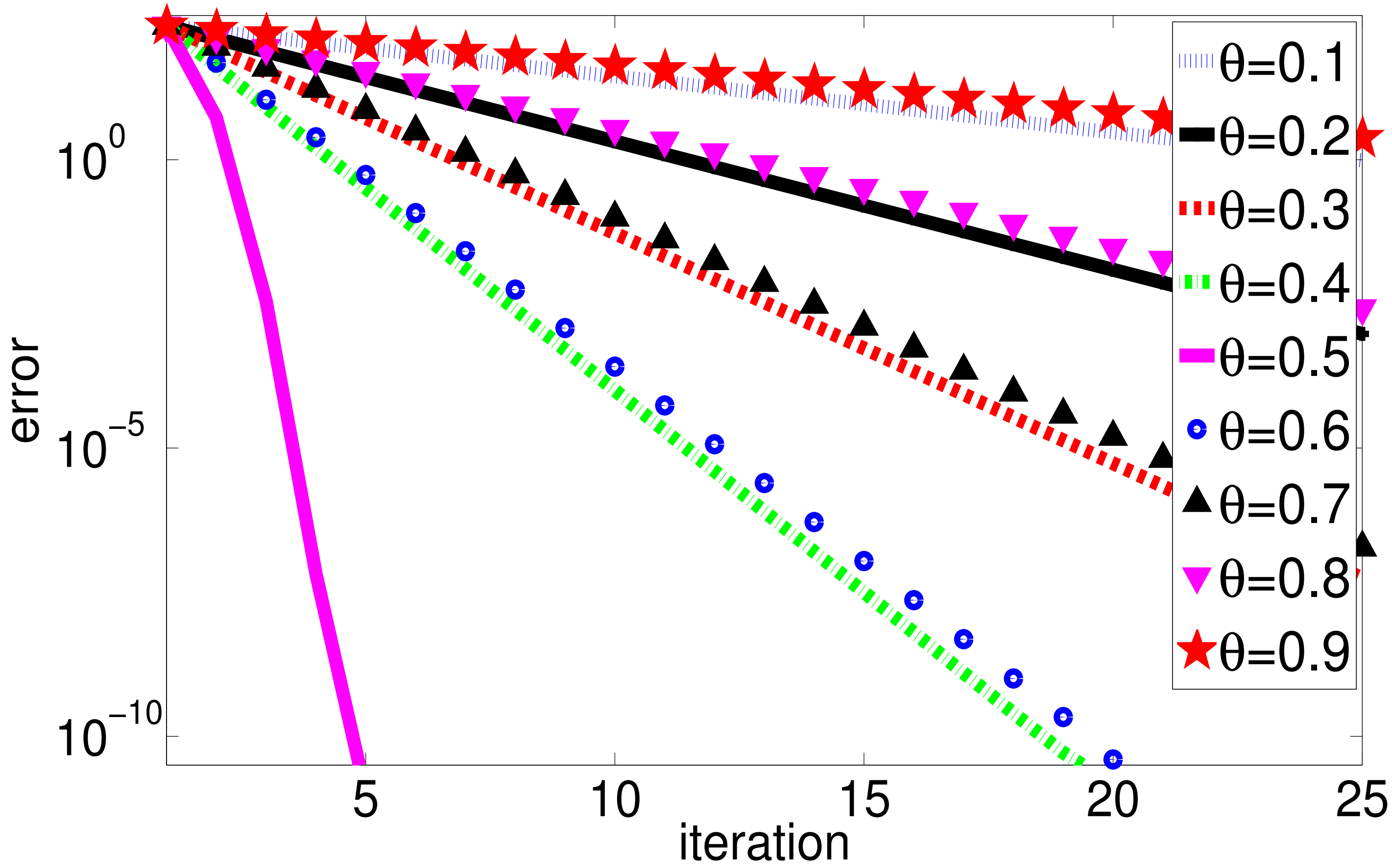
Update condition

$$h^k(t) = (1-\theta)h^{k-1}(t) + \theta u_2^k(0,t),$$

θ : positive relaxation parameter.

Superlinear Convergence of DNWR

$\Omega = (-3, 2)$. Two subdomains: $\Omega_1 = (-3, 0), \Omega_2 = (0, 2)$. Time $T = 2$.



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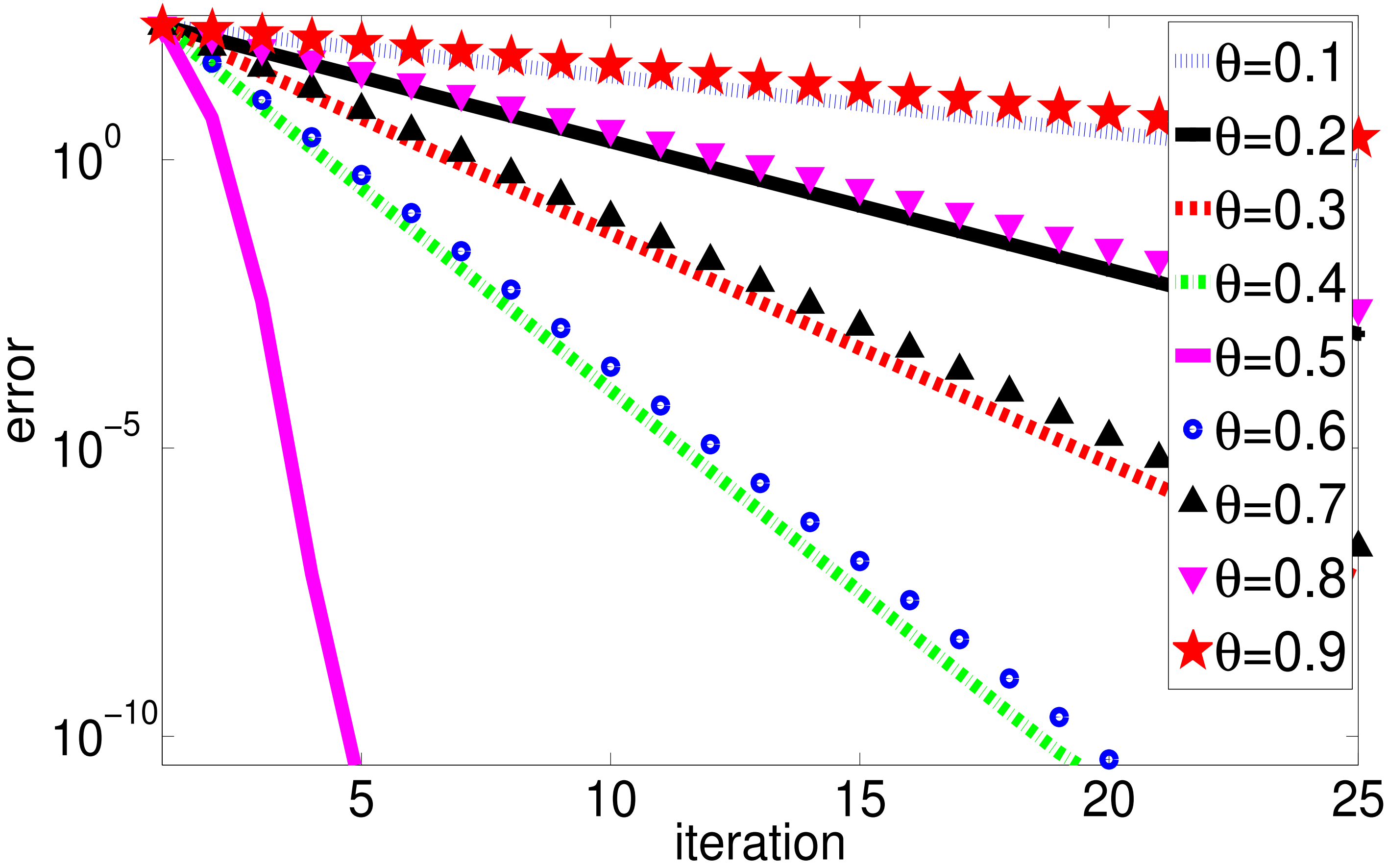


Goal: Estimate a bound for the error in case of $\theta = 1/2$.

Convergence Estimates

Dirichlet bigger than Neumann : $a > b$

Theorem(Gander,Kwok,M., 2012)

Let $\theta = 1/2$. On a finite time interval $t \in (0, T)$, the DNWR satisfies

$$\| h^k \|_{L^\infty(0,T)} \leq \left(\frac{a-b}{a}\right)^k \operatorname{erfc}\left(\frac{kb}{2\sqrt{\nu T}}\right) \| h^0 \|_{L^\infty(0,T)} .$$

Theorem(*Linear convergence estimate*)

For $\theta = 1/2$, the DNWR satisfies for $t \in (0, \infty)$

$$\| h^k \|_{L^\infty(0,\infty)} \leq \left(\frac{a-b}{2a}\right)^k \| h^0 \|_{L^\infty(0,\infty)},$$

$k = 1, 2, 3, \ldots$

Bounds on the error

Short time interval

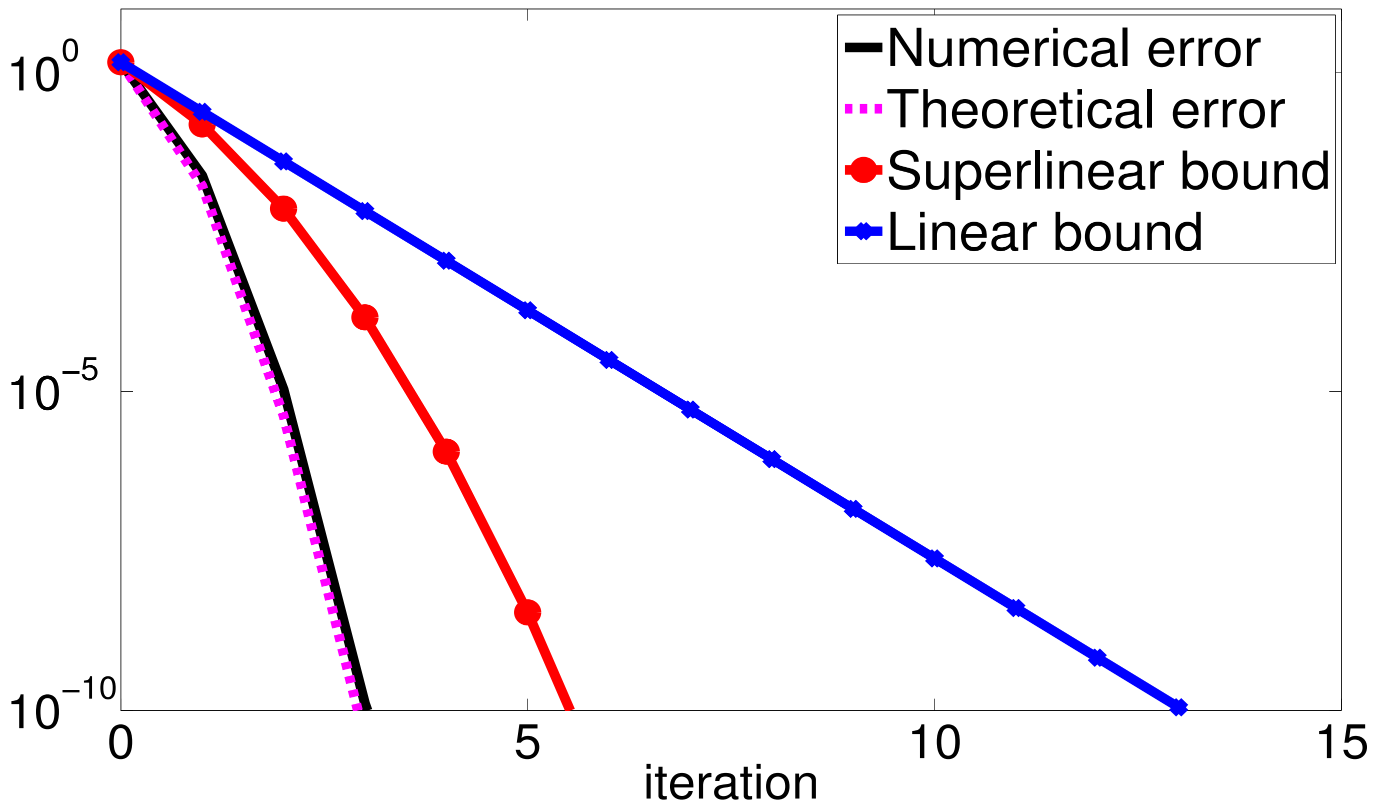


Figure: $a = 3, b = 2, T = 2$

Bounds on the error

Large time interval

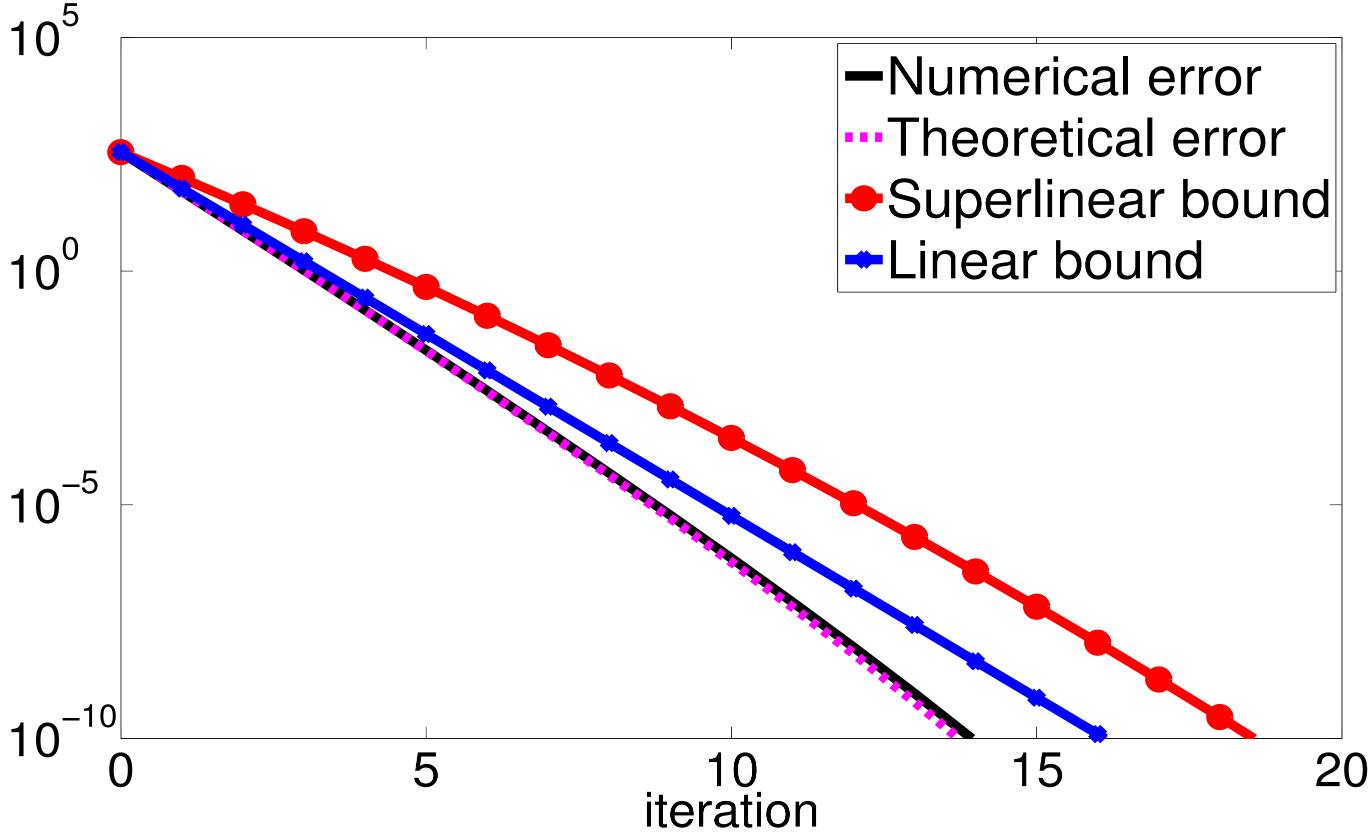
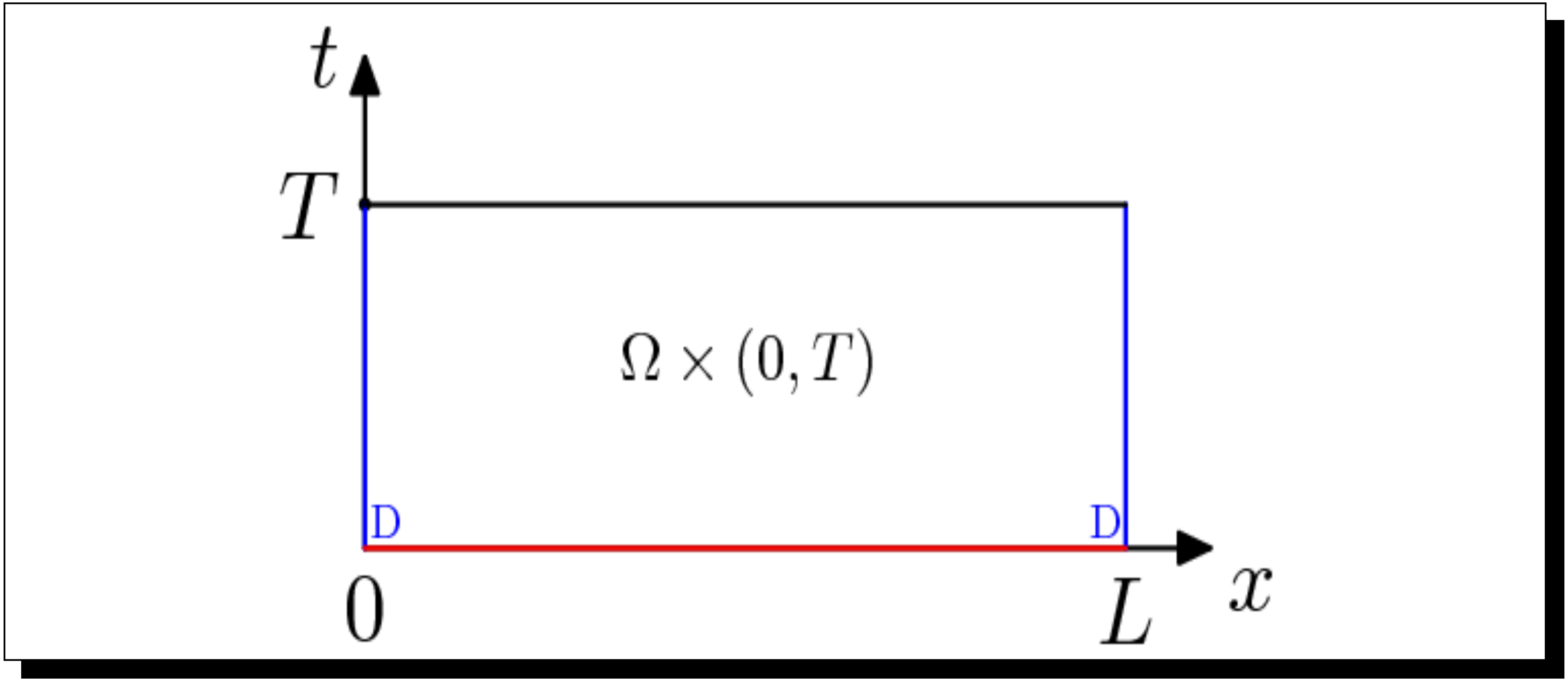
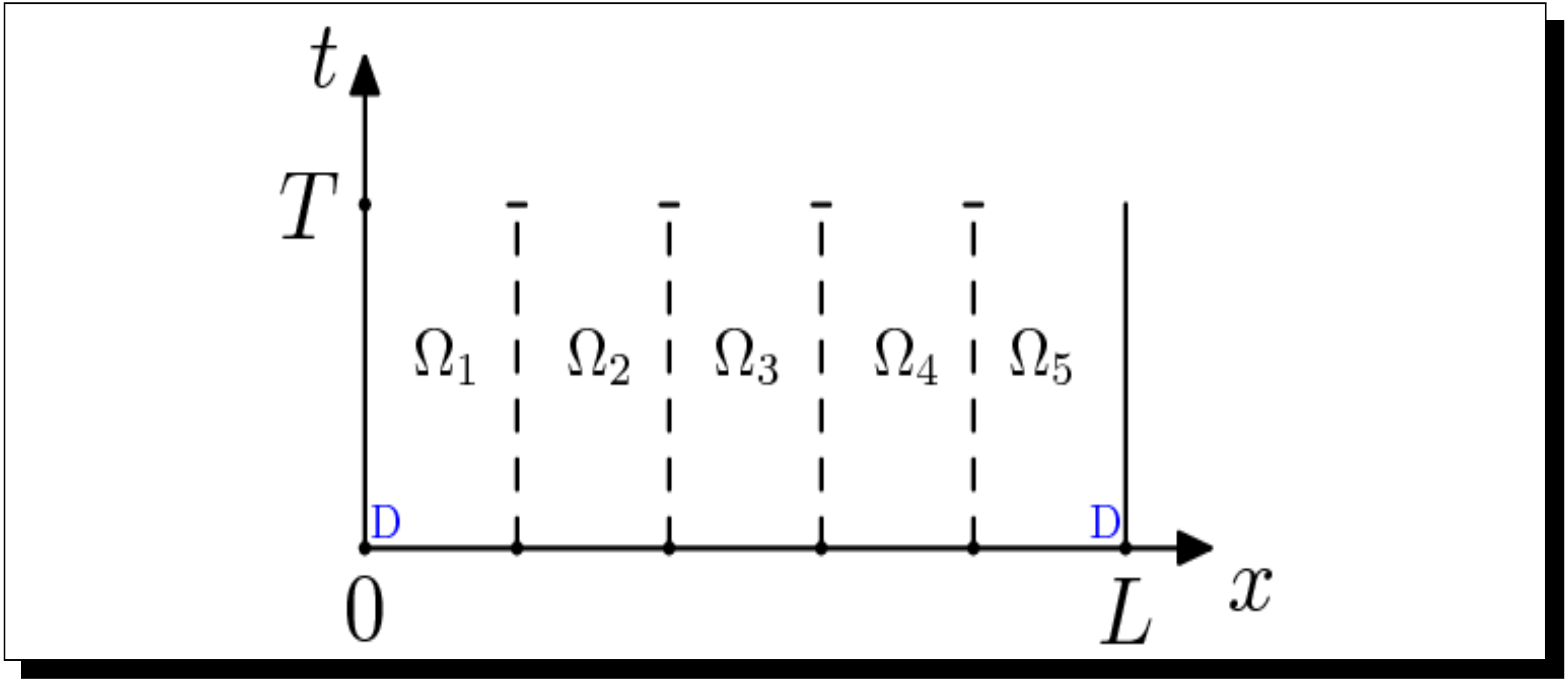


Figure: $a = 3$, $b = 2$, $T = 50$

DNWR Method : Many Subdomains



DNWR Method : Many Subdomains



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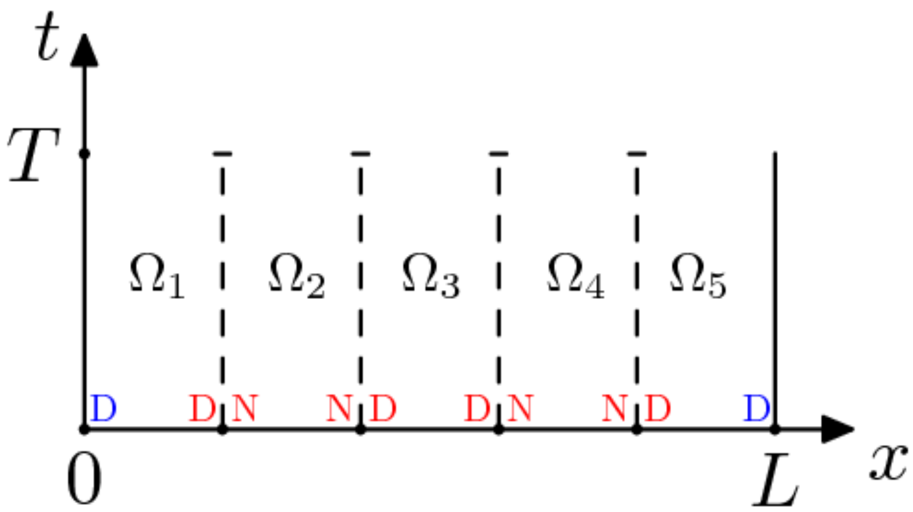
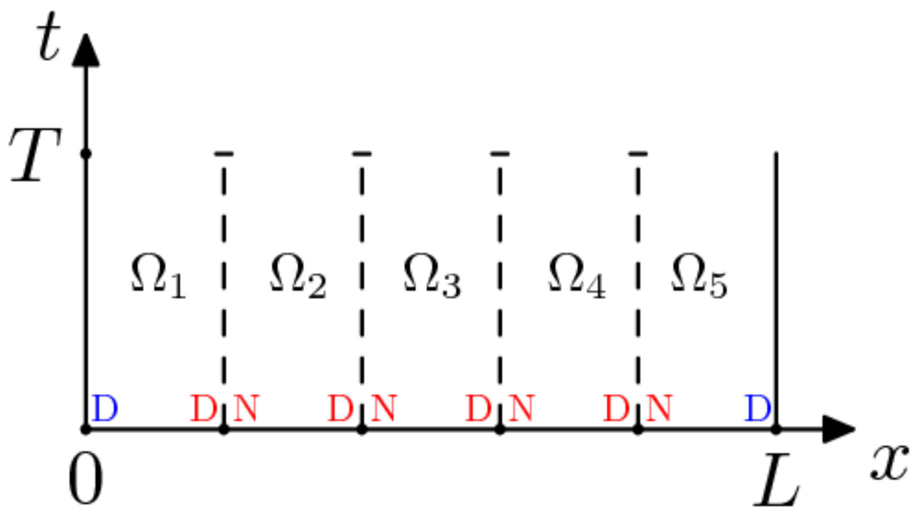
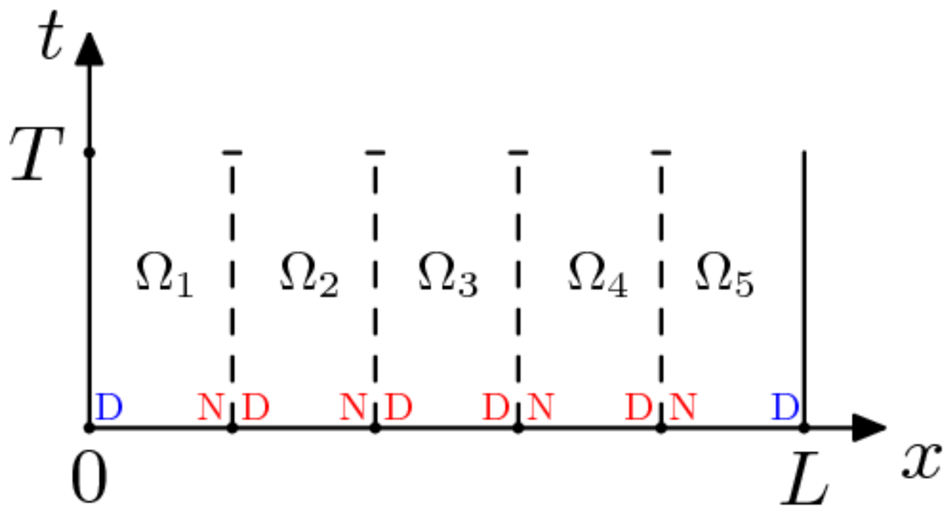
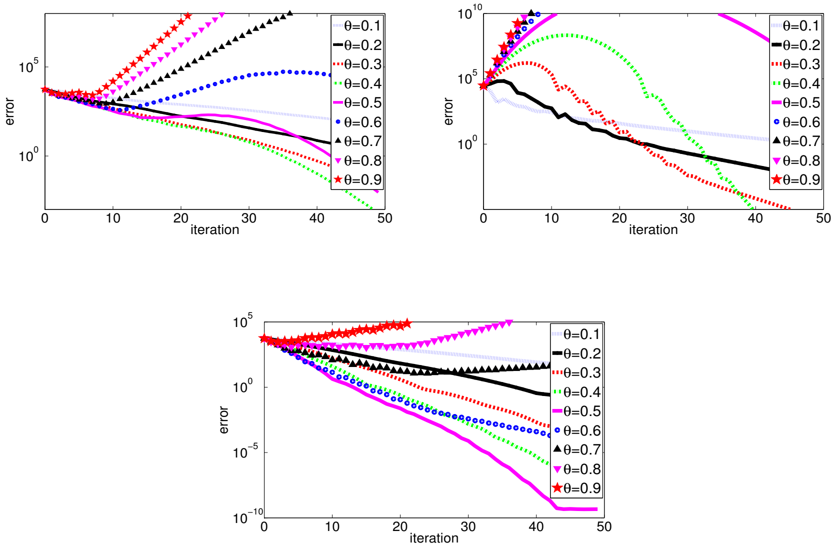


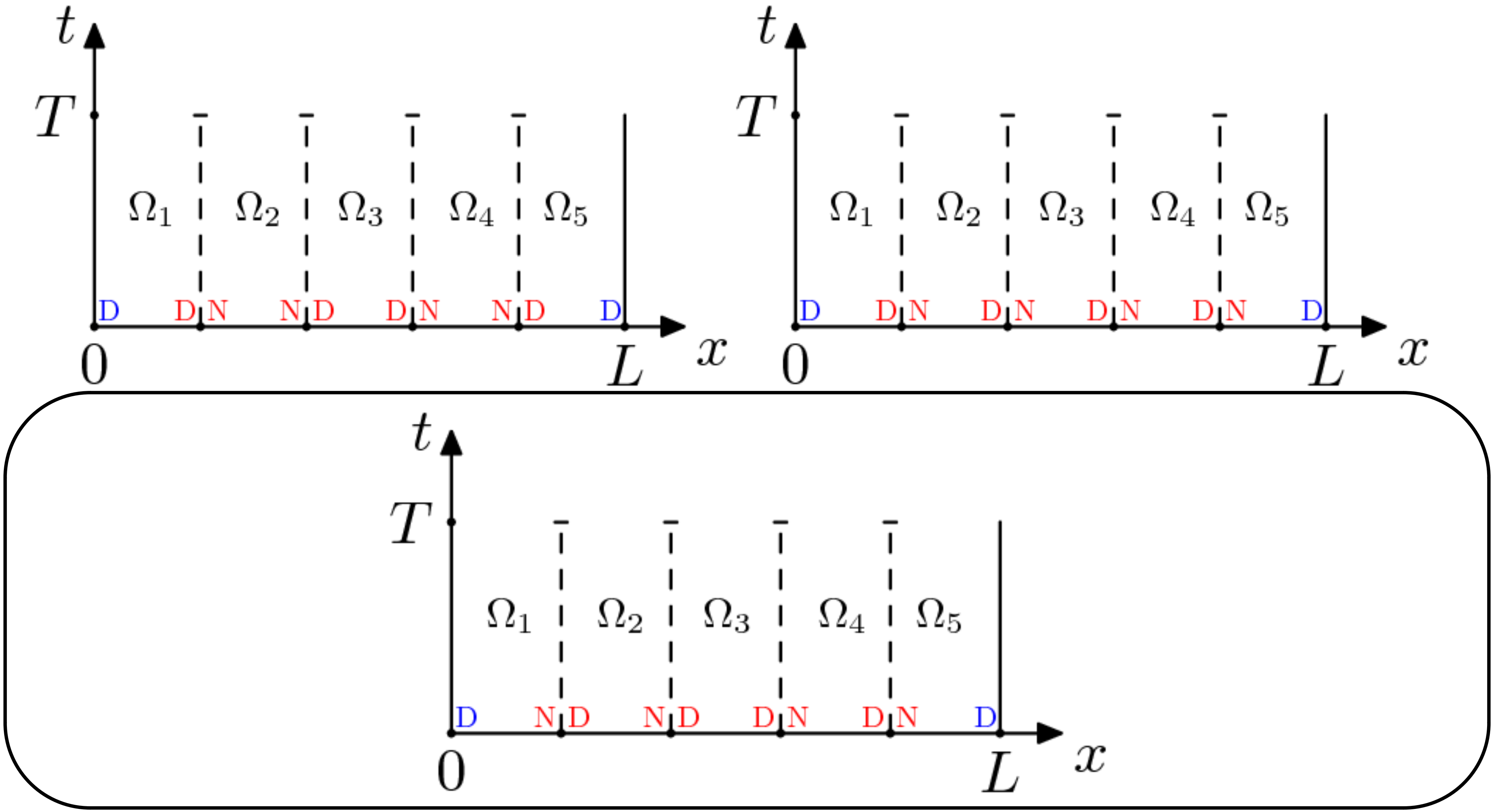




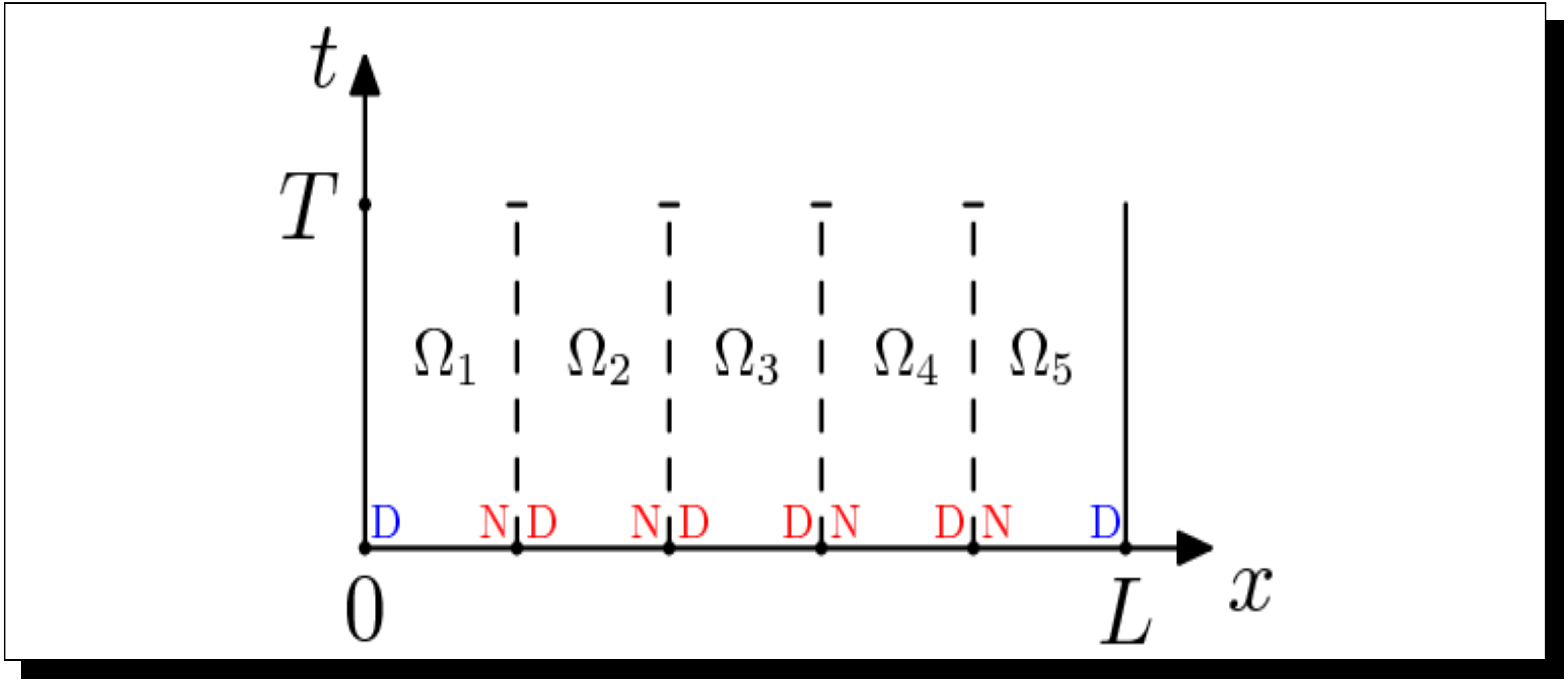
DNWR Method : Many Subdomains



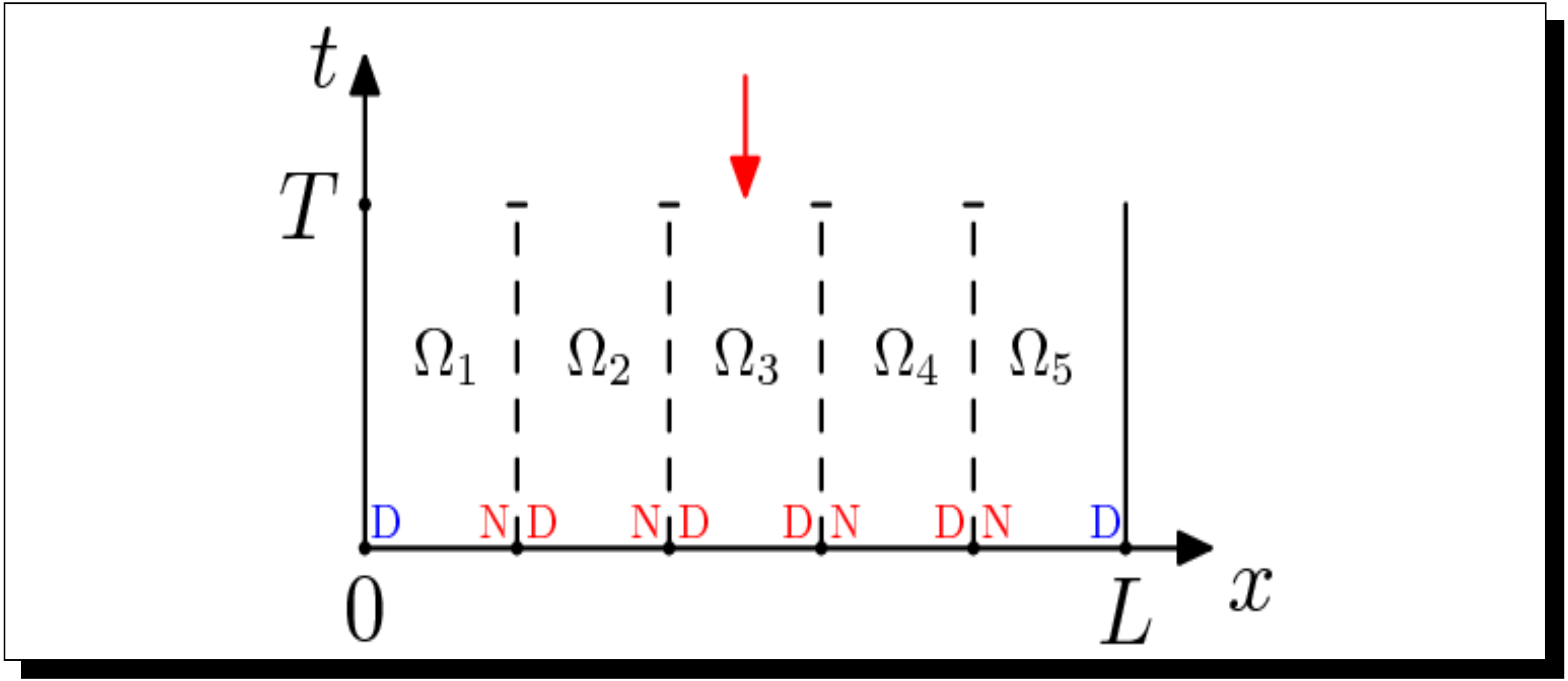
DNWR Method : Funaro, Quarteroni (1988)



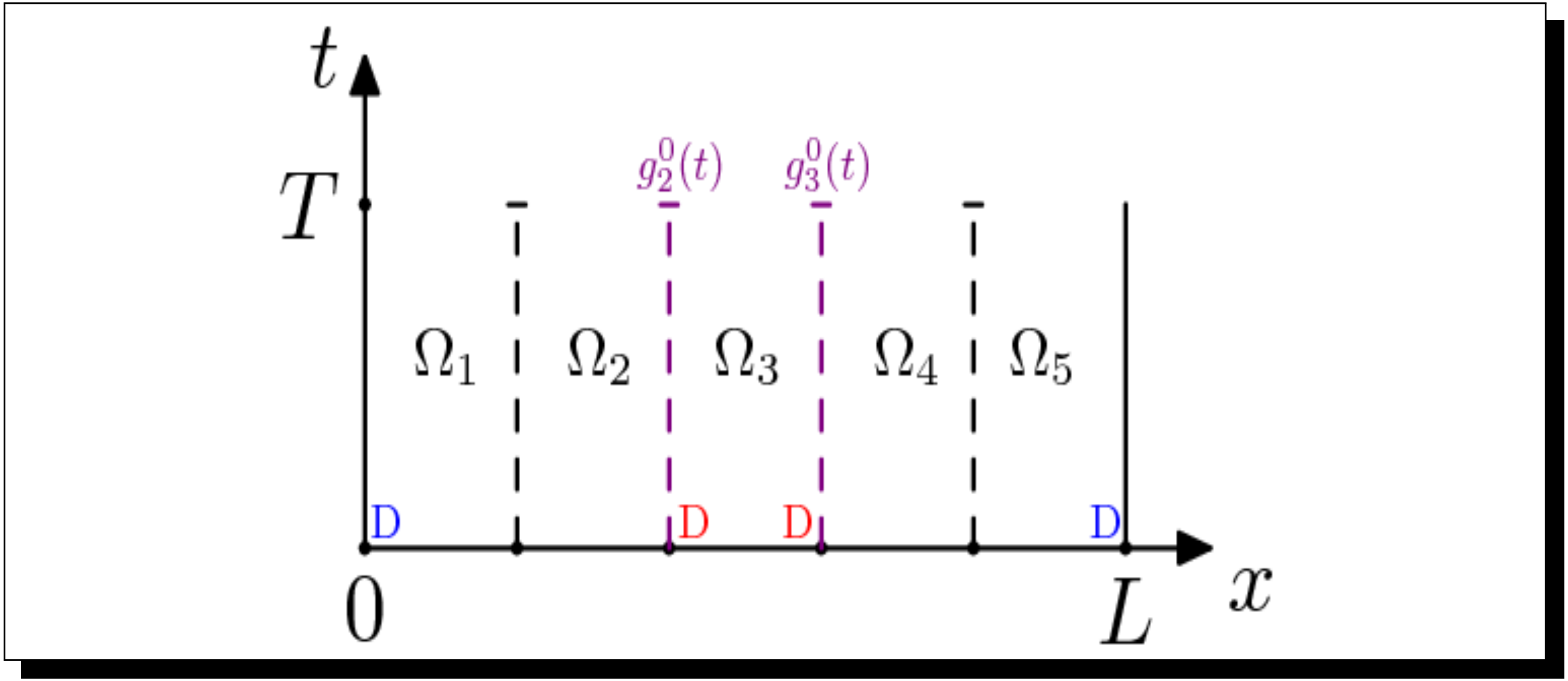
DNWR Method : Many Subdomains



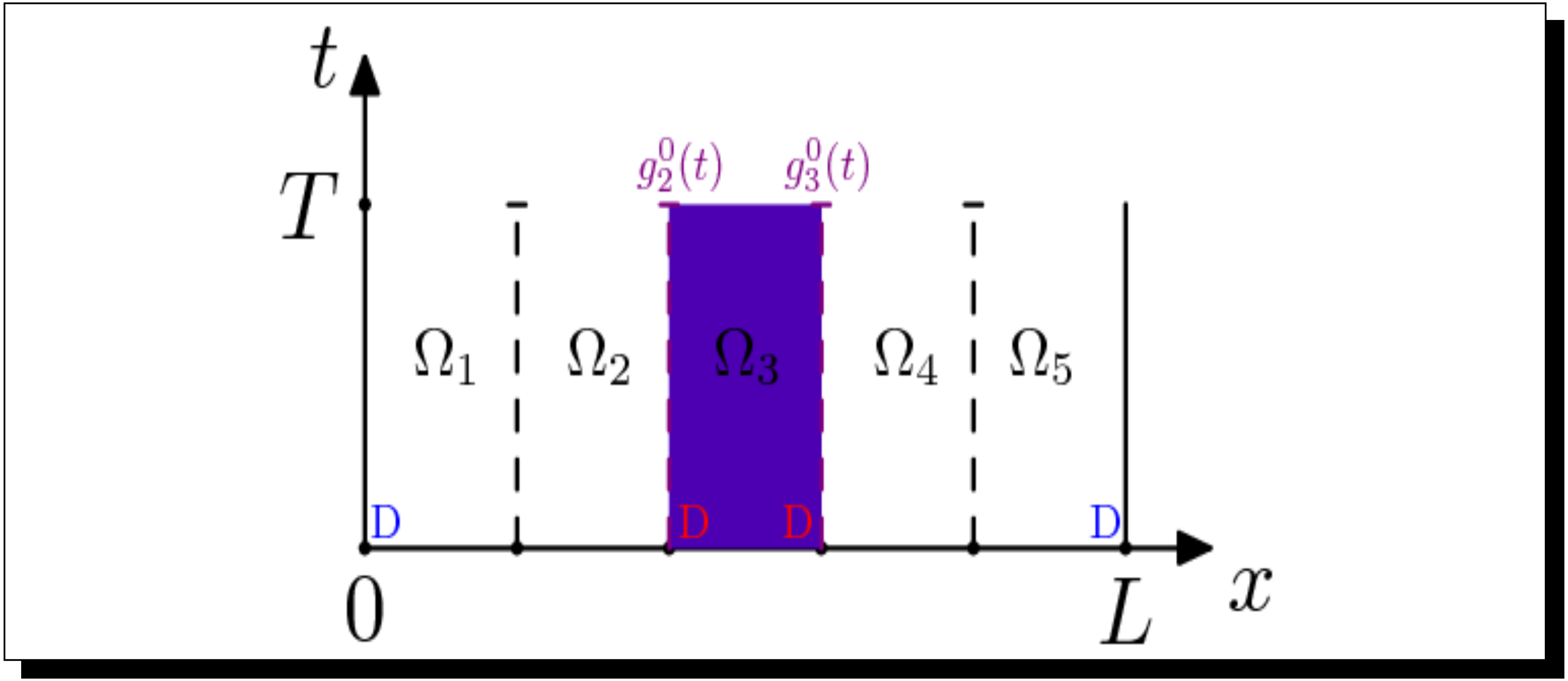
DNWR Method : Many Subdomains



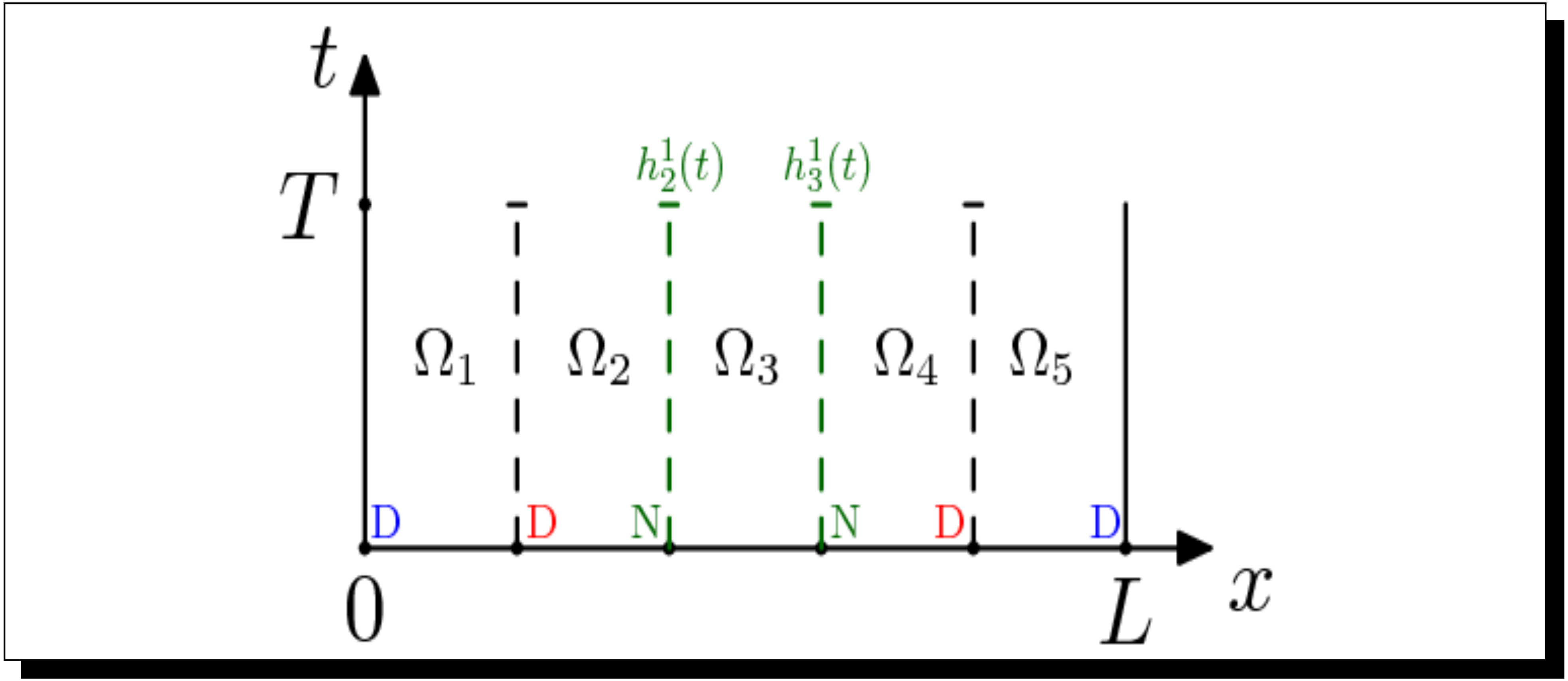
DNWR Method : Many Subdomains



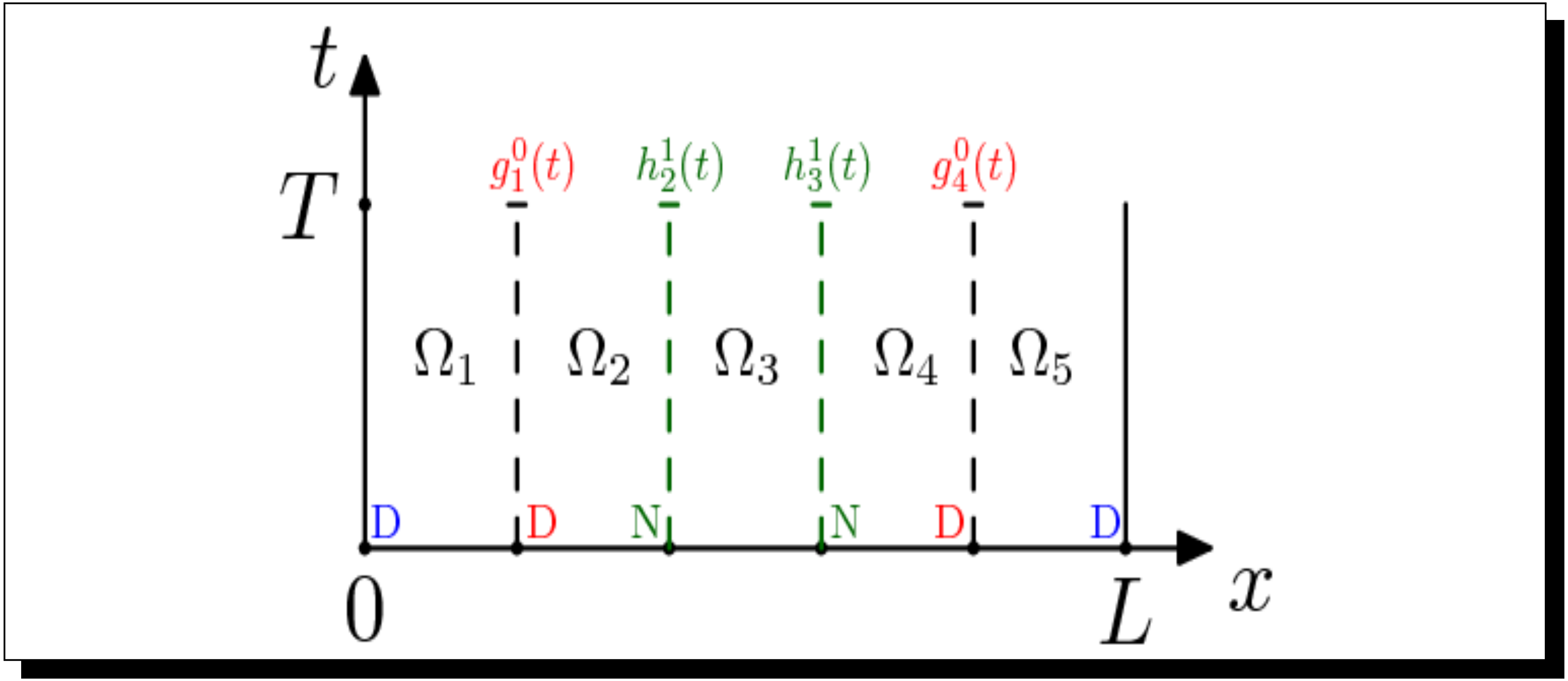
DNWR Method : Many Subdomains



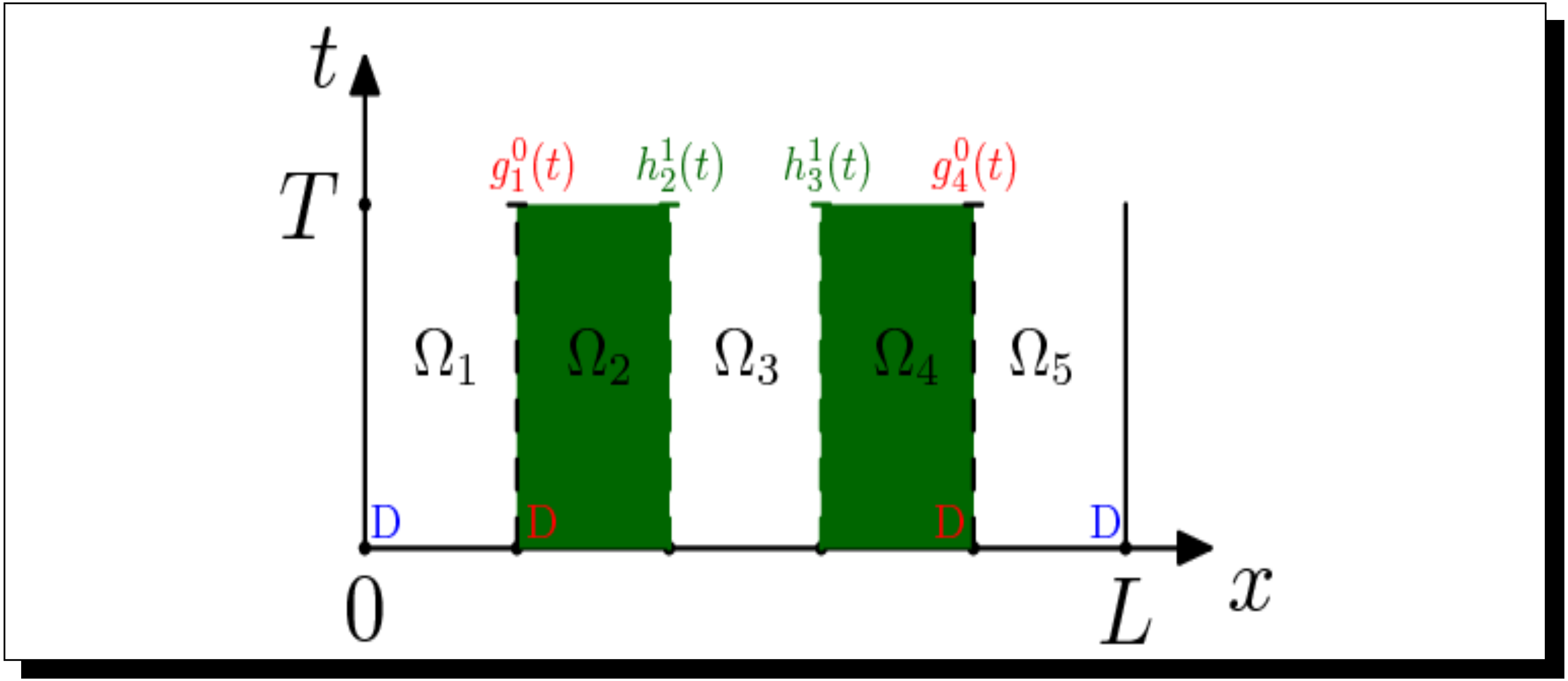
DNWR Method : Many Subdomains



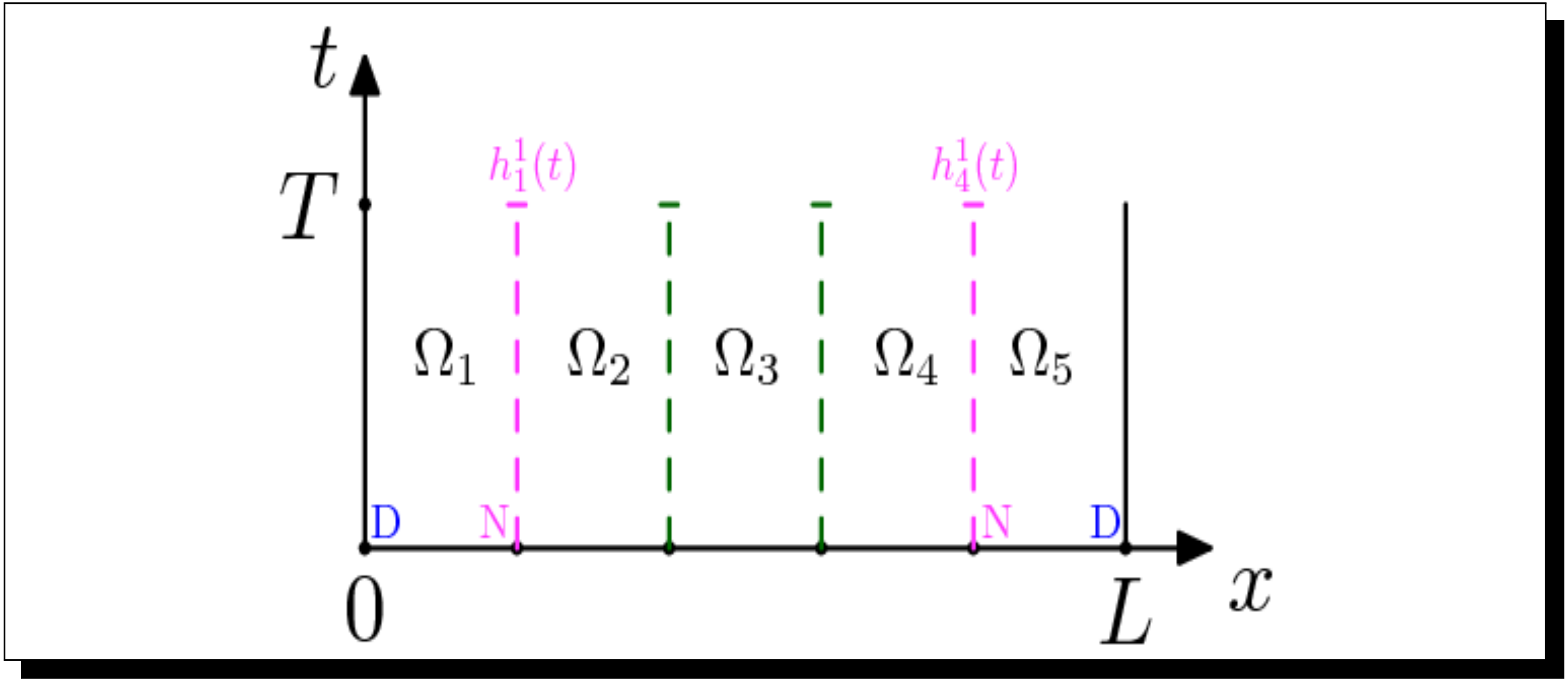
DNWR Method : Many Subdomains



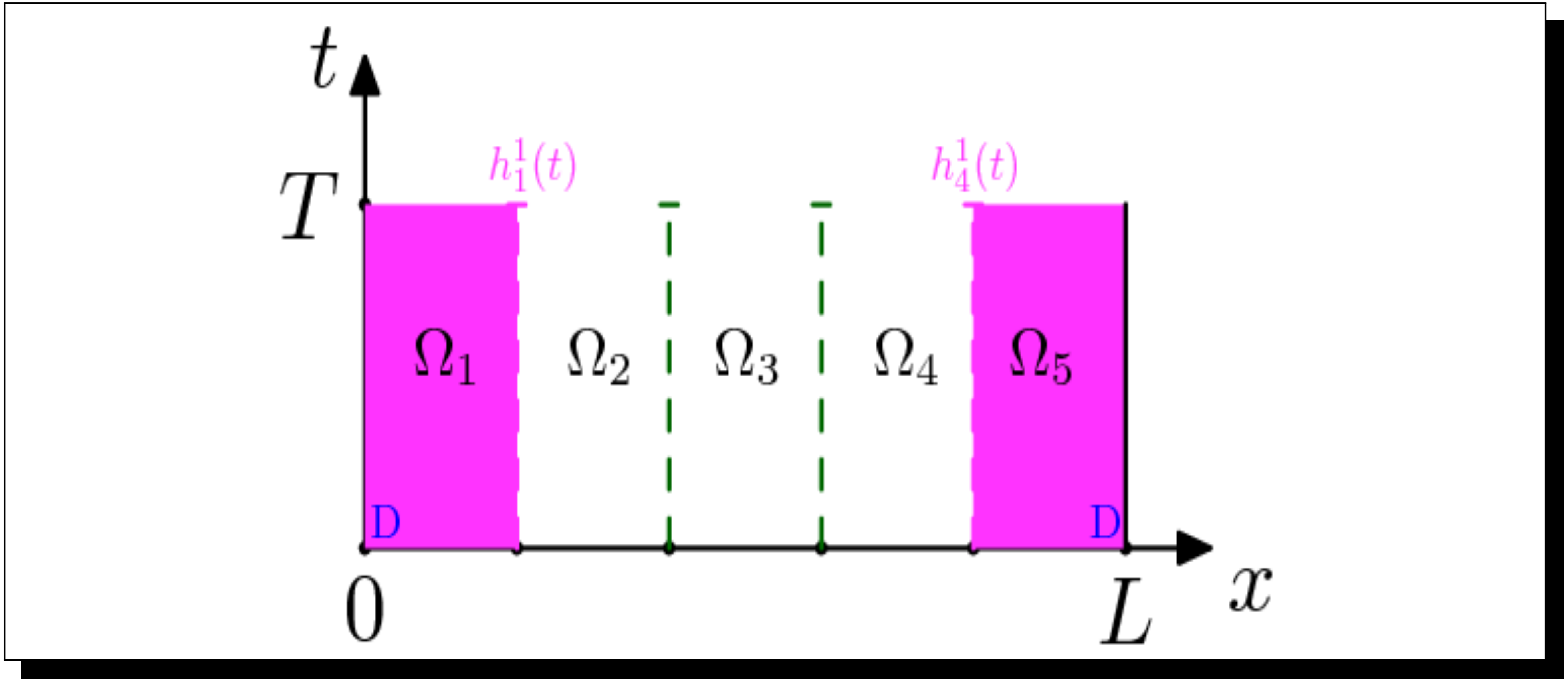
DNWR Method : Many Subdomains



DNWR Method : Many Subdomains



DNWR Method : Many Subdomains



Convergence result: Heat equation

Theorem(*Convergence of DNWR for N subdomains)[GKM, '13]*

Suppose N is odd. Then for $\theta = 1/2$ and for a finite time interval $(0, T)$, the DNWR algorithm for N subdomains converges superlinearly with the estimate

$$\max_{1 \leq i \leq N-1} \| g_i^k \|_{L^\infty(0,T)} \leq \psi^k \operatorname{erfc}\left(\frac{kh}{2\sqrt{T}}\right) \max_{1 \leq i \leq N-1} \| g_i^0 \|_{L^\infty(0,T)},$$

where $\psi(N, T) = \min\{(N-2), \phi(N, T)\}$

with $\phi(N, T) = 2 \operatorname{erfc}\left(\frac{h}{2\sqrt{T}}\right) + \sum_{i=0}^{(N-3)/2} 2^{i+1} \operatorname{erfc}\left(\frac{ih}{2\sqrt{T}}\right).$

Convergence estimates

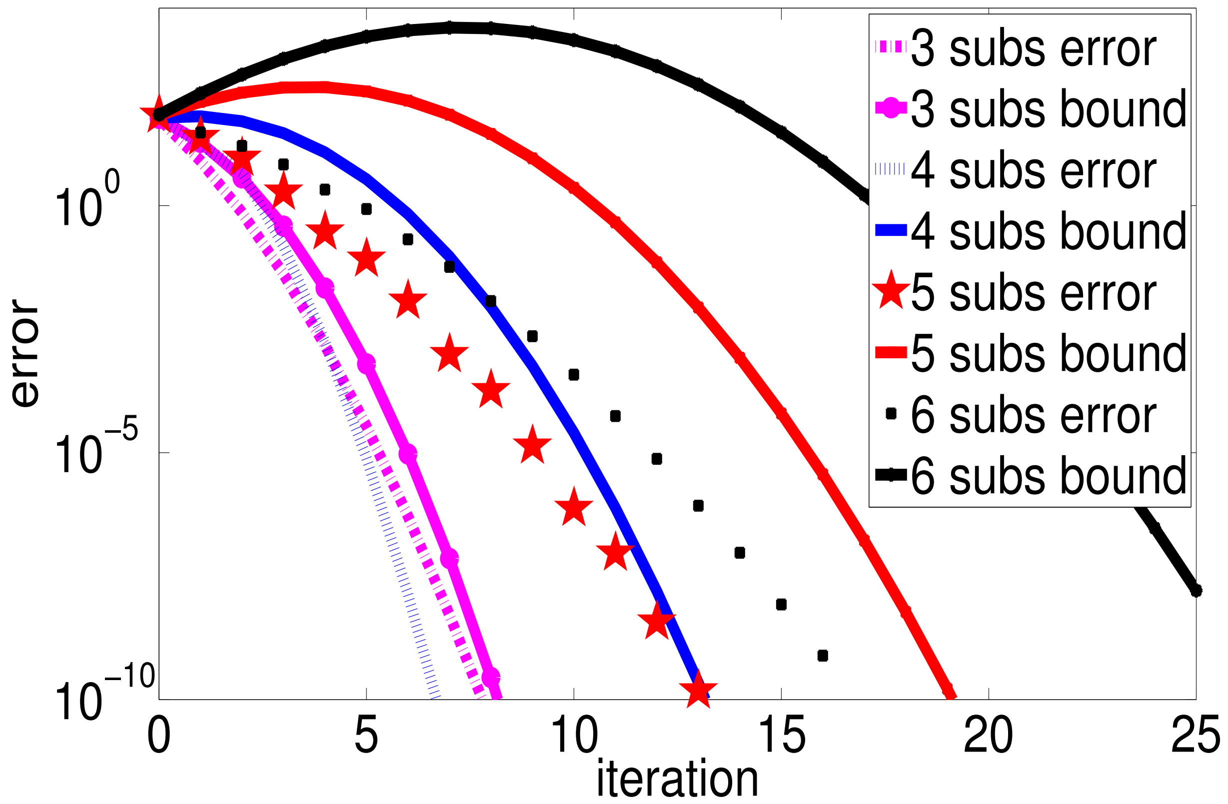


Figure: Estimates for different number of subdomains, $T = 2$.

$$\text{Minimize } J(y,u) = \frac{1}{2}\int_0^T\int_0^1 (y-\hat{y})^2\,dxdt + \frac{\lambda}{2}\int_0^T\int_0^1 u^2 dxdt,$$

$$\text{subject to } \begin{cases} \partial_t y(x,t) - \nu\Delta y(x,t) = u(x,t), & x\in\Omega, t\in(0,T),\\ y(x,0) = y_0(x), & x\in\Omega,\\ y(x,t) = 0, & x\in\partial\Omega\times(0,T). \end{cases} \tag{3}$$

The adjoint equation would be:

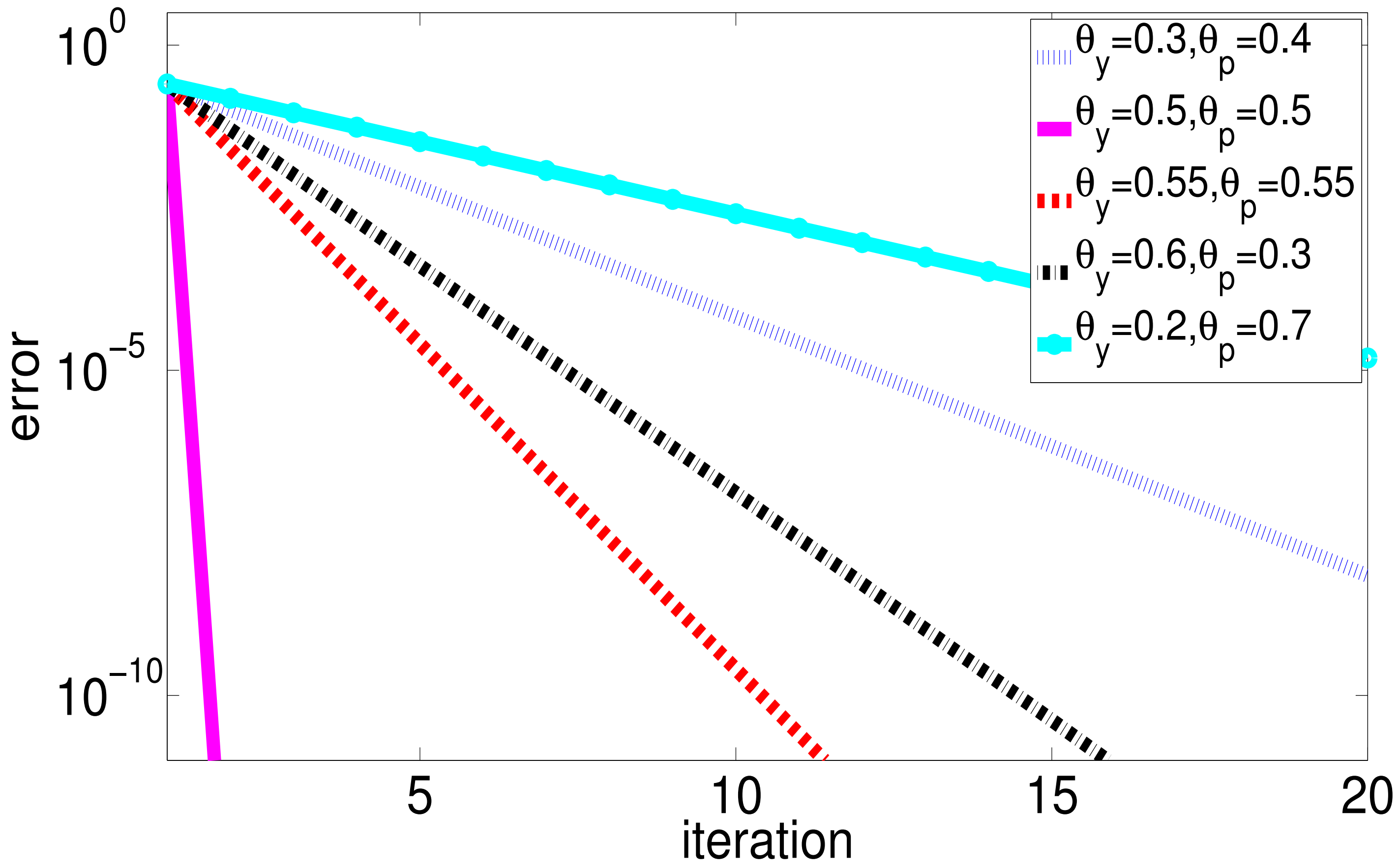
$$\begin{cases} -\partial_t p(x,t) - \nu\Delta p(x,t) = y(x,t) - \hat{y}(x,t), & x\in\Omega, t\in(0,T),\\ p(x,T) = 0, & x\in\Omega,\\ p(x,t) = 0, & x\in\partial\Omega\times(0,T), \end{cases} \tag{4}$$

with the optimality condition:

$$p(x,t) + \lambda u(x,t) = 0.$$

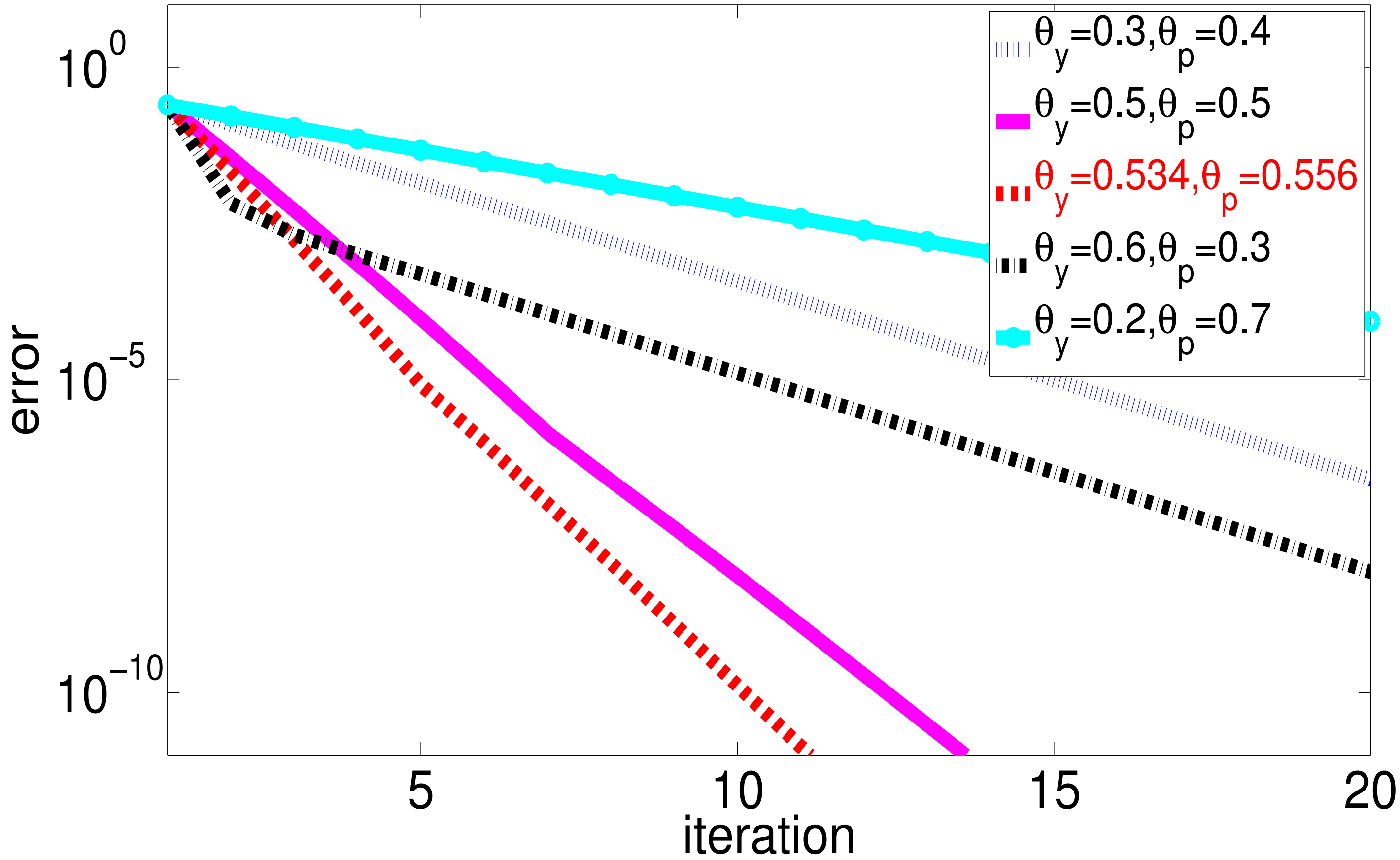
Numerical Results: DNWR

Experiment 1: $\alpha = 0.5, \lambda = 1, T = 2. \Rightarrow \theta_y^* = 1/2 = \theta_p^*.$



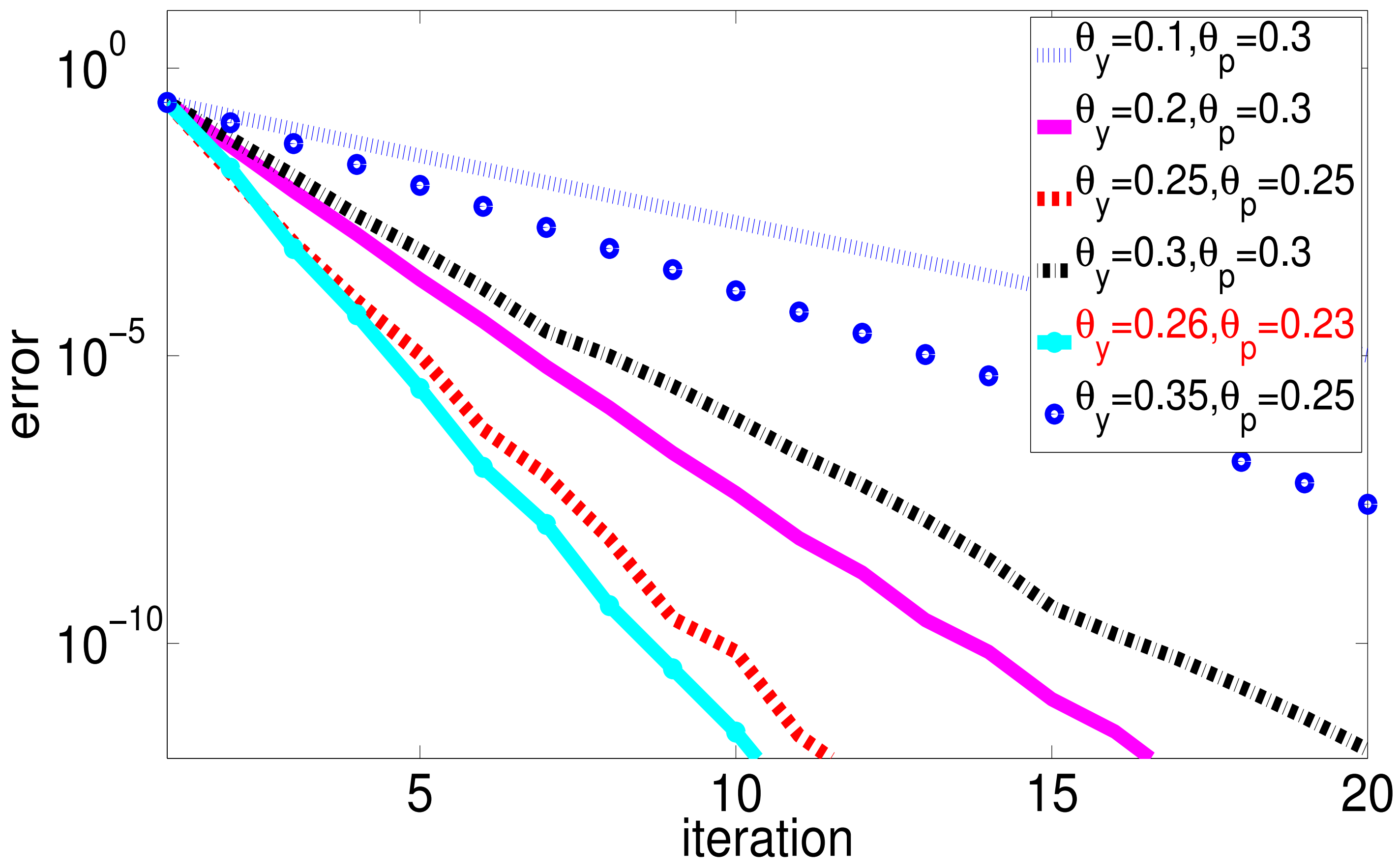
Numerical Results: DNWR

Experiment 2: $\alpha = 0.6, \lambda = 1, T = 2. \Rightarrow \theta_y^* \approx 0.534, \theta_p^* \approx 0.556.$



Numerical Results: NNWR

Experiment: $\alpha = 0.6, \lambda = 1, T = 2. \Rightarrow \theta_y^* = 0.26, \theta_p^* = 0.23.$



$$\text{Minimize } J(y,u) = \frac{1}{2}\|Cy - \hat{y}\|^2_{L^2} + \frac{\lambda}{2}\|u\|^2_{L^2},$$

$$\text{subject to } \begin{cases} \partial_t y(x,t) - \Delta f(y) + \epsilon^2 \Delta^2 y = u(x,t), & x \in \Omega, t \in (0,T), \\ y(x,0) = y_0(x), & x \in \Omega, \\ y(x,t) = 0 = \Delta y(x,t), & x \in \partial\Omega \times (0,T). \end{cases}$$

The adjoint equation would be:

$$\begin{cases} -\partial_t p(x,t) - f'(y)\Delta p + \epsilon^2 \Delta^2 p = C^T(Cy(x,t) - \hat{y}), & x \in \Omega, t \in (0,T), \\ p(x,T) = 0, & x \in \Omega, \\ p(x,t) = 0 = \Delta p(x,t) & x \in \partial\Omega \times (0,T), \end{cases}$$

$f(y) = y^3 - y$ with the optimality condition:

$$J'(y,u)(v-u) \geq 0 \quad \forall v \in L^2(\Omega \times (0,T))$$

where $J'(y,u)$ is the Gateaux derivative of $J(y,v)$ at $v = u$.
[1]

[1] Optimal control for the multi-dimensional viscous Cahn-Hilliard equation, Ning Duan and Xiufang Zhao, Elec. J. Differential Equations, 2015

Cahn-Hilliard Equation

$$\begin{aligned}
\frac{\partial u}{\partial t} &= \Delta v, \quad \text{for } (x,t) \in \Omega \times (0,T], \\
v &= F'(u) - \epsilon^2 \Delta u, \quad \text{for } (x,t) \in \Omega \times (0,T], \\
u(x,0) &= u_0(x), \;\; x \in \Omega,
\end{aligned}$$

where $\Omega \subset \mathbb{R}^d$, with $\frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0$ on $\partial\Omega$, for all $t \in (0,T]$.

- represents the evolution of a binary melted alloy below the critical temperature.

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- represents the evolution of a binary melted alloy below the critical temperature.

- it describes energy minimization and the total mass conservation while the system evolves:

$$
\frac{d}{dt}\mathcal{E}(u) \leq 0, \qquad \frac{d}{dt}\int_\Omega u = 0,
$$

where $F(u) = \frac{1}{4}(u^2-1)^2$, $\mathcal{E}(u) := \int_\Omega \left(F(u) + \frac{\epsilon^2}{2}|\nabla u|^2 \right) d\boldsymbol{x}$.

Discretized scheme can be written as:

$$
\begin{aligned}
u_j^{n+1} - \delta_t \Delta_h v_j^{n+1} &= u_j^n, \\
v_j^{n+1} + \epsilon^2 \Delta_h u_j^{n+1} - (u_j^{n+1})^3 &= -u_j^n,
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[2] Convergence of Linear and Nonlinear Substructuring Methods for the Cahn-Hilliard Equation, Gobinda Garai and Bankim Mandal, preprint.

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Linearized discrete scheme can be written as:

$$u_j^{n+1} - \delta_t \Delta_h v_j^{n+1} = u_j^n,$$
$$v_j^{n+1} + \epsilon^2 \Delta_h u_j^{n+1} - (u_j^n)^2 u_j^{n+1} = -u_j^n,$$

- which is an unconditionally gradient stable scheme and has the same accuracy as the nonlinear scheme (Eyre, 1998).
- at each time level obtain a system of elliptic equations

$$\begin{bmatrix} I & -\delta_t \Delta \\ \epsilon^2 \Delta - c^2 & I \end{bmatrix} \begin{bmatrix} u_j^{n+1} \\ v_j^{n+1} \end{bmatrix} = \begin{bmatrix} u_j^n \\ -u_j^n \end{bmatrix}, \quad \text{in } \Omega.$$

[2]

[2] Convergence of Linear and Nonlinear Substructuring Methods for the Cahn-Hilliard Equation, Gobinda Garai and Bankim Mandal, preprint.

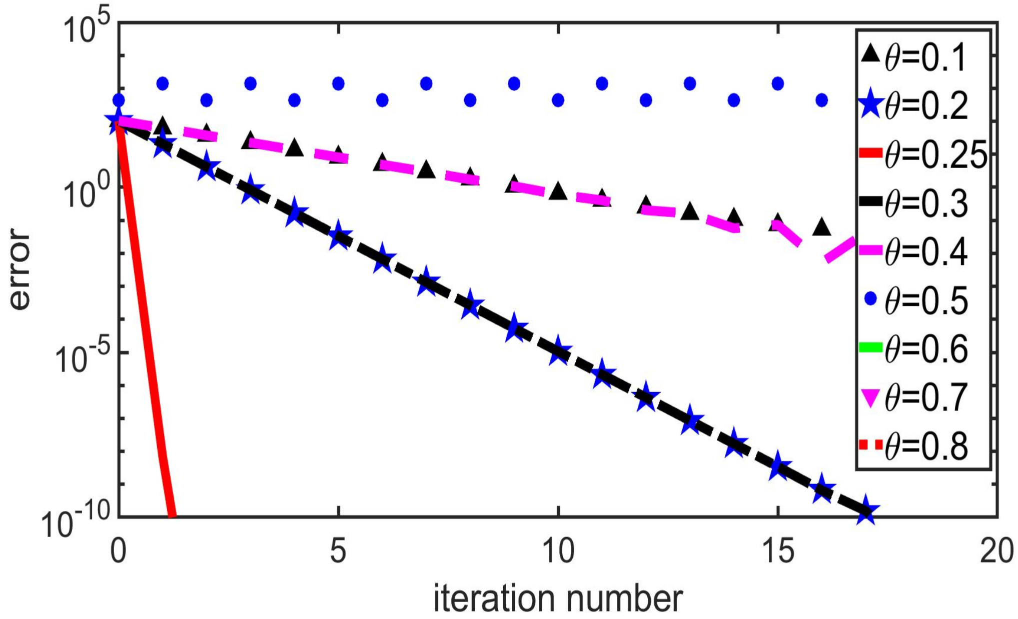
Convergence Result: NN

Theorem (Non-symmetric subdomains (Garai, M.))

For $\theta = 1/4$, the error of the NN method for two subdomains satisfies,

$$\| g^{[k]} \|_{L^\infty(\Gamma)} \leq \begin{cases} \left(\frac{(a-b)^2}{4ab}\right)^k \max\left\{\| g^{[0]} \|_{L^\infty(\Gamma)}, \| h^{[0]} \|_{L^\infty(\Gamma)}\right\}, & \text{if } \delta_t > \frac{4\epsilon^2}{c^4}, \\ \left(\frac{(a-b)^2}{2ab}\right)^k \max\left\{\| g^{[0]} \|_{L^\infty(\Gamma)}, \| h^{[0]} \|_{L^\infty(\Gamma)}\right\}, & \text{if } \delta_t < \frac{4\epsilon^2}{c^4}, \end{cases}$$

where $g^{[0]}$ and $h^{[0]}$ are the initial guesses for u and v.



THEOREM (NON-SYMMETRIC SUBDOMAINS (GARAI, M.))

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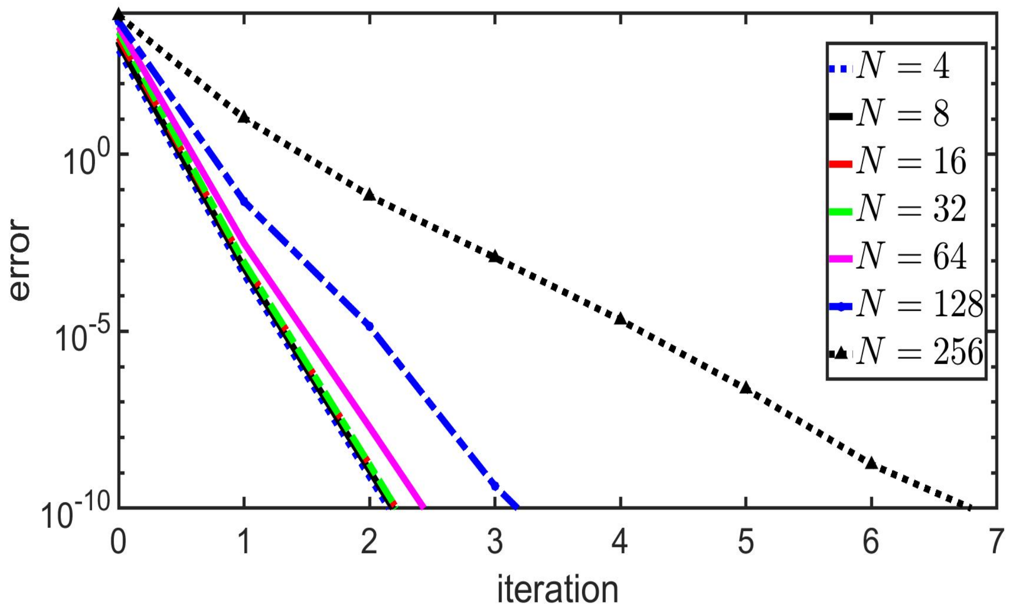

Time-Fractional Diffusion Equation

$$\begin{cases} D_t^\alpha u = \nabla \cdot (\kappa(\boldsymbol{x}, t)\nabla u) + f(\boldsymbol{x}, t), & \text{in } \Omega \times (0, T), \\ u(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}), & \text{in } \Omega, \\ u(\boldsymbol{x}, t) = g(\boldsymbol{x}, t), & \text{on } \partial\Omega \times (0, T). \end{cases}$$

D_t^α is the Caputo fractional derivative, defined for order α, $n - 1 < \alpha < n$ and $n \in \mathbb{N}$ as follows:

$$D_t^\alpha x(t) := \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-\tau)^{n-\alpha-1} x^{(n)}(\tau) d\tau.$$

[3] appear in viscoelasticity, fractional capacitor theory, electrical circuits, control theory etc.

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$\alpha \in (0,1)$ corresponds to sub-diffusion and $\alpha \in (1,2)$ corresponds to super-diffusion case. [3]

[3] appear in viscoelasticity, fractional capacitor theory, electrical circuits, control theory etc.

Theorem (DNWR for $\alpha \leq 1$ (Sana, M.))

In sub-diffusion and normal diffusion cases the interface error $w^{(k)}(t)$ follows the following super-linear estimates for $\theta = 1/(1+\sqrt{\kappa_1/\kappa_2})$:

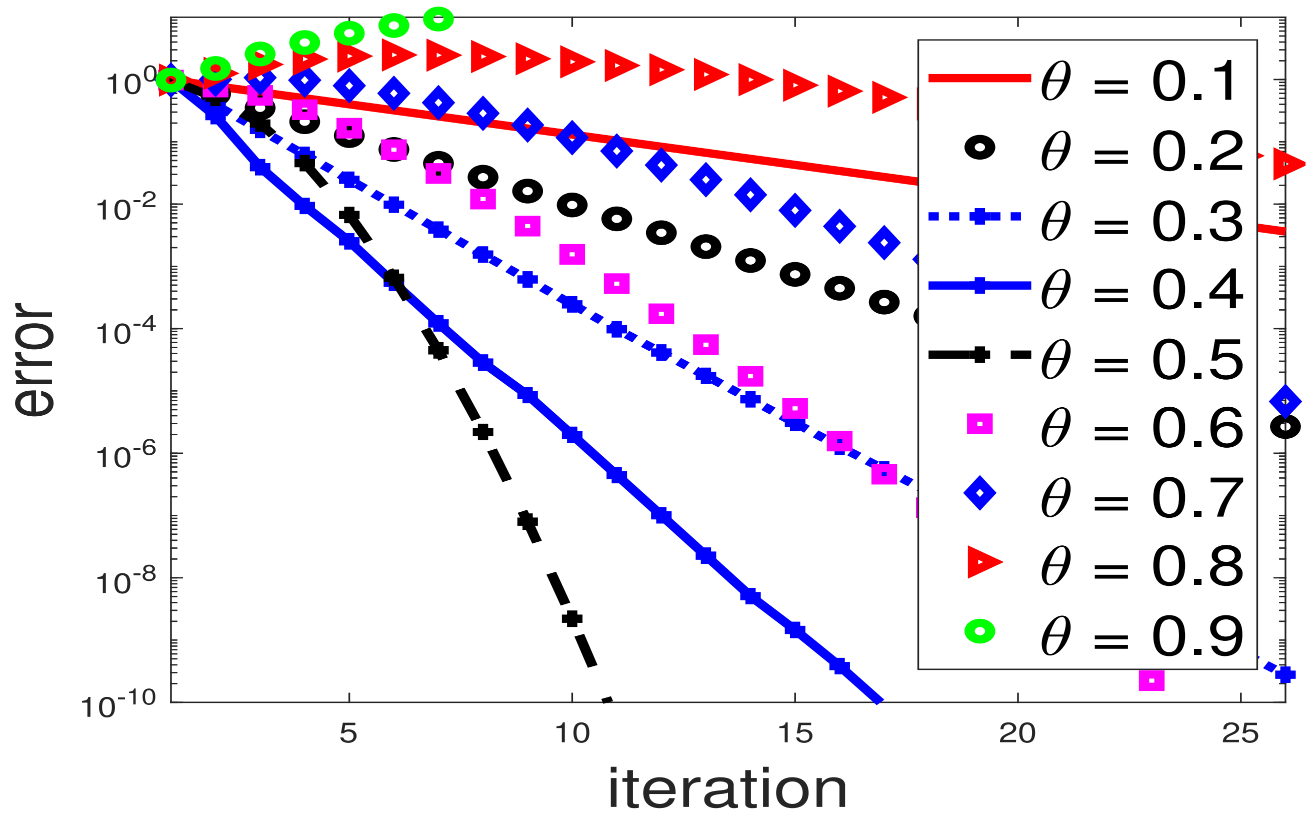
$$\|w^{(k)}\|_{L^\infty(0,T)} \leq (C(a,b,\kappa_1,\kappa_2))^k \exp\left(-\nu k^{2/(2-\alpha)}\right) \|w^{(0)}\|_{L^\infty(0,T)},$$

ν is a constant depending only on T, α, κ.

$\Rightarrow$ A similar super-linear estimate is proved for super-diffusion case $1 < \alpha < 2$.

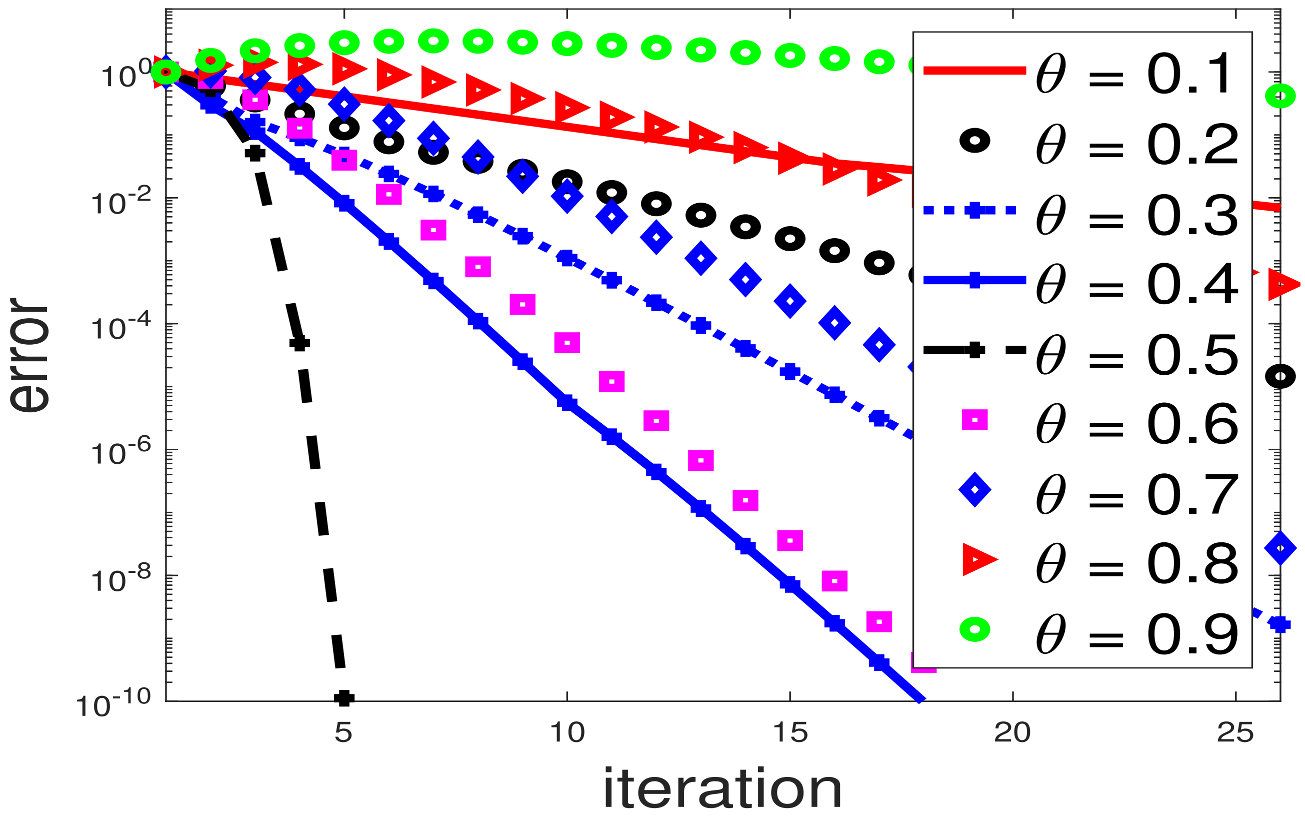
Convergence Result: Sub-diffusion case

$\alpha = 0.25$



Convergence Result: Super-diffusion case

$\alpha = 1.5$



- Increase number of communications,
- Decreased size of communications,
- Multiple waveform levels simultaneously,
- Use upto $2NK$ processors for NNWR, and upto NK processors for DNWR.

[4]

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[4] Pipeline Implementations of Neumann-Neumann and Dirichlet-Neumann Waveform Relaxation Methods, Ong and M., Numer. Algorithms, 2018

Waveform iteration, $K = 4$, Subdomains, $N = 8$

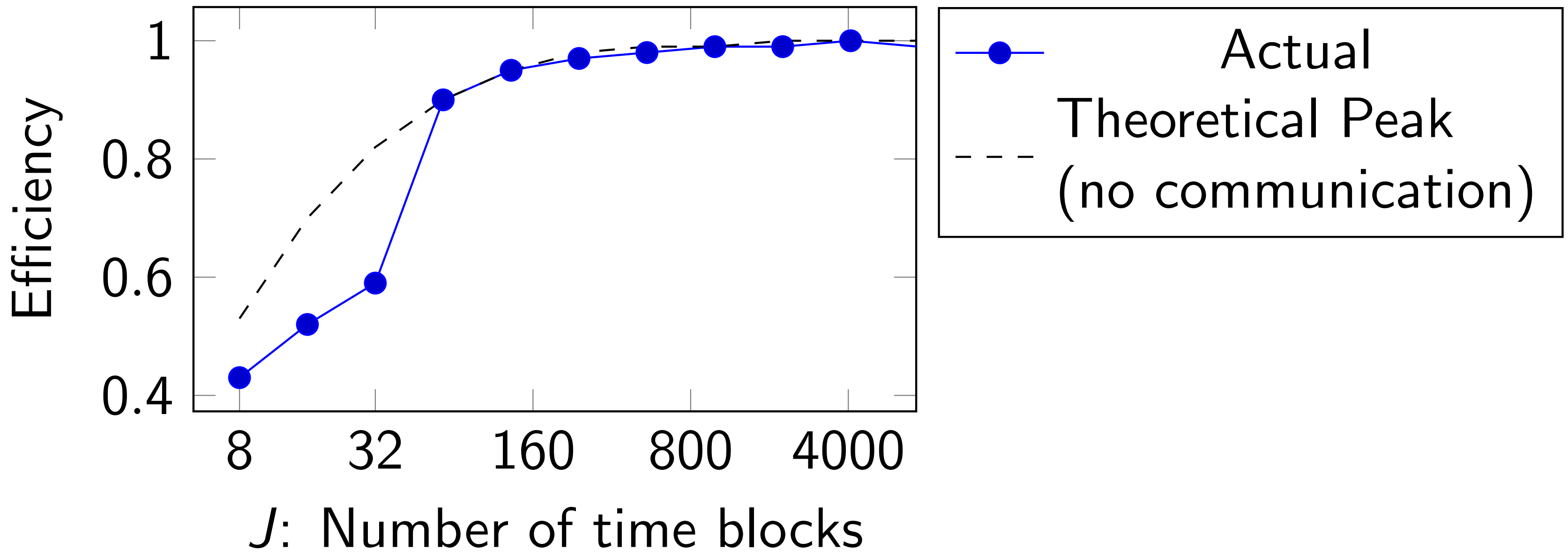

FIGURE: For a large number of time blocks, J, the algorithm is able to utilize all processors in a pipeline fashion for a larger percentage of the computation, leading to higher efficiency.

Waveform iteration, $K = 4$, Subdomains, $N = 8$

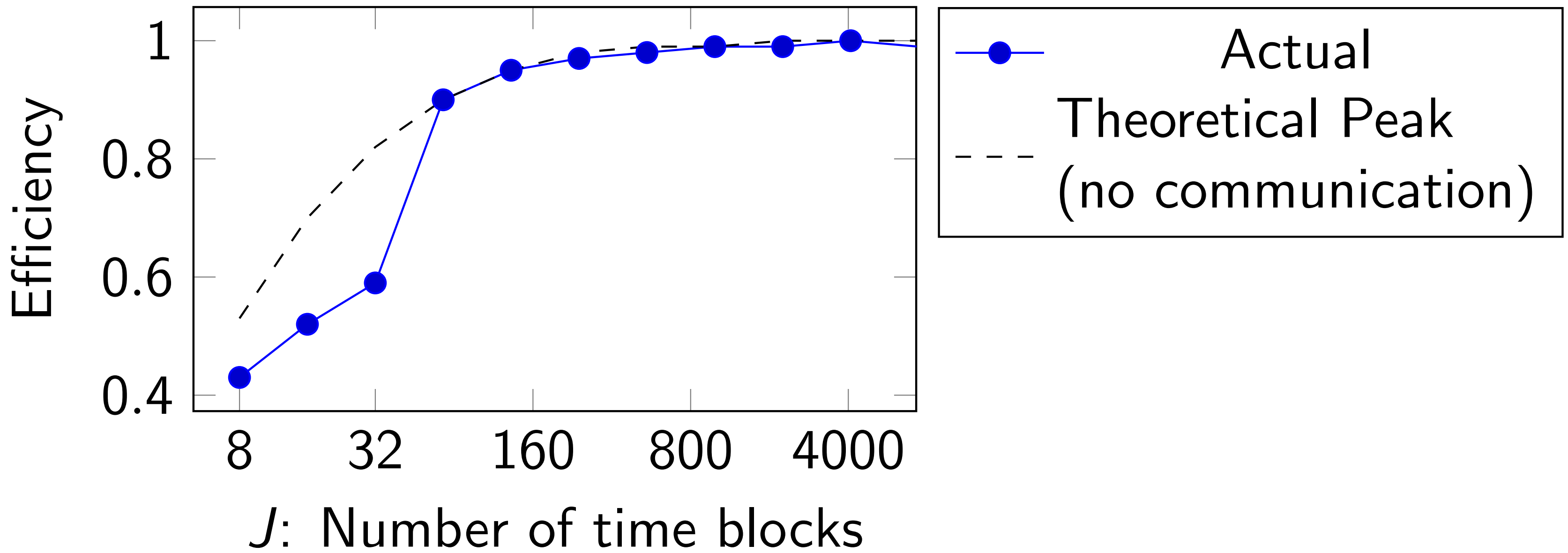

FIGURE: For a large number of time blocks, J, the algorithm is able to utilize all processors in a pipeline fashion for a larger percentage of the computation, leading to higher efficiency.

$\Rightarrow$ The pipeline NNWR implementation with $2KN$ processing cores is able to compute K full waveform iterates $2K$ times faster than the the classical NNWR implementation using N processors.

Pipeline NNWR: numerical results

weak scaling

K	$\#$ procs	Walltime (s)	Parallel Efficiency μs
1	16	211	1.00
2	32	209	1.01
4	64	214	0.99
8	128	212	1.00
16	256	212	1.00
32	512	212	1.00
64	1024	212	1.00

Table: An efficiency of 1 means that the pipeline NNWR implementation is able to compute K full waveform iterates using $2NK$ processing cores in half the time it takes N processing cores to compute one full waveform iterate.

Concluding Remarks

1. Steady Problems:
   - Three-step convergence for both DN and NN methods applied to OCP.
   - Analytical formulae for optimal parameters θ_y^*, θ_p^*.
2. Evolution Problems:
   - DNWR and NNWR to solve space-time problems.
   - Heat equation: Superlinear convergence for DNWR and NNWR.
   - Nonlinear equations: Convergence is superlinear.
   - Application to Optimal control problems with PDE constraints.
   - Easy to parallelize, scalable methods.

Thank You For Your Attention!

To know more about DNWR & NNWR, see...

1. *Convergence of Substructuring Methods for Elliptic Optimal Control Problems*, Gander, Kwok, M., DD24, 2017.
2. *Dirichlet-Neumann and Neumann-Neumann Waveform Relaxation Algorithms for Parabolic Problems*, Gander, Kwok, M., Electron. Trans. Numer. Anal. 45, 2016.
3. *Convergence of Linear and Nonlinear Substructuring Methods for the Cahn-Hilliard Equation*, Garai, M., preprint, arXiv:2112.01699, 2022
4. *Dirichlet-Neumann and Neumann-Neumann Waveform Relaxation Algorithms for the Time-Fractional Diffusion Problems*, Sana, M., preprint, 2022