Domain Decomposition Methods: Schwarz, Schur, Waveform Relaxation and the Parareal Algorithm

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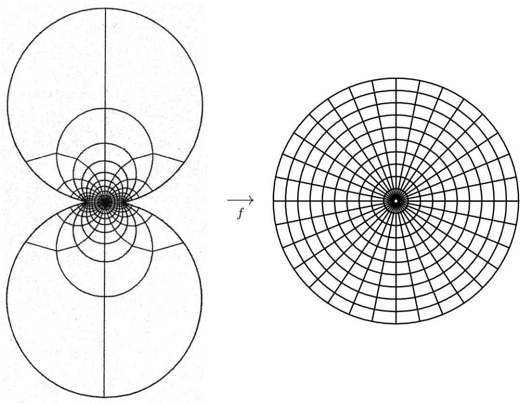
History: Riemann Mapping Theorem

"Zwei gegebene einfach zusammenhängende Flächen können stets so aufeinander bezogen werden, dass jedem Punkte der einen ein mit ihm stetig fortrückender Punkt entspricht...;"



(drawing M. Gutknecht 18.12.1975)

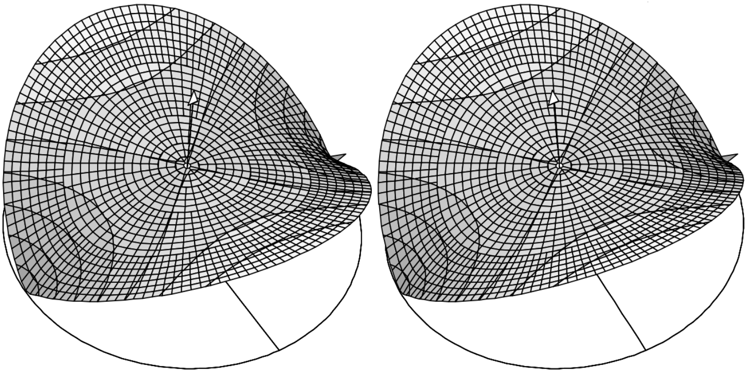
Proof: Riemann uses existence of harmonic functions

International Challenge

Find harmonic functions $\Delta u = 0$ on any domain Ω with prescribed boundary conditions $u = g$ for $(x, y) \in \partial\Omega$.

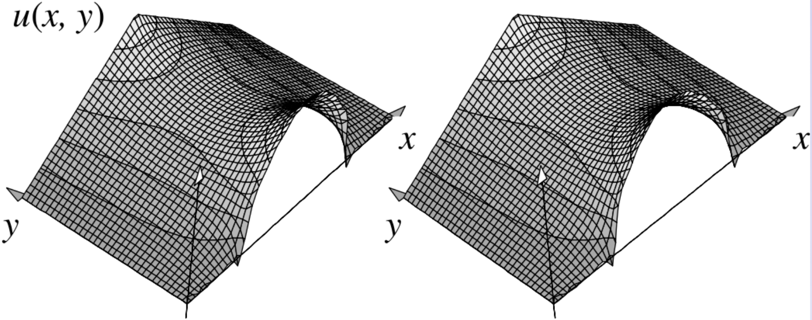
Solution easy for circular domain (Poisson 1815) ...

$$u(r,\phi) = \frac{1}{2\pi}\int_0^{2\pi} \frac{1-r^2}{1-2r\cos(\phi-\psi)+r^2} f(\psi)\, d\psi \; .$$



International Challenge

... and for rectangular domains (Fourier 1807):



But existence of solutions of Laplace equation on arbitrary domains appears hopeless !

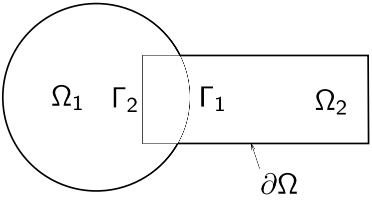
Proof without Dirichlet Principle

H.A. Schwarz (1870, Crelle 74, 1872) Über einen Grenzübergang durch alternierendes Verfahren

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

Classical Alternating Schwarz Method

Schwarz invents a method to proof that the infimum is attained: for a general domain $\Omega := \Omega_1 \cup \Omega_2$:



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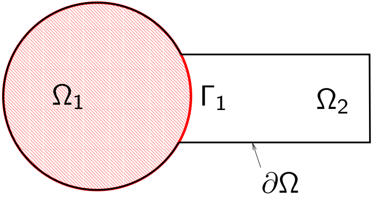

$$\begin{aligned} \Delta u_1^1 &= 0 && \text{in } \Omega_1 \\ u_1^1 &= g && \text{on } \partial\Omega \cap \overline{\Omega}_1 \\ u_1^1 &= u_2^0 && \text{on } \Gamma_1 \end{aligned}$$

solve on the disk $u_2^0 = 0$

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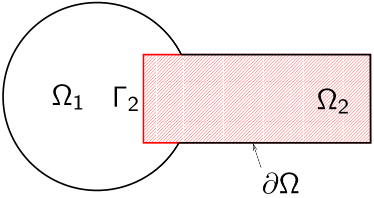

$$
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\end{aligned}
$$

solve on the rectangle

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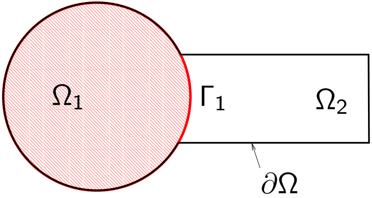

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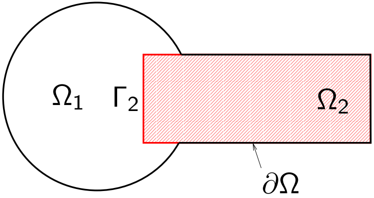

$$\begin{aligned} \Delta u_2^2 &= 0 && \text{in } \Omega_2 \\ u_2^2 &= g && \text{on } \partial\Omega \cap \overline{\Omega}_2 \\ u_2^2 &= u_1^2 && \text{on } \Gamma_2 \end{aligned}$$

solve on the rectangle

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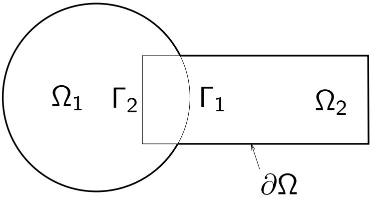

$$
\begin{aligned}
\Delta u_1^n &= 0 && \text{in } \Omega_1 \\
u_1^n &= g && \text{on } \partial\Omega \cap \overline{\Omega}_1 \\
u_1^n &= u_2^{n-1} && \text{on } \Gamma_1
\end{aligned}
\qquad
\begin{aligned}
\Delta u_2^n &= 0 && \text{in } \Omega_2 \\
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solve on the disk — solve on the rectangle

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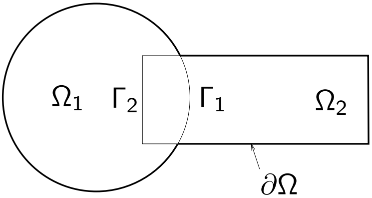
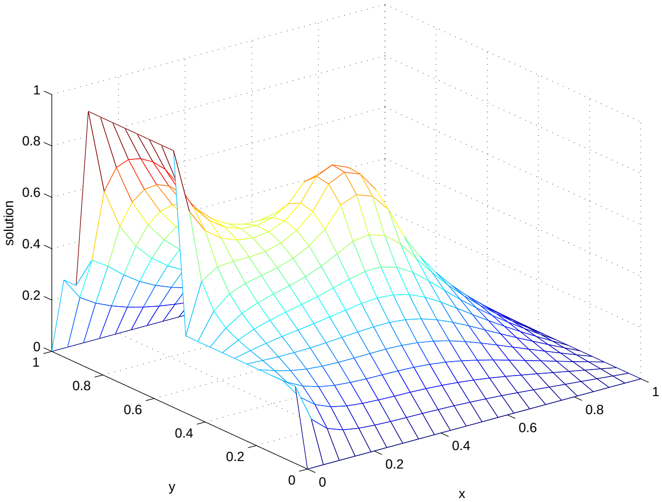


$$\begin{array}{rlcrl} \Delta u_1^n = 0 & \text{in } \Omega_1 & \quad & \Delta u_2^n = 0 & \text{in } \Omega_2 \\ u_1^n = g & \text{on } \partial\Omega \cap \overline{\Omega}_1 & & u_2^n = g & \text{on } \partial\Omega \cap \overline{\Omega}_2 \\ u_1^n = u_2^{n-1} & \text{on } \Gamma_1 & & u_2^n = u_1^n & \text{on } \Gamma_2 \end{array}$$

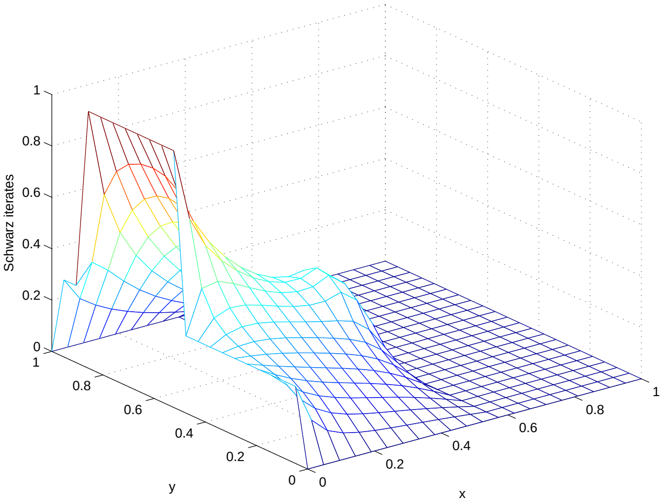
solve on the disk — solve on the rectangle

- Schwarz proved convergence in 1869 using the maximum principle.

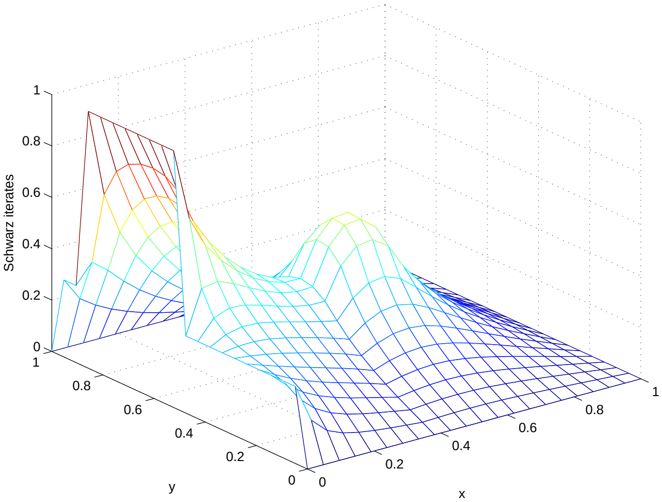
Example: Heating a Room



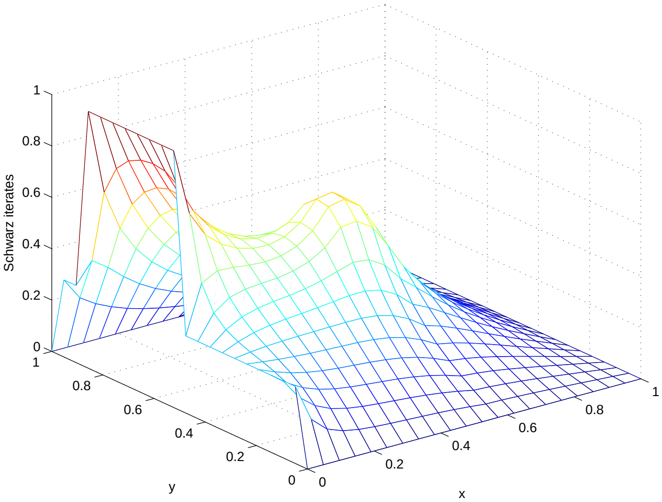
Iteration 1



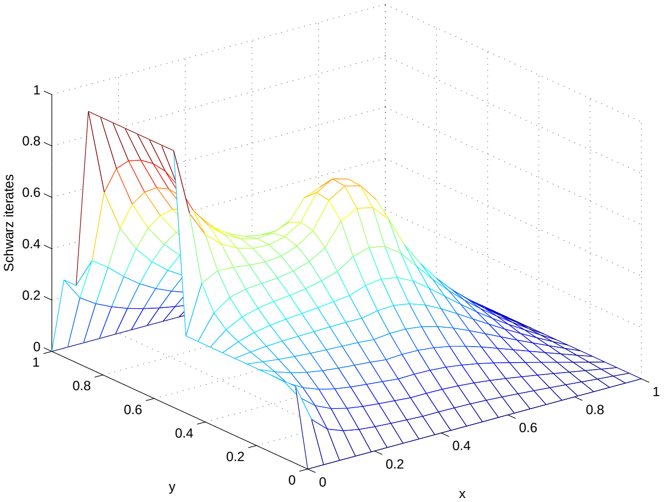
Iteration 2



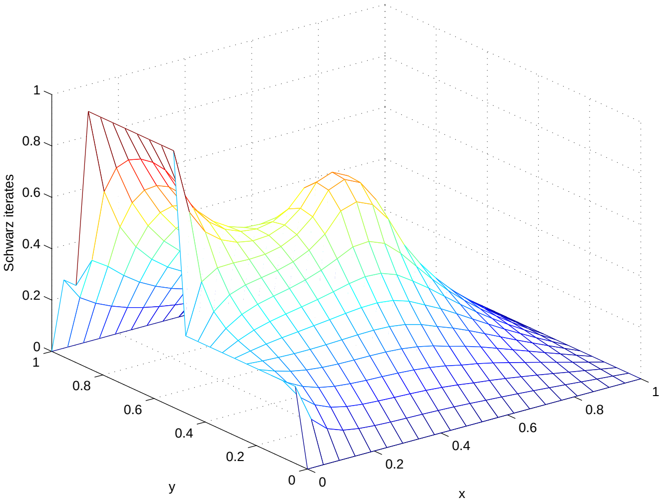
Iteration 3



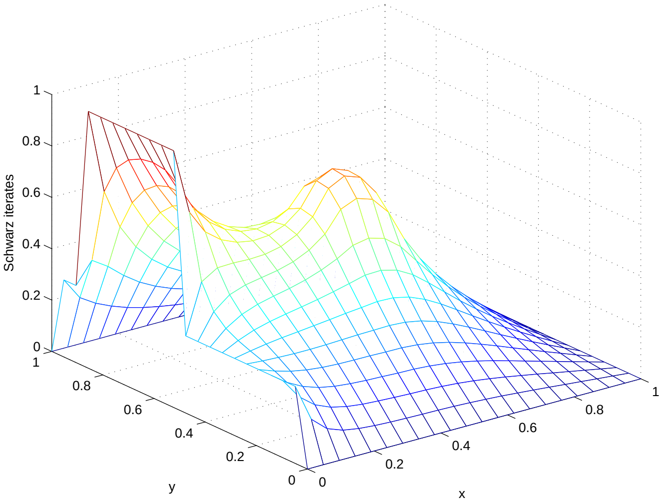
Iteration 4



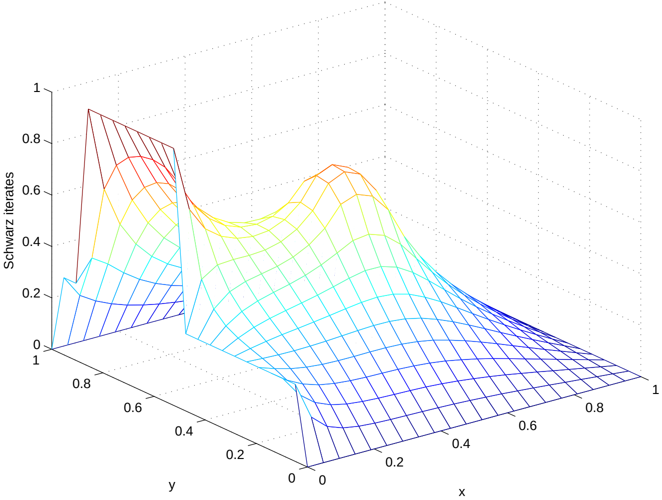
Iteration 5



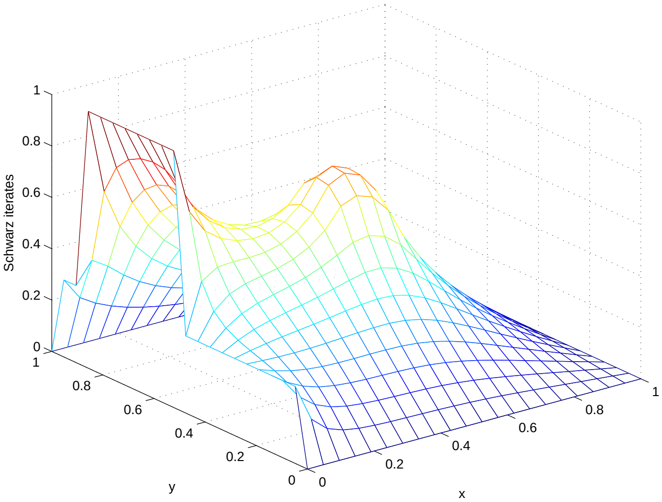
Iteration 6



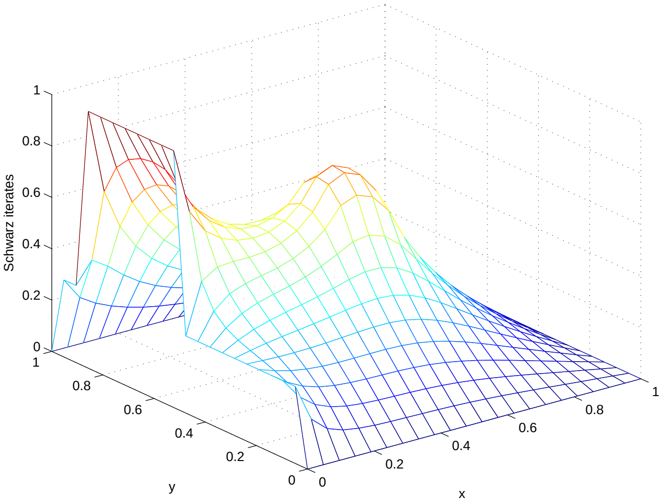
Iteration 7



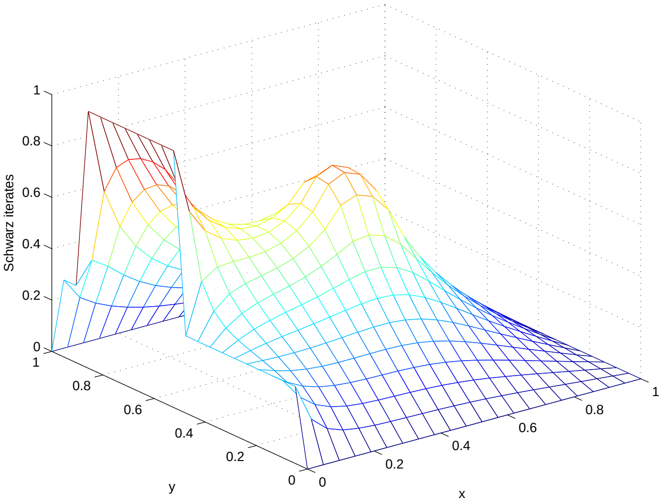
Iteration 8



Iteration 9



Iteration 10



Substructuring

Invented in the engineering community for the finite element design of aircraft (Boeing)

Przemieniecki 1963: Matrix structural analysis of substructures

The necessity for dividing a structure into substructures arises either from the requirement that different types of analysis have to be used on different components, or because the capacity of the digital computer is not adequate to cope with the analysis of the complete structure.

Idea of Przemieniecki

Przemieniecki 1963: In the present method each substructure is first analyzed separately, assuming that all common boundaries with adjacent substructures are completely fixed: these boundaries are then relaxed simultaneously and the actual boundary displacements are determined from the equations of equilibrium of forces at the boundary joints. The substructures are then analyzed separately again under the action of specified external loading and the previously determined boundary displacements.

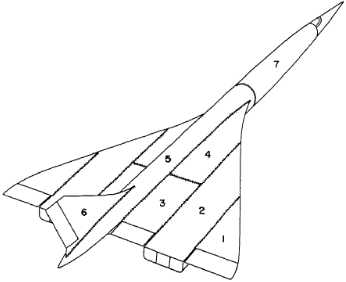


FIG. 3. Typical substructure arrangement for delta aircraft.

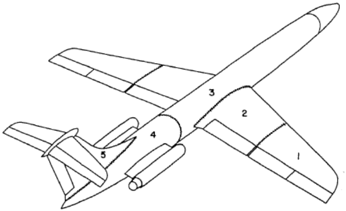


FIG. 4. Typical substructure arrangement for conventional aircraft.

Historical Example of Przemieniecki

Let P be the exterior forces, K the stiffness matrix, and U the displacement vector satisfying

$$KU = P.$$

Partition U into U_i interior in each substructure, and U_b on the interfaces between substructures:

$$K \begin{bmatrix} U_b \\ U_i \end{bmatrix} := \begin{bmatrix} K_{bb} & K_{bi} \\ K_{ib} & K_{ii} \end{bmatrix} \begin{bmatrix} U_b \\ U_i \end{bmatrix} = \begin{bmatrix} P_b \\ P_i \end{bmatrix}.$$

Physical motivation of Przemieniecki:

$$P = P^{(\alpha)} + P^{(\beta)} = \begin{bmatrix} P_b^{(\alpha)} \\ P_i \end{bmatrix} + \begin{bmatrix} P_b^{(\beta)} \\ 0 \end{bmatrix},$$

$$U = U^{(\alpha)} + U^{(\beta)} = \begin{bmatrix} 0 \\ U_i^{(\alpha)} \end{bmatrix} + \begin{bmatrix} U_b \\ U_i^{(\beta)} \end{bmatrix}.$$

Two Physically Relevant Systems

By linearity, Przemieniecki obtains two systems

$$(\alpha): \begin{bmatrix} K_{bb} & K_{bi} \\ K_{ib} & K_{ii} \end{bmatrix} \begin{bmatrix} 0 \\ U_i^{(\alpha)} \end{bmatrix} = \begin{bmatrix} P_b^{(\alpha)} \\ P_i \end{bmatrix}$$

$$(\beta): \begin{bmatrix} K_{bb} & K_{bi} \\ K_{ib} & K_{ii} \end{bmatrix} \begin{bmatrix} U_b \\ U_i^{(\beta)} \end{bmatrix} = \begin{bmatrix} P_b^{(\beta)} \\ 0 \end{bmatrix},$$

Rewriting the first one leads to

$$(\alpha): \begin{cases} K_{bi} U_i^{(\alpha)} = P_b^{(\alpha)}, \\ K_{ii} U_i^{(\alpha)} = P_i, \end{cases}$$

Knowing the forces P_i in each substructure, (α) permits to compute the interior displacements keeping interfaces fixed:

$$U_i^{(\alpha)} = K_{ii}^{-1} P_i.$$

This uncovers the unknown splitting of the interface forces

$$P_b^{(\alpha)} = K_{bi} K_{ii}^{-1} P_i,$$

Toward the Schur Complement System

Hence the remaining forces acting on the interfaces are

$$P_b^{(\beta)} := P_b - P_b^{(\alpha)} = P_b - K_{bi}K_{ii}^{-1}P_i \, ,$$

One can now solve the system

$$(\beta) : \begin{cases} K_{bb}U_b + K_{bi}U_i^{(\beta)} = P_b^{(\beta)}, \\ K_{ib}U_b + K_{ii}U_i^{(\beta)} = 0, \end{cases}$$

which represents the response of the structures to the interface loading $P_b^{(\beta)}$. The second equation gives the internal displacement $U_i^{(\beta)}$ based on the boundary displacement U_b,

$$U_i^{(\beta)} = -K_{ii}^{-1}K_{ib}U_b,$$

and inserting this into the first equation, Przemieniecki obtains the interface system

$$(K_{bb} - K_{bi}K_{ii}^{-1}K_{ib})U_b = P_b - K_{bi}K_{ii}^{-1}P_i,$$

Primal Schur Method

This gives the complete interface displacement

$$U_b = (K_{bb} - K_{bi}K_{ii}^{-1}K_{ib})^{-1}(P_b - K_{bi}K_{ii}^{-1}P_i),$$

and interior displacements are obtained by summing $U_i^{(\beta)}$ and $U_i^{(\alpha)}$ (or solving $K_{ib}U_b + K_{ii}U_i = P_i$ for U_i).

Procedure of Przemieniecki:

1. Invert the block diagonal matrix K_{ii}
2. Invert the smaller matrix $S = K_{bb} - K_{bi}K_{ii}^{-1}K_{ib}$

The matrix S is called Schur complement matrix after Emilie Virginia Haynsworth (On the Schur complement 1968, Basel) after a determinant lemma of Issai Schur.

Remark: The name Schur method is more precise than substructuring, since any method can be substructured, also Schwarz methods.

Waveform Relaxation

Émile Picard (1893): Sur l'application des méthodes d'approximations successives à l'étude de certaines équations différentielles ordinaires

Les méthodes d'approximation dont nous faisons usage sont théoriquement susceptibles de s'appliquer à toute équation, mais elles ne deviennent vraiment intéressantes pour l'étude des propriétés des fonctions définies par les équations différentielles que si l'on ne reste pas dans les généralités et si l'on envisage certaines classes d'équations.

The Method of ...

14. Indiquons une autre méthode pour établir l'existence des intégrales des équations différentielles ordinaires (¹). Nous envisageons, comme plus haut, en changeant seulement un peu les notations, le système des n équations du premier ordre

$$\frac{du}{dx} = f_1(x, u, v, \ldots, w),$$
$$\frac{dv}{dx} = f_2(x, u, v, \ldots, w),$$
$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots,$$
$$\frac{dw}{dx} = f_n(x, u, v, \ldots, w).$$

Les fonctions f sont des fonctions continues réelles des quantités réelles $x, u, v, \ldots, w$ dans le voisinage de $x_0, u_0, v_0, \ldots, w_0$. Elles sont définies quand $x, u, v, \ldots, w$ restent respectivement compris dans les intervalles

$$(x_0 - a, x_0 + a), \quad (u_0 - b, u_0 + b), \quad \ldots, \quad (w_0 - b, w_0 + b),$$

… Successive Approximations

Considérons d'abord le système

$$\frac{du_1}{dx} = f_1(x, u_0, v_0, \ldots, w_0), \qquad \ldots, \qquad \frac{dw_1}{dx} = f_n(x, u_0, v_0, \ldots, w_0),$$

nous en tirons, par quadratures, les fonctions $u_1, v_1, \ldots, w_1$, en les déterminant de manière qu'elles prennent pour x_0 les valeurs $u_0, v_0, \ldots, w_0$. On forme ensuite les équations

$$\frac{du_2}{dx} = f_1(x, u_1, v_1, \ldots, w_1), \qquad \ldots, \qquad \frac{dw_2}{dx} = f_n(x, u_1, v_1, \ldots, w_1),$$

et l'on détermine $u_2, v_2, \ldots, w_2$ par la condition qu'elles prennent respectivement pour x_0 les valeurs $u_0, v_0, \ldots, w_0$. On continue ainsi indéfiniment. Les fonctions $u_{m-1}, v_{m-1}, \ldots, w_{m-1}$ seront liées aux suivantes $u_m, v_m, \ldots, w_m$ par les relations

$$\frac{du_m}{dx} = f_1(x, u_{m-1}, v_{m-1}, \ldots, w_{m-1}),$$

$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots,$$

$$\frac{dw_m}{dx} = f_n(x, u_{m-1}, v_{m-1}, \ldots, w_{m-1}),$$

Detailed Historical Convergence Analysis

Ernest Lindelöf (1894): Sur l'application des méthodes d'approximations successives à l'étude des intégrales réelles des équations différentielles ordinaires

La présente étude a pour but de donner une exposition succincte de la méthode d'approximations successives de M. Picard en tant qu'elle s'applique aux équations différentielles ordinaires.

Theorem (Superlinear Convergence (Lindelöf 1894))

On bounded time intervals $t \in [0, T]$, the iterates satisfy the superlinear error bound

$$||\mathbf{v} - \mathbf{v}^n|| \leq \frac{(CT)^n}{n!} ||\mathbf{v} - \mathbf{v}^0||,$$

where C is a positive constant.

Classical Waveform Relaxation

Lelarasmee, Ruehli and Sangiovanni-Vincentelli (1982): The Waveform Relaxation Method for Time-Domain Analysis of Large Scale Integrated Circuits.

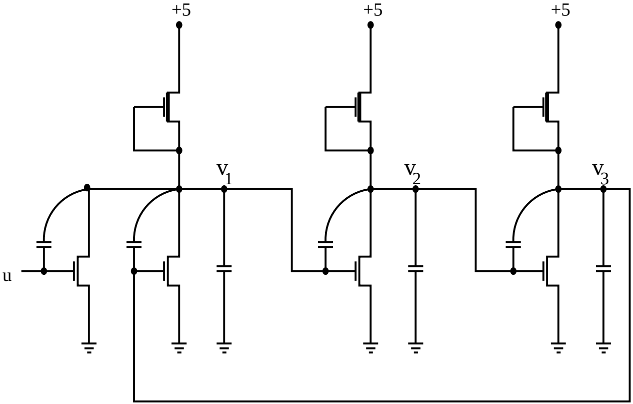
"The spectacular growth in the scale of integrated circuits being designed in the VLSI era has generated the need for new methods of circuit simulation. "Standard" circuit simulators, such as SPICE and ASTAP, simply take too much CPU time and too much storage to analyze a VLSI circuit".

Nevanlinna and Odeh (1987): Remarks on the Convergence of Waveform Relaxation Methods.

"Recently an approach called waveform relaxation methods (WR) has captured considerable attention in solving certain classes of large scale digital circuit equations."

A Historical Example

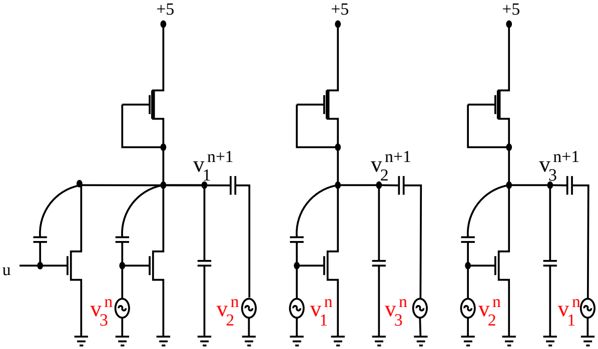
Example: a MOS ring oscillator (Lelarasmee et al 1982):



The equations for such a circuit can be written in form of a system of ordinary differential equations

$$\begin{aligned} \frac{\partial \mathbf{v}}{\partial t} &= f(\mathbf{v}), \qquad 0 < t < T \\ \mathbf{v}(0) &= \mathbf{g} \end{aligned}$$

Waveform Relaxation Decomposition

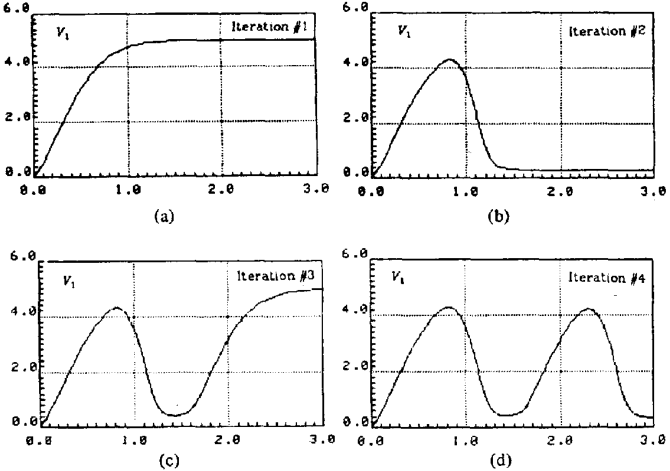


Iteration using subcircuit solutions only:

$$\begin{aligned} \partial_t v_1^{n+1} &= f_1(v_1^{n+1}, v_2^n, v_3^n) \\ \partial_t v_2^{n+1} &= f_2(v_1^n, v_2^{n+1}, v_3^n) \\ \partial_t v_3^{n+1} &= f_3(v_1^n, v_2^n, v_3^{n+1}) \end{aligned}$$

Signals along cables are called 'waveforms', which gave the algorithm its name Waveform Relaxation.

Historical Numerical Convergence Study



"Note that since the oscillator is highly nonunidirectional due to the feedback from v_3 to the NOR gate, the convergence of the iterated solutions is achieved with the number of iterations being proportional to the number of oscillating cycles of interest"

Alternating and Parallel Schwarz Method

For $\mathcal{L}u = f$ in $\Omega = \mathbb{R}^2$, $\Omega_1 = (-\infty, L) \times \mathbb{R}$, $\Omega_2 = (0, \infty) \times \mathbb{R}$

Alternating Schwarz method (Schwarz 1869):

$$\begin{array}{rcl} \mathcal{L}u_1^n &=& f, \text{ in } \Omega_1 \\ u_1^n &=& u_2^{n-1}, \text{ on } x = L \end{array} \qquad \begin{array}{rcl} \mathcal{L}u_2^n &=& f, \text{ in } \Omega_2 \\ u_2^n &=& u_1^n, \text{ on } x = 0 \end{array}$$

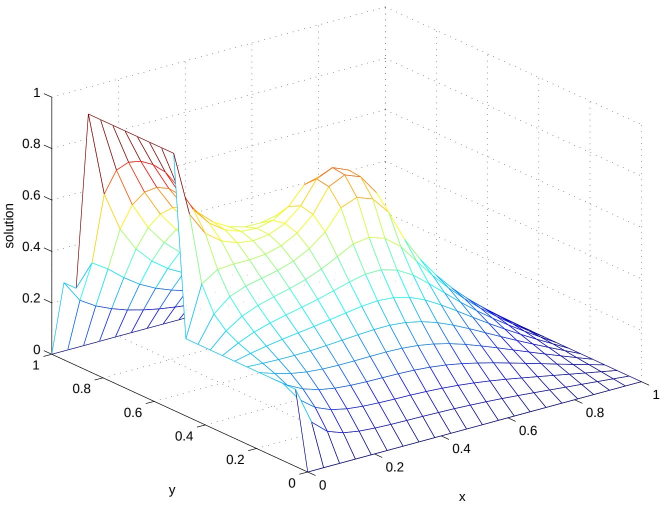
Parallel Schwarz method (P-L. Lions 1988):

> *The final extension we wish to consider concerns "parallel" versions of the Schwarz alternating method ..., ..., u_i^{n+1} is solution of $-\Delta u_i^{n+1} = f$ in Ω_i and $u_i^{n+1} = u_j^n$ on $\partial\Omega_i \cap \Omega_j$.*

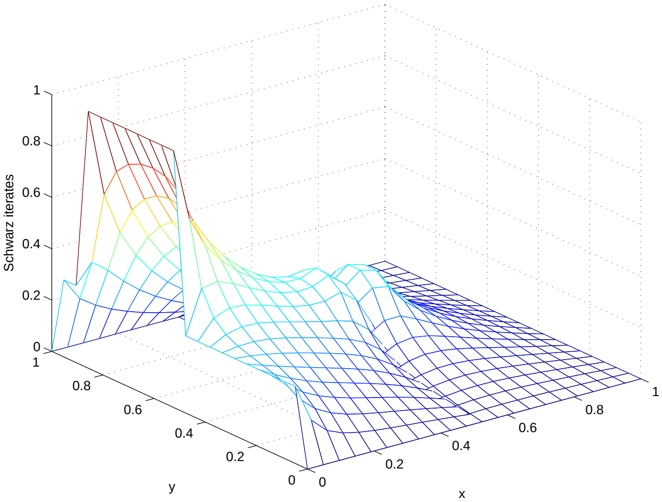
$$\begin{array}{rcl} \mathcal{L}u_1^n &=& f, \text{ in } \Omega_1 \\ u_1^n &=& u_2^{n-1}, \text{ on } x = L \end{array} \qquad \begin{array}{rcl} \mathcal{L}u_2^n &=& f, \text{ in } \Omega_2 \\ u_2^n &=& u_1^{n-1}, \text{ on } x = 0 \end{array}$$

Can solve with two processors in parallel, one computes for Ω_1 and one computes for Ω_2!

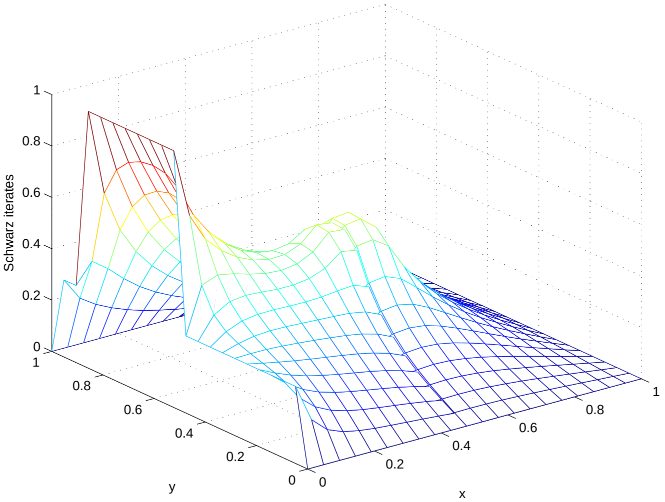
Example: Heating a Room



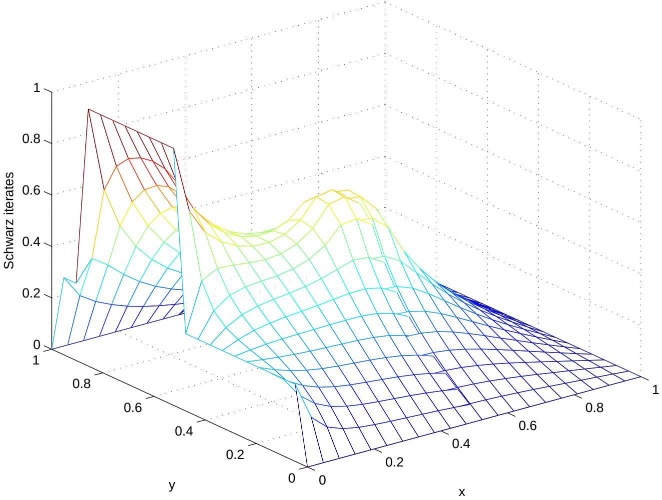
Iteration 1



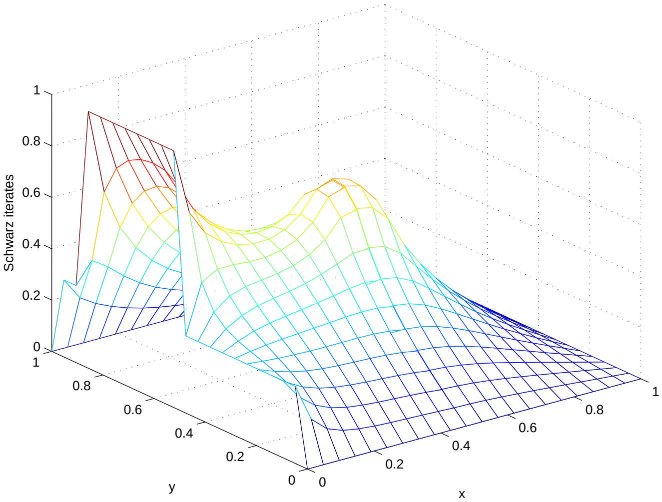
Iteration 2



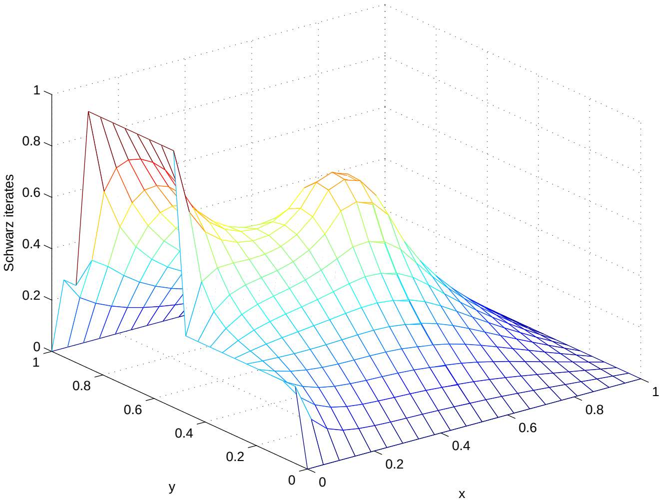
Iteration 3



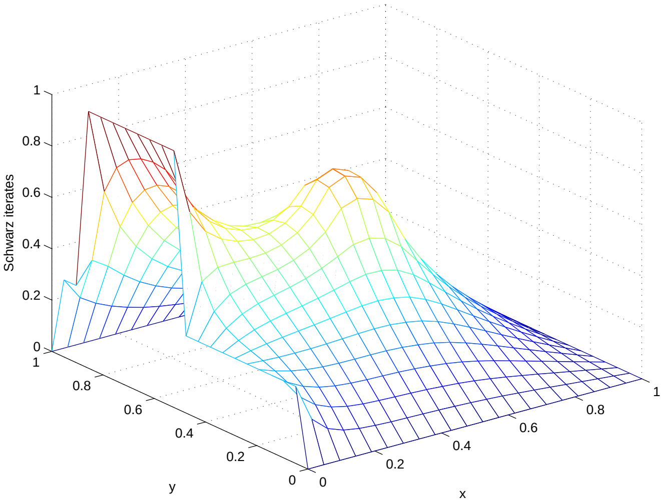
Iteration 4



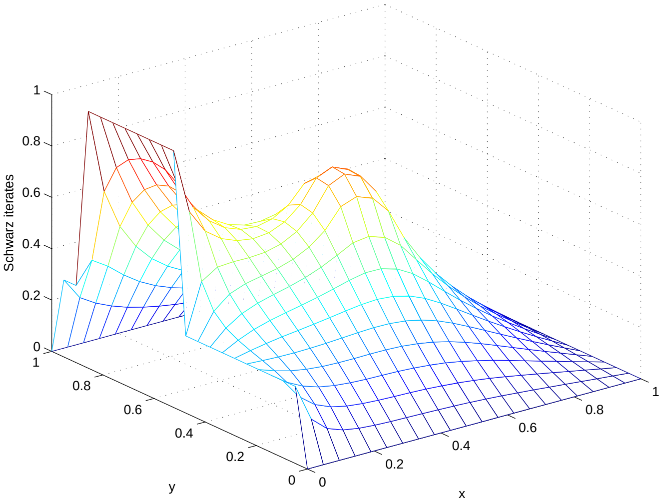
Iteration 5



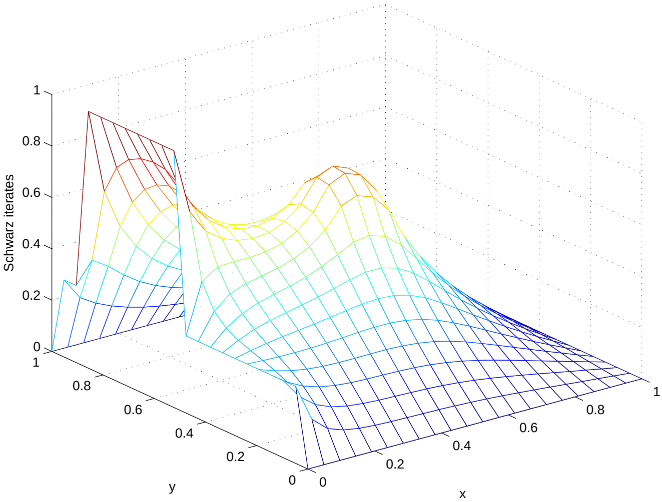
Iteration 6



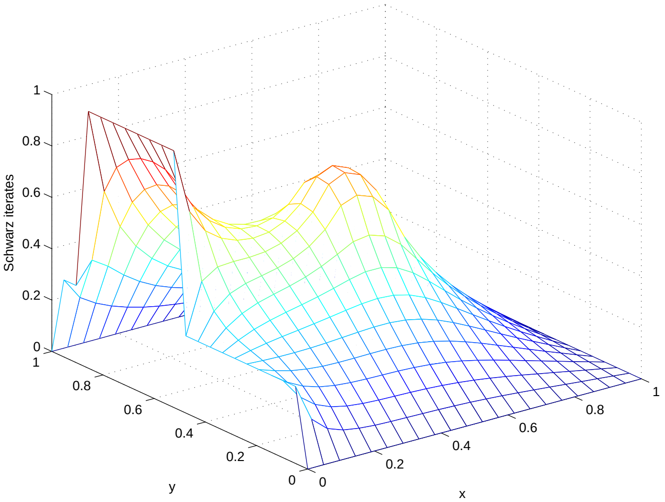
Iteration 7



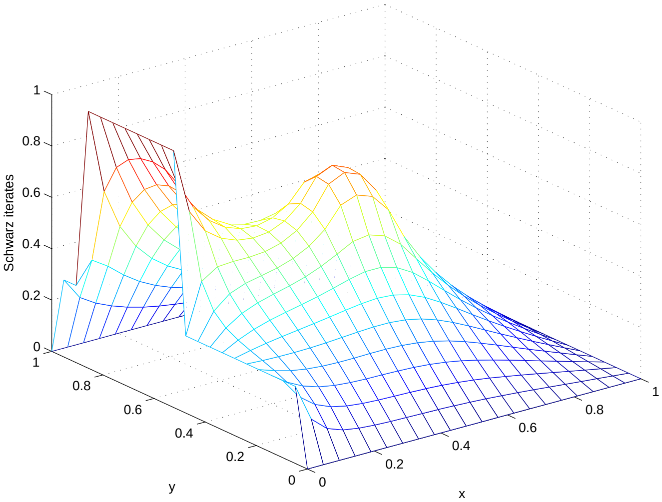
Iteration 8



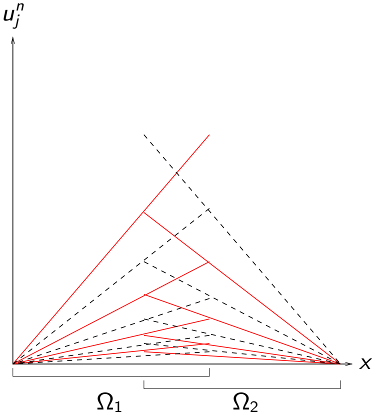
Iteration 9

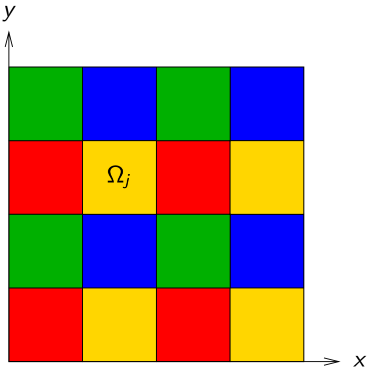


Iteration 10



Comparison of Alternating and Parallel Schwarz





For $\frac{\partial^2 u}{\partial x^2}u = 0$: alternating Schwarz method red + alternating Schwarz method dashed = parallel Schwarz method

Alternating Schwarz methods with many subdomain can also be parallel: solve red, then yellow, then blue, then green and so on.

Convergence with Fourier Analysis

For the model problem $\mathcal{L}u := (\eta - \Delta)u = 0$ on $\Omega = \mathbb{R}^2$, $\Omega_1 = (-\infty, L) \times \mathbb{R}$ and $\Omega_2 = (0, \infty) \times \mathbb{R}$,

$$\begin{aligned} (\eta - \Delta)u_1^n &= 0 \quad \text{in } \Omega_1, \\ u_1^n &= u_2^{n-1} \quad \text{on } x = L, \end{aligned} \qquad \begin{aligned} (\eta - \Delta)u_2^n &= 0 \quad \text{in } \Omega_2, \\ u_2^n &= u_1^n \quad \text{on } x = 0, \end{aligned}$$

we obtain after a Fourier transform in y

$$\begin{aligned} \hat{u}_j^n(x,k) &= \mathcal{F}(u_j^n) := \int_{-\infty}^{\infty} e^{-iky} u_j^n(x,y)dy, \quad k \in \mathbb{R}, \\ u_j^n(x,y) &= \mathcal{F}^{-1}(\hat{u}_j^n) := \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{iky} \hat{u}_j^n(x,k)dk, \end{aligned}$$

the Schwarz iteration in the Fourier domain (note how derivatives in y become multiplications by ik)

$$\begin{aligned} (\eta + k^2 - \partial_{xx})\hat{u}_1^n &= 0 \quad \text{in } \Omega_1, \\ \hat{u}_1^n &= \hat{u}_2^{n-1} \quad \text{on } x = L, \end{aligned} \qquad \begin{aligned} (\eta + k^2 - \partial_{xx})\hat{u}_2^n &= 0 \quad \text{in } \Omega_2, \\ \hat{u}_2^n &= \hat{u}_1^n \quad \text{on } x = 0. \end{aligned}$$

Convergence Analysis

Now the ordinary differential equations

$$(\eta + k^2 - \partial_{xx})\hat{u}_j^n = 0$$

can easily be solved:

$$\hat{u}_j^n(x,k) = A_j^n e^{\sqrt{\eta+k^2}x} + B_j^n e^{-\sqrt{\eta+k^2}x}.$$

On domain Ω_1, solutions must stay bounded at $-\infty$, hence

$$\hat{u}_1^n(x,k) = A_1^n e^{\sqrt{\eta+k^2}x},$$

and on domain Ω_2, solutions must stay bounded at ∞,

$$\hat{u}_2^n(x,k) = B_2^n e^{-\sqrt{\eta+k^2}x}.$$

To determine the constants A_j^n and B_j^n, we use the transmission conditions

$$\hat{u}_1^n(L,k) = \hat{u}_2^{n-1}(L,k), \quad \hat{u}_2^n(0,k) = \hat{u}_1^n(0,k),$$

which give

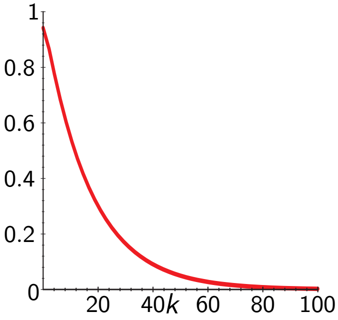
$$A_1^n e^{\sqrt{\eta+k^2}L} = B_2^{n-1} e^{-\sqrt{\eta+k^2}L} = A_1^{n-1} e^{-\sqrt{\eta+k^2}L}.$$

Convergence Result

After one iteration of the alternating Schwarz method, we obtain the convergence factor

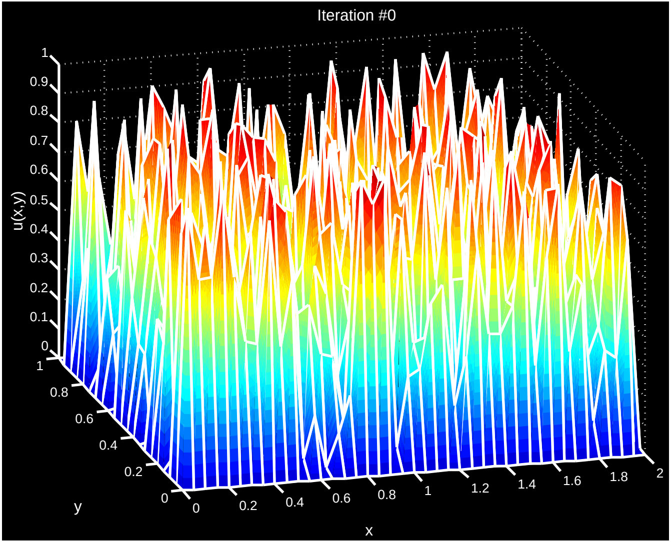
$$\rho(\eta, k, L) := \frac{A_1^n}{A_1^{n-1}} = e^{-2\sqrt{\eta+k^2}L}.$$

Graph of $\rho(k)$ for $\eta = 1$, $L = 1/10$:

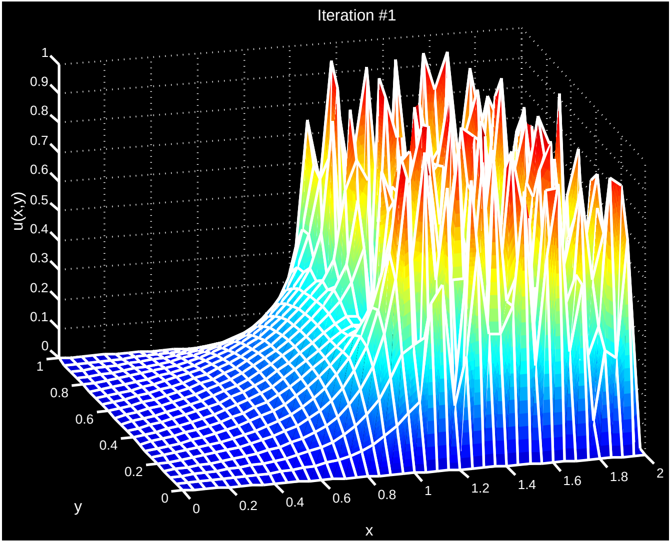


$\Longrightarrow$ Low frequencies converge slowly, high frequencies fast

Example how Error Decreases in Schwarz Method

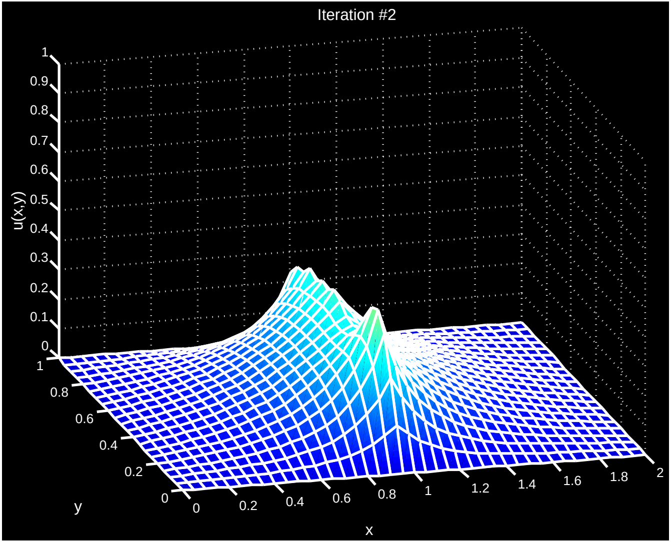


Iteration 1



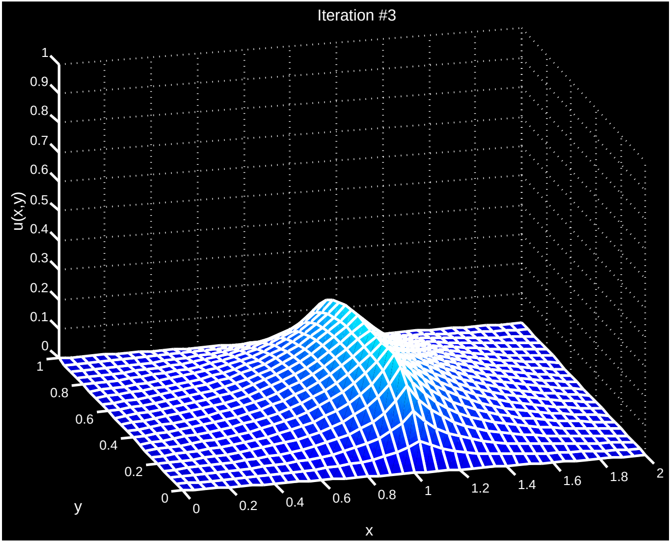
solve on the left subdomain

Iteration 2



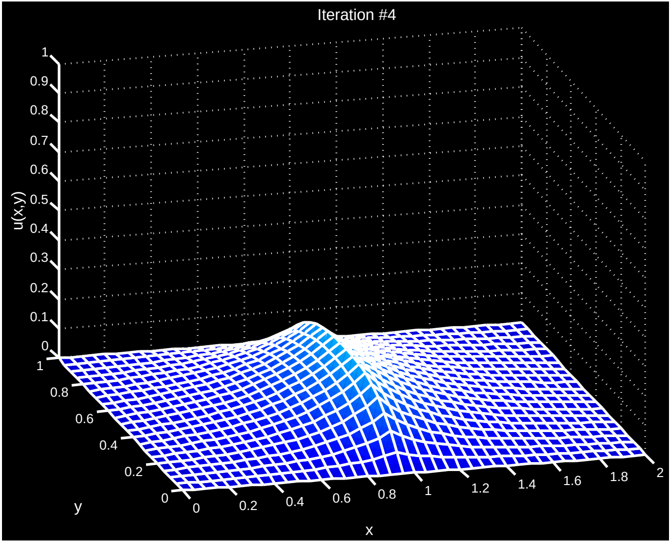
solve on the right subdomain

Iteration 3



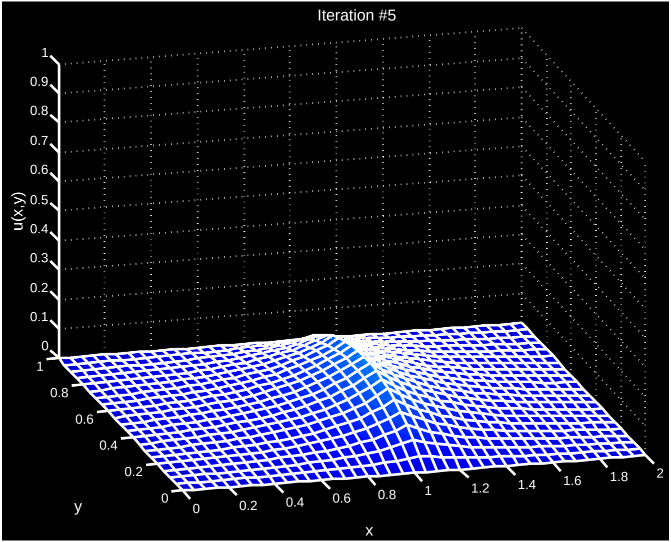
solve on the left subdomain

Iteration 4



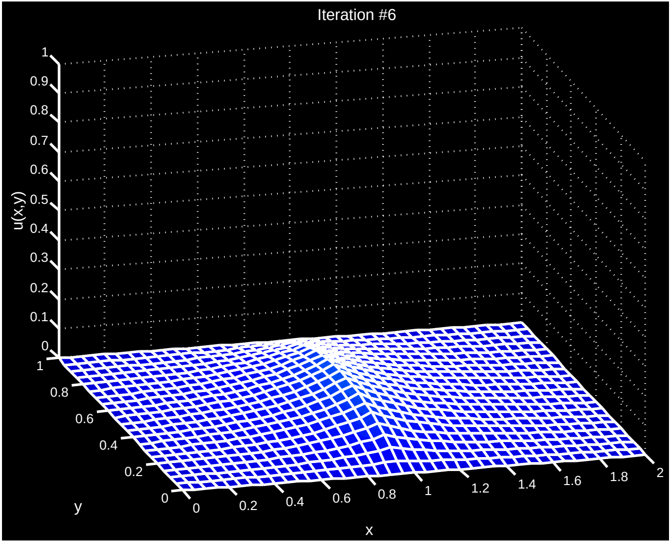
solve on the right subdomain

Iteration 5



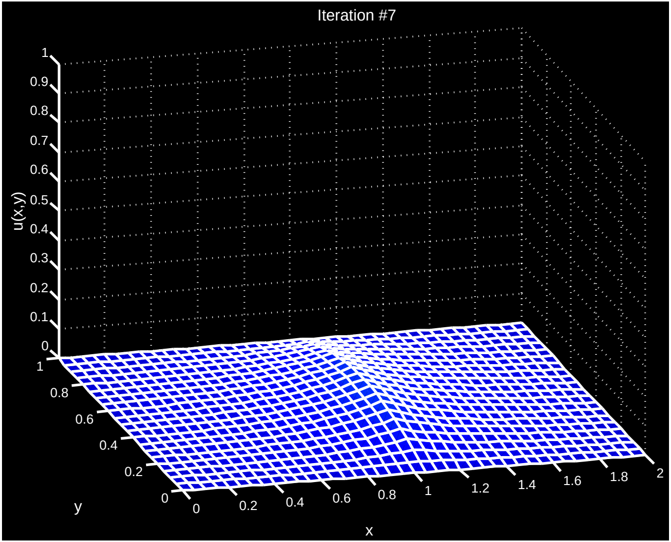
solve on the left subdomain

Iteration 6



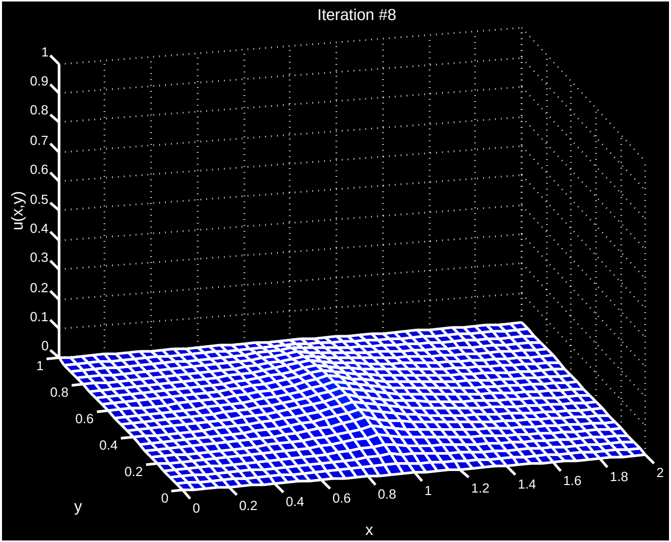
solve on the right subdomain

Iteration 7



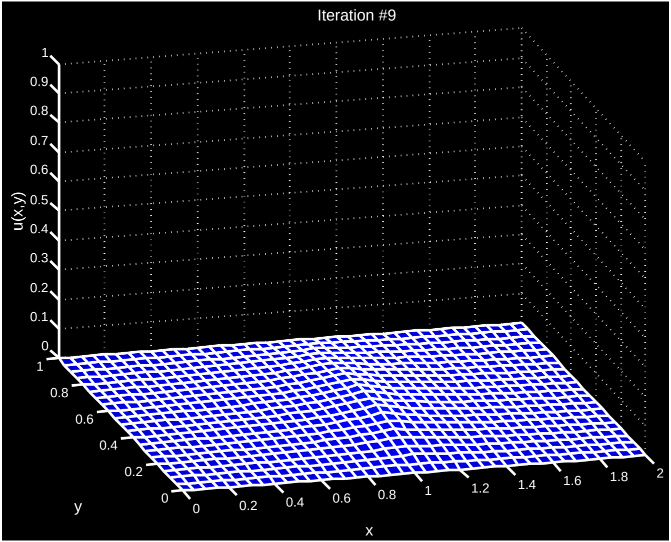
solve on the left subdomain

Iteration 8



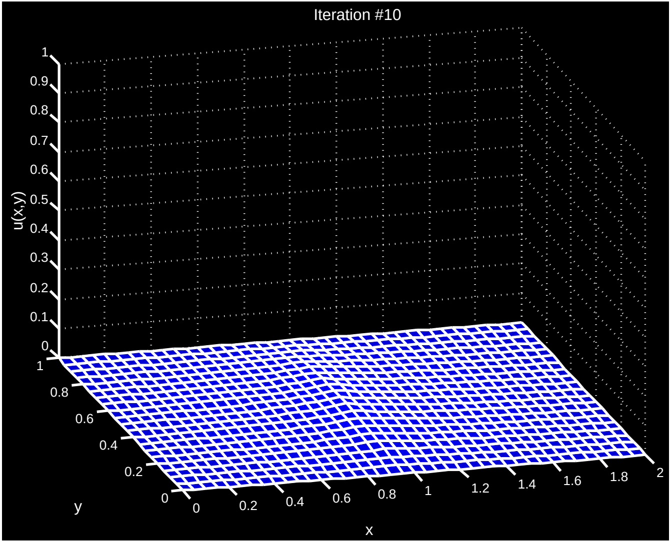
solve on the right subdomain

Iteration 9



solve on the left subdomain

Iteration 10



solve on the right subdomain

The Multiplicative Schwarz Method (MS)

The discretized PDE $\mathcal{L}u = f$ leads to the linear system

$$A\mathbf{u} = \mathbf{f}, \qquad A \text{ a large sparse matrix}$$

With the restriction matrices

$$R_1 = \begin{bmatrix} 1 & & & \\ & \ddots & & \\ & & 1 & \end{bmatrix} R_2 = \begin{bmatrix} & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}$$

and $A_j = R_j A R_j^T$ the multiplicative Schwarz method is

$$\begin{aligned} \mathbf{u}^{n+\frac{1}{2}} &= \mathbf{u}^n + R_1^T A_1^{-1} R_1(\mathbf{f} - A\mathbf{u}^n) \\ \mathbf{u}^{n+1} &= \mathbf{u}^{n+\frac{1}{2}} + R_2^T A_2^{-1} R_2(\mathbf{f} - A\mathbf{u}^{n+\frac{1}{2}}). \end{aligned}$$

Questions:

- Is MS a discretization of a continuous Schwarz method?
- How is the algebraic overlap related to the physical one?

Relation with Alternating Schwarz

If the R_j are non-overlapping, and we partition accordingly

$$A = \begin{bmatrix} A_1 & A_{12} \\ A_{21} & A_2 \end{bmatrix}, \qquad \mathbf{f} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{pmatrix},$$

we obtain from the first relation of MS, i.e.

$$\mathbf{u}^{n+\frac{1}{2}} = \mathbf{u}^n + R_1^T A_1^{-1} R_1(\mathbf{f} - A\mathbf{u}^n)$$

an interesting cancellation:

$$\begin{aligned}
R_1(\mathbf{f} - A\mathbf{u}^n) &= \mathbf{f}_1 - A_1\mathbf{u}_1^n - A_{12}\mathbf{u}_2^n \\
A_1^{-1}R_1(\mathbf{f} - A\mathbf{u}^n) &= A_1^{-1}(\mathbf{f}_1 - A_{12}\mathbf{u}_2^n) - \mathbf{u}_1^n \\
\begin{pmatrix} \mathbf{u}_1^{n+\frac{1}{2}} \\ \mathbf{u}_2^{n+\frac{1}{2}} \end{pmatrix} &= \begin{pmatrix} \mathbf{u}_1^n \\ \mathbf{u}_2^n \end{pmatrix} + \begin{pmatrix} A_1^{-1}(\mathbf{f}_1 - A_{12}\mathbf{u}_2^n) - \mathbf{u}_1^n \\ 0 \end{pmatrix} \\
&= \begin{pmatrix} A_1^{-1}(\mathbf{f}_1 - A_{12}\mathbf{u}_2^n) \\ \mathbf{u}_2^n \end{pmatrix}
\end{aligned}$$

Relation with Alternating Schwarz

Similarly, from the second relation of MS, i.e.

$$\mathbf{u}^{n+1} = \mathbf{u}^{n+\frac{1}{2}} + R_2^T A_2^{-1} R_2(\mathbf{f} - A\mathbf{u}^{n+\frac{1}{2}})$$

we obtain

$$\begin{pmatrix} \mathbf{u}_1^{n+1} \\ \mathbf{u}_2^{n+1} \end{pmatrix} = \begin{pmatrix} A_1^{-1}(\mathbf{f}_1 - A_{12}\mathbf{u}_2^n) \\ A_2^{-1}(\mathbf{f}_2 - A_{21}\mathbf{u}_1^{n+1}) \end{pmatrix},$$

which can be rewritten in the equivalent form

$$A_1\mathbf{u}_1^{n+1} = \mathbf{f}_1 - A_{12}\mathbf{u}_2^n, \qquad A_2\mathbf{u}_2^{n+1} = \mathbf{f}_2 - A_{21}\mathbf{u}_1^{n+1}$$

and is therefore a discretization of the alternating Schwarz method from 1869,

$$\begin{array}{rcl} \mathcal{L}u_1^{n+1} & = & f, \text{ in } \Omega_1 \\ u_1^{n+1} & = & u_2^n, \text{ on } \Gamma_1 \end{array} \qquad \begin{array}{rcl} \mathcal{L}u_2^{n+1} & = & f, \text{ in } \Omega_2 \\ u_2^{n+1} & = & u_1^{n+1}, \text{ on } \Gamma_2 \end{array}$$

General proof for many subdomains (G 2008)

MS is also a block Gauss Seidel method

MS is also equivalent to a block Gauss Seidel method, since

$$A_1\mathbf{u}_1^{n+1} = \mathbf{f}_1 - A_{12}\mathbf{u}_2^{n}, \quad A_2\mathbf{u}_2^{n+1} = \mathbf{f}_2 - A_{21}\mathbf{u}_1^{n+1}$$

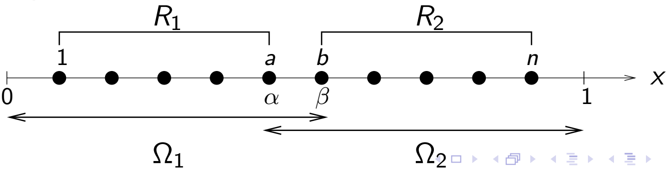
leads in matrix form to the iteration

$$\begin{bmatrix} A_1 & 0 \\ A_{21} & A_2 \end{bmatrix} \begin{pmatrix} \mathbf{u}_1^{n+1} \\ \mathbf{u}_2^{n+1} \end{pmatrix} = \begin{bmatrix} 0 & -A_{12} \\ 0 & 0 \end{bmatrix} \begin{pmatrix} \mathbf{u}_1^{n} \\ \mathbf{u}_2^{n} \end{pmatrix} + \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{pmatrix}$$

So why the complicated R_j notation ?

- With R_j, one can also use overlapping blocks.
- With R_j, there is a global approximate solution $\mathbf{u}^n$.

Note that even the algebraically non-overlapping case above implies overlap at the PDE level:



The Additive Schwarz Method (AS)

M. Drjya and O. Widlund 1989:

> *The basic idea behind the additive form of the algorithm is to work with the simplest possible polynomial in the projections. Therefore the equation $(P_1 + P_2 + \ldots + P_N)u_h = g_h'$ is solved by an iterative method.*

Using the same notation as before, $P_j = R_j^T A_j^{-1} R_j A$, the preconditioned system is

$$(R_1^T A_1^{-1} R_1 + R_2^T A_2^{-1} R_2) A\mathbf{u} = (R_1^T A_1^{-1} R_1 + R_2^T A_2^{-1} R_2)\mathbf{f}$$

Writing this as a stationary iterative method yields

$$\mathbf{u}^n = \mathbf{u}^{n-1} + (R_1^T A_1^{-1} R_1 + R_2^T A_2^{-1} R_2)(\mathbf{f} - A\mathbf{u}^{n-1})$$

Question: Is AS equivalent to a discretization of Lions parallel Schwarz method ?

Algebraically non-overlapping case

If the R_j are non-overlapping, we obtain now

$$\begin{pmatrix} \mathbf{u}_1^{n+1} \\ \mathbf{u}_2^{n+1} \end{pmatrix} = \begin{pmatrix} A_1^{-1}(\mathbf{f}_1 - A_{12}\mathbf{u}_2^n) \\ A_2^{-1}(\mathbf{f}_2 - A_{21}\mathbf{u}_1^n) \end{pmatrix},$$

which can be rewritten in the equivalent form

$$A_1\mathbf{u}_1^{n+1} = \mathbf{f}_1 - A_{12}\mathbf{u}_2^n, \qquad A_2\mathbf{u}_2^{n+1} = \mathbf{f}_2 - A_{21}\mathbf{u}_1^n.$$

This is a discretization of Lions' parallel Schwarz method from 1988,

$$\begin{array}{rcl} \mathcal{L}u_1^{n+1} & = & f, \text{ in } \Omega_1 \\ u_1^{n+1} & = & u_2^n, \text{ on } \Gamma_1 \end{array} \qquad \begin{array}{rcl} \mathcal{L}u_2^{n+1} & = & f, \text{ in } \Omega_2 \\ u_2^{n+1} & = & u_1^n, \text{ on } \Gamma_2 \end{array}$$

In the algebraically non-overlapping case, AS is also equivalent to a block Jacobi method,

$$\begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix} \begin{pmatrix} \mathbf{u}_1^{n+1} \\ \mathbf{u}_2^{n+1} \end{pmatrix} = \begin{bmatrix} 0 & -A_{12} \\ -A_{21} & 0 \end{bmatrix} \begin{pmatrix} \mathbf{u}_1^n \\ \mathbf{u}_2^n \end{pmatrix} + \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{pmatrix}$$

What happens if the R_j overlap ?

If the R_j overlap, the cancellation is more complicated:

$$\mathbf{u}^{n+1}=\mathbf{u}^n+\begin{pmatrix}\boxed{A_1^{-1}(\mathbf{f}_1-A_{12}\mathbf{u}_2^n)-\mathbf{u}_1^n}\\ \mathbf{0}\end{pmatrix}+\begin{pmatrix}\mathbf{0}\\ \boxed{A_2^{-1}(\mathbf{f}_2-A_{21}\mathbf{u}_1^n)-\mathbf{u}_2^n}\end{pmatrix}$$

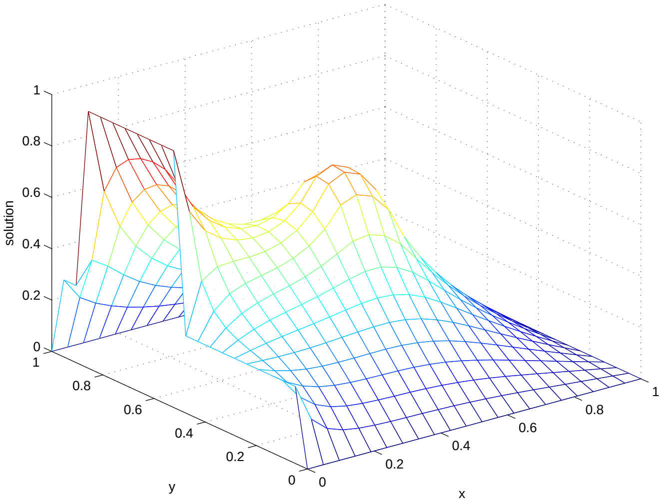
In the overlap, the current iterate is subtracted twice, and a new approximation from the left and right solve is added.

Remarks:

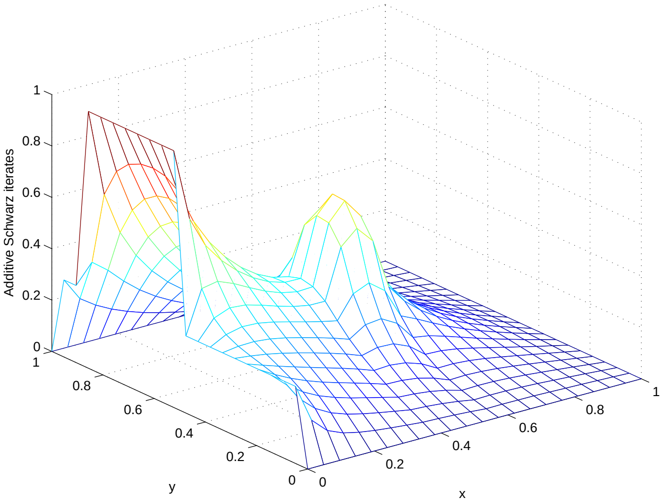
- Method does not converge in the overlap: the spectral radius of the AS iteration operator equals 1 for two subdomains.
- The method converges outside of the overlap for two subdomains.
- For more than two subdomains with cross points the method diverges everywhere.

AS is thus not equivalent to a discretization of Lions parallel Schwarz method for more than minimal physical overlap.

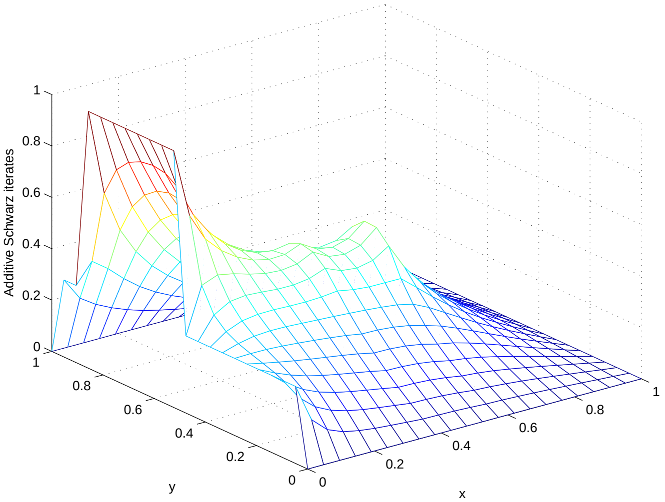
Example: Heating a Room



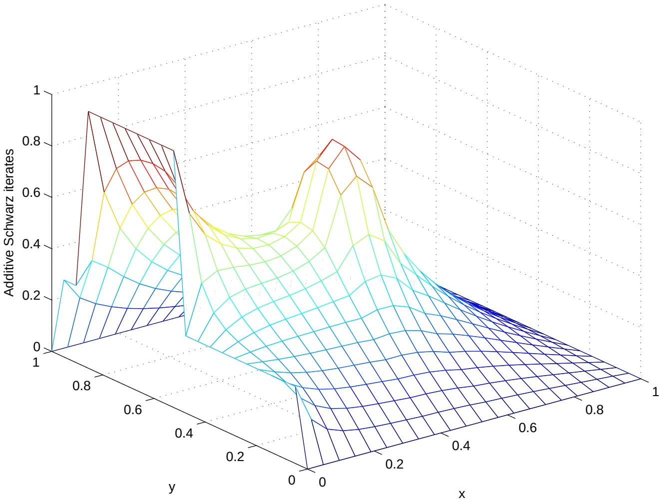
Iteration 1


Additive Schwarz iterates
1
0.8
0.6
0.4
0.2
0
1
0.8
0.6
0.4
0.2
0
y
0
0.2
0.4
0.6
0.8
1
x

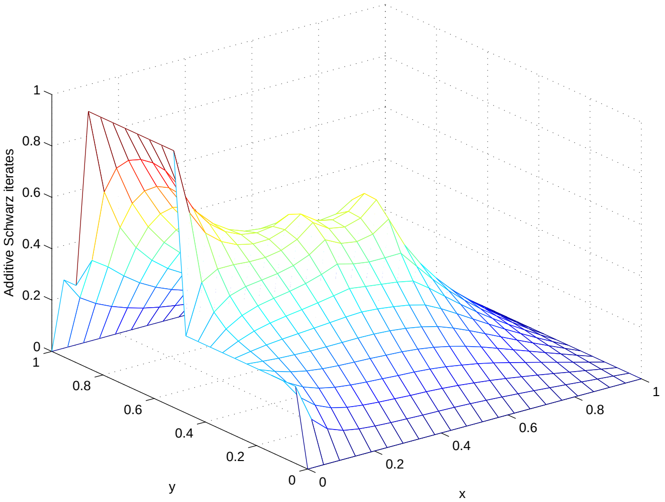
Iteration 2



Iteration 3

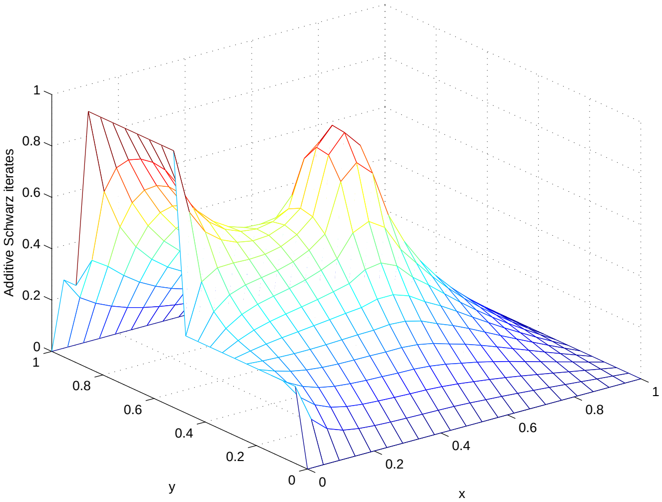

Additive Schwarz iterates
1
0.8
0.6
0.4
0.2
0
1
0.8
0.6
0.4
0.2
0
y
0
0.2
0.4
0.6
0.8
1
x

Iteration 4



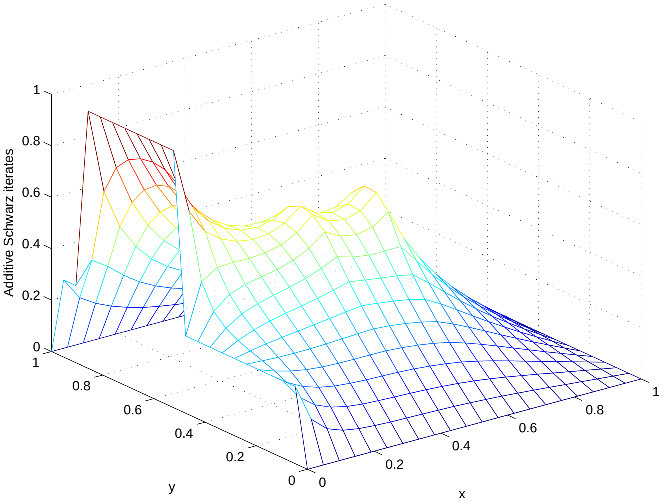
Additive Schwarz iterates
1
0.8
0.6
0.4
0.2
0
1
0.8
0.6
0.4
0.2
0
y
0
0.2
0.4
0.6
0.8
1
x

Iteration 5

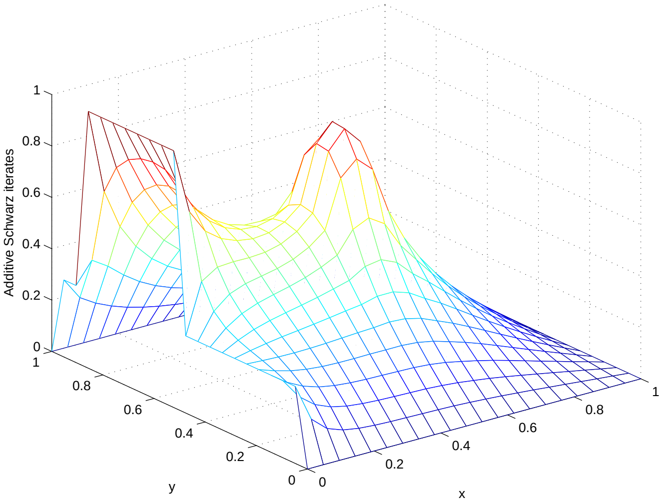


Additive Schwarz iterates
1
0.8
0.6
0.4
0.2
0
1
0.8
0.6
0.4
0.2
0
y
0
0.2
0.4
0.6
0.8
1
x

Iteration 6

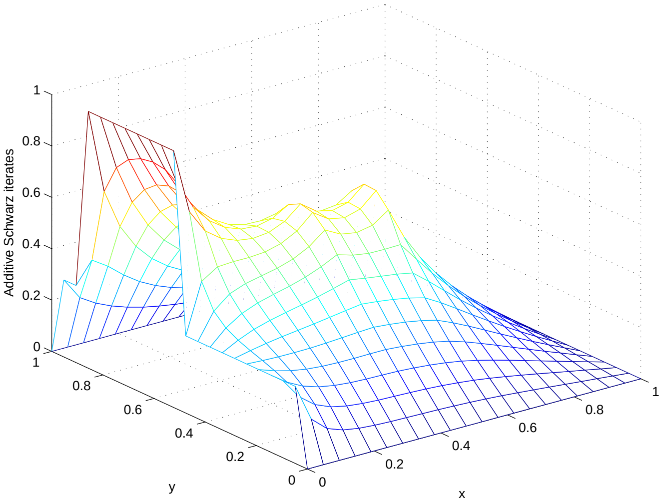


Iteration 7



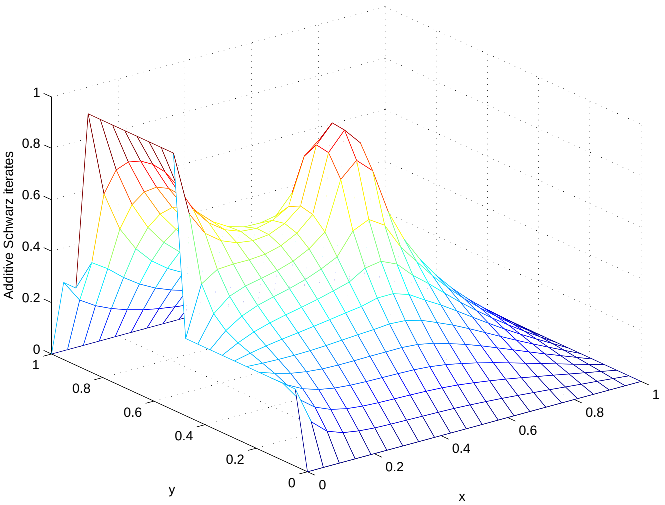
Additive Schwarz iterates
1
0.8
0.6
0.4
0.2
0
1
0.8
0.6
0.4
0.2
0
y
0
0.2
0.4
0.6
0.8
1
x

Iteration 8

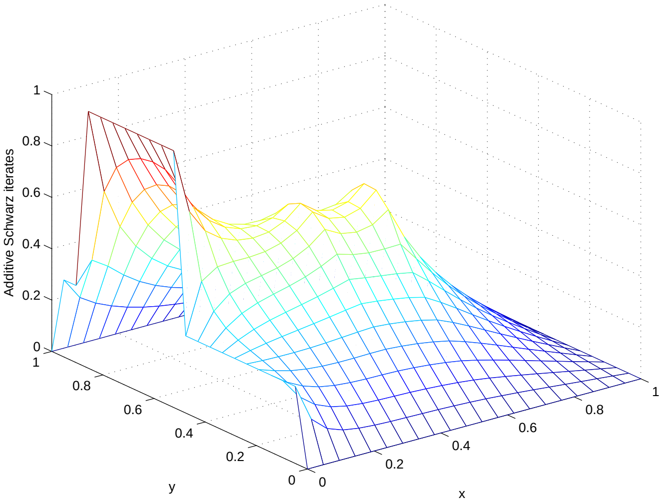


1
0.8
0.6
0.4
0.2
0
Additive Schwarz iterates
1
0.8
0.6
0.4
0.2
0
y
0
0.2
0.4
0.6
0.8
1
x

Iteration 9


Additive Schwarz iterates
1
0.8
0.6
0.4
0.2
0
y
1
0.8
0.6
0.4
0.2
0
x
0
0.2
0.4
0.6
0.8
1

Iteration 10



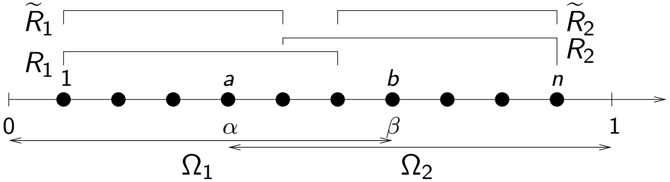
Restricted Additive Schwarz (RAS)

X. Cai and M. Sarkis 1998:

> *While working on an AS/GMRES algorithm in an Euler simulation, we removed part of the communication routine and surprisingly the "then AS" method converged faster in both terms of iteration counts and CPU time.*

Replace R_j^T in AS by $\widetilde{R}_j^T$:

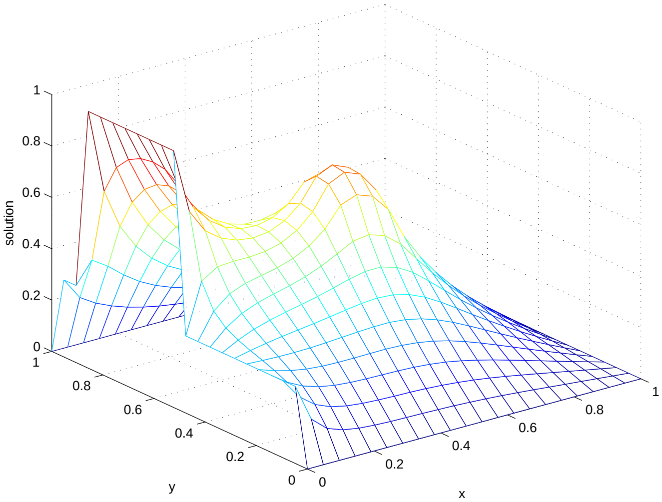
$$u^{n+1} = u^n + (\widetilde{R}_1^T A_1^{-1} R_1 + \widetilde{R}_2^T A_2^{-1} R_2)(f - Au^n)$$



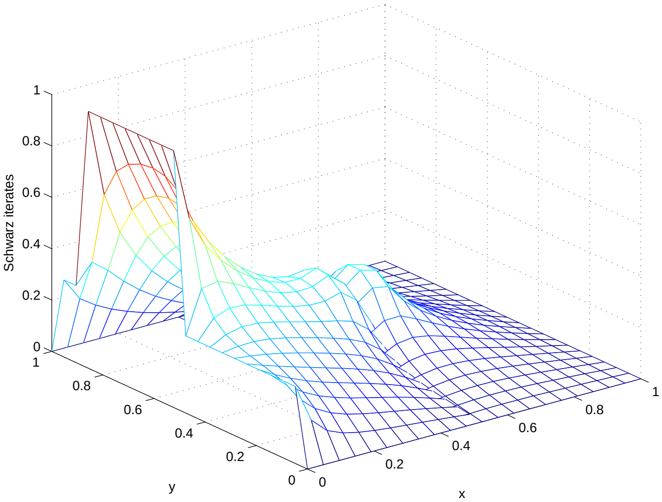
Remarks:

- RAS is equivalent to a discretization of Lions parallel Schwarz method (Efstathiou, G. 2003, general G. 2008)
- the preconditioner is **non symmetric**, even if A_j is symmetric

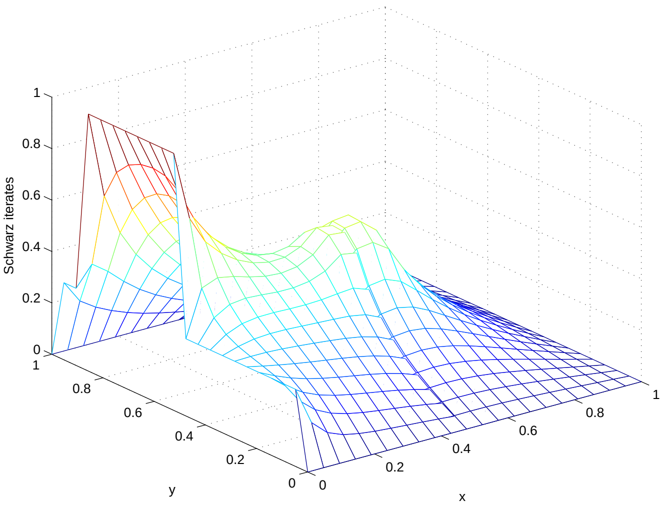
Example: Heating a Room



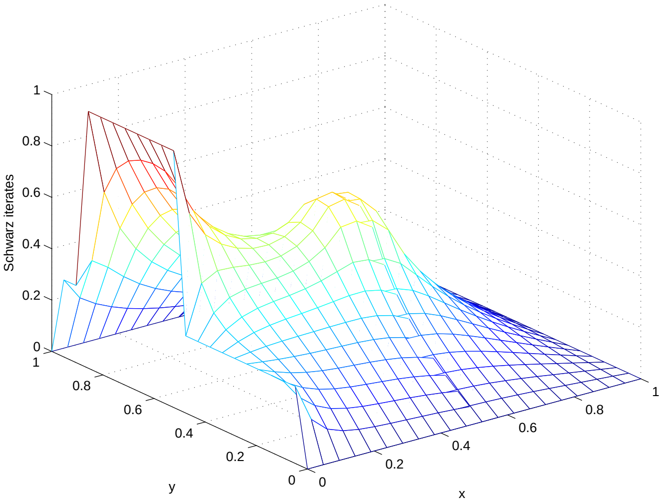
Iteration 1



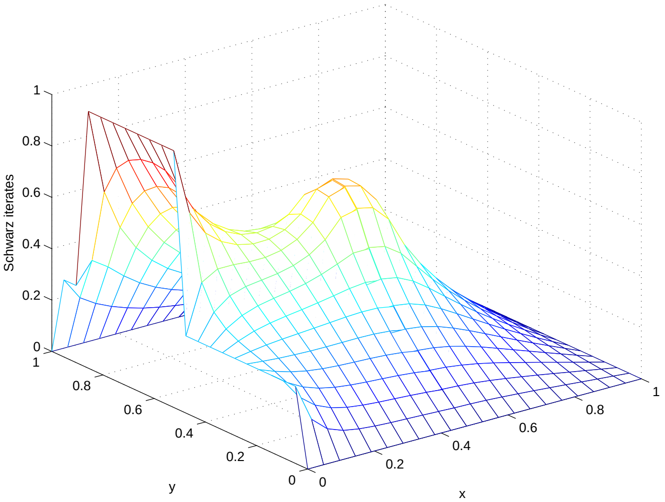
Iteration 2



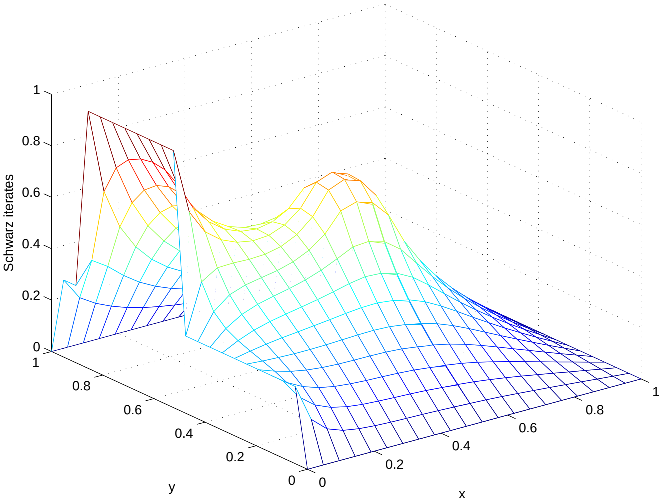
Iteration 3



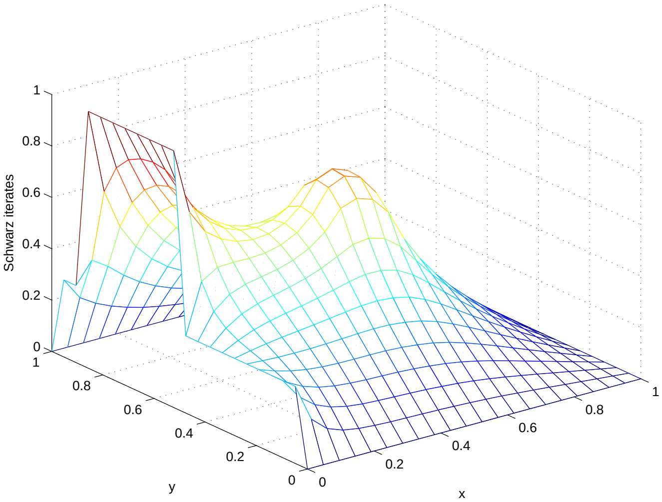
Iteration 4



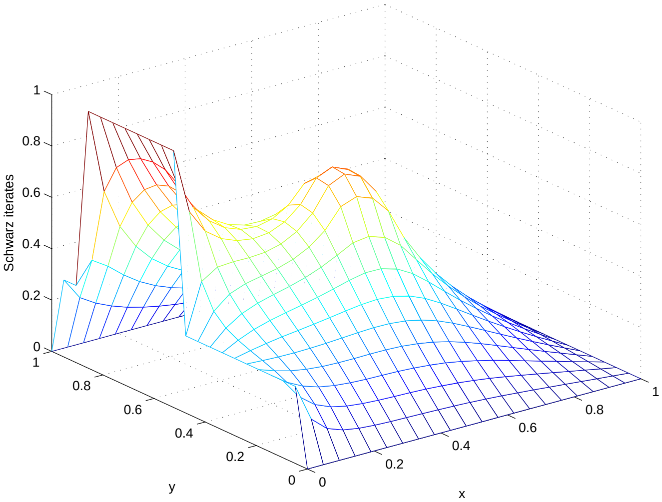
Iteration 5



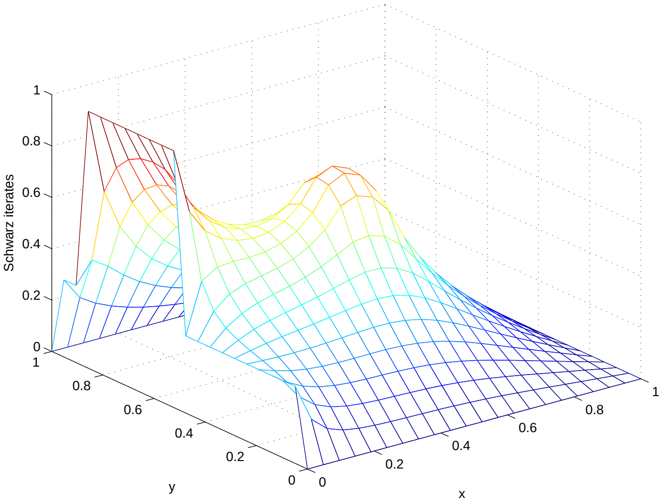
Iteration 6



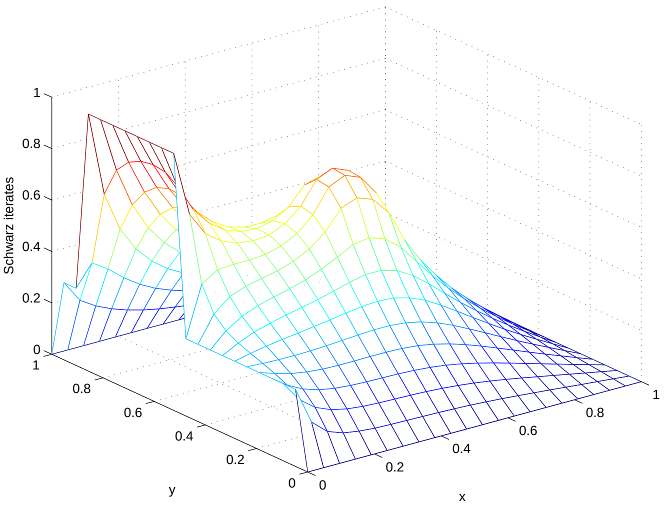
Iteration 7



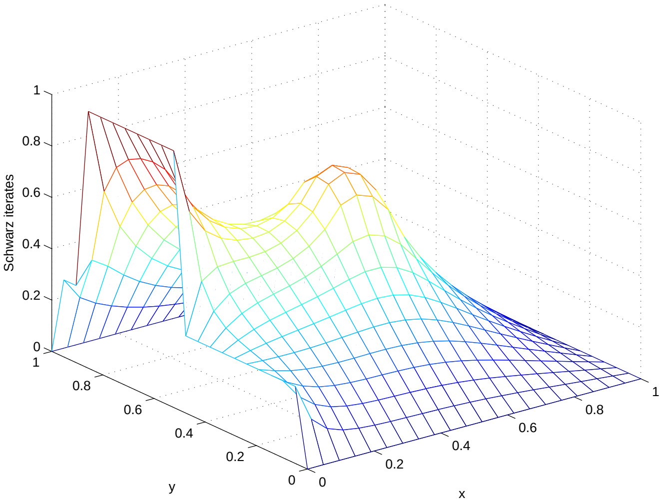
Iteration 8



Iteration 9



Iteration 10



Idea of Preconditioning

Let $A\mathbf{u} = \mathbf{f}$ be a discretization of the PDE $(\eta - \Delta)u = f$ on the unit square.

Solving this linear system using conjugate gradients leads to the convergence factor estimate

$$\rho_{CG} = \frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \qquad \kappa(A) := \|A\| \, \|A^{-1}\|$$

For the discretized PDE,

$$\kappa(A) = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)} \sim \frac{2}{\eta + 2\pi^2} \frac{1}{h^2} \implies \rho_{CG} = 1 - O(h)$$

For fast convergence, it would be better to solve the preconditioned system $M^{-1}A\mathbf{u} = M^{-1}\mathbf{f}$ with M s.t. $\kappa(M^{-1}A) << \kappa(A)$.

How to choose M ?

- M should be easy to invert
- M^{-1} should be close to A^{-1}

Given a stationary iterative method for $A\mathbf{u} = \mathbf{f}$,

$$M\mathbf{u}^{n+1} = (M - A)\mathbf{u}^n - \mathbf{f},$$

at convergence, the system

$$M\mathbf{u} = (M - A)\mathbf{u} - \mathbf{f} \quad \Longleftrightarrow \quad M^{-1}A\mathbf{u} = M^{-1}\mathbf{f}$$

is solved. Hence every station-nary iterative method gives raise to a preconditioner!

Example: Block Jacobi or Additive Schwarz without algebraic overlap

$$\begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix} \begin{pmatrix} \mathbf{u}_1^{n+1} \\ \mathbf{u}_2^{n+1} \end{pmatrix} = \begin{bmatrix} 0 & -A_{12} \\ -A_{21} & 0 \end{bmatrix} \begin{pmatrix} \mathbf{u}_1^n \\ \mathbf{u}_2^n \end{pmatrix} + \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{pmatrix}$$

Does this Give a Good Preconditioner ?

The stationary iterative method

$$M\mathbf{u}^{n+1} = (M - A)\mathbf{u}^n - \mathbf{f},$$

converges fast, if $\rho(I - M^{-1}A) << 1$. This is equivalent to saying that the spectrum of the preconditioned operator $M^{-1}A$ is close to one. This implies, if the spectrum is real, that

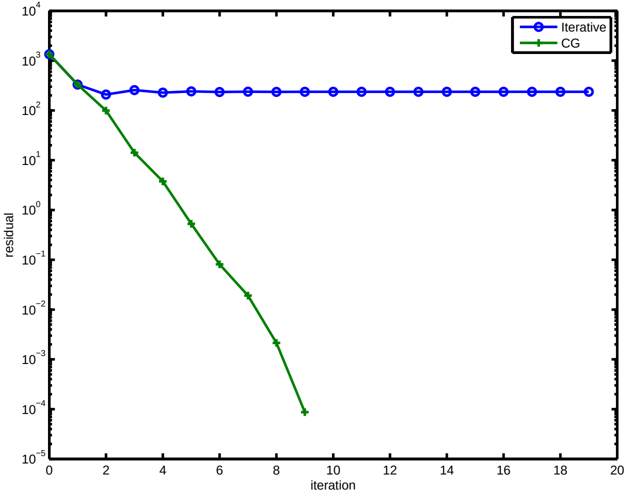
$$\kappa(M^{-1}A) = \frac{\lambda_{\max}(M^{-1}A)}{\lambda_{\min}(M^{-1}A)} \approx 1.$$

For Schwarz methods, there are two possibilities:

1. Preconditioning in volume (for AS, MS, RAS)
2. Substructured formulation (for iterations formulated on the interfaces only)

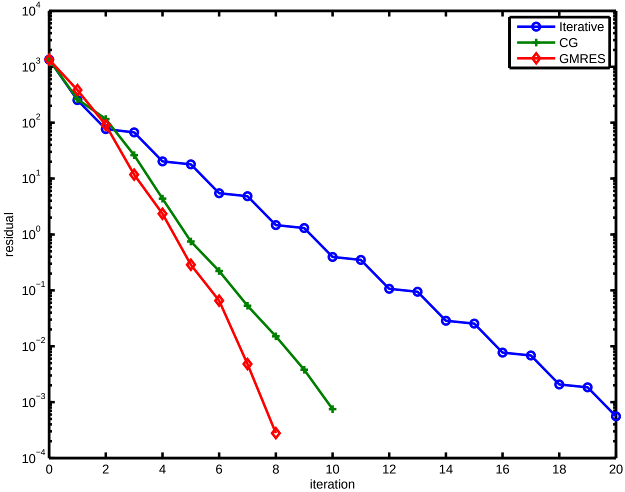
Additive Schwarz Preconditioner

$$M_{AS}^{-1} := \sum_{i=1}^{I} R_i^T A_i^{-1} R_i$$

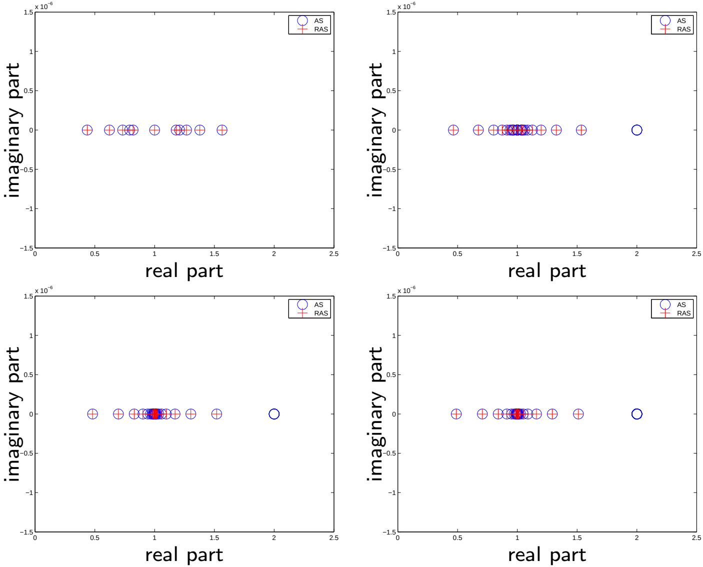


Restricted Additive Schwarz Preconditioner

$$M_{RAS}^{-1} := \sum_{i=1}^{I} \widetilde{R}_i^T A_i^{-1} R_i$$

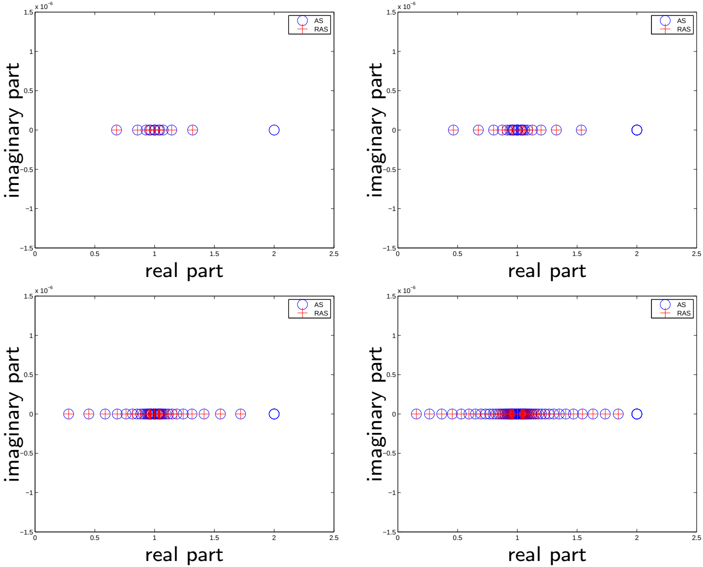


Comparison of the Spectra of AS and RAS



Fixed overlap δ, independent of the mesh size

Comparison of the Spectra of AS and RAS



Overlap depending on the mesh size $\delta = 2h$

Substructured Formulation

Applying the trace operator $\begin{pmatrix} G_1 & 0 \\ 0 & G_2 \end{pmatrix}$ to the discretized parallel Schwarz method

$$\begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix} \begin{pmatrix} \mathbf{u}_1^{n+1} \\ \mathbf{u}_2^{n+1} \end{pmatrix} = \begin{bmatrix} 0 & -A_{12} \\ -A_{21} & 0 \end{bmatrix} \begin{pmatrix} \mathbf{u}_1^{n} \\ \mathbf{u}_2^{n} \end{pmatrix} + \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{pmatrix}$$

we get

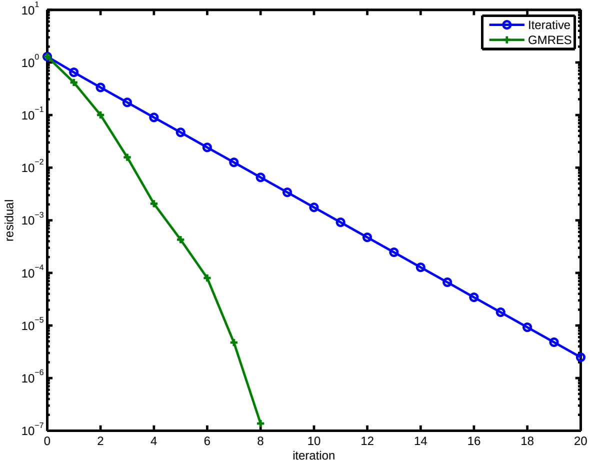
$$\begin{pmatrix} G_1\mathbf{u}_1^{n+1} \\ G_2\mathbf{u}_2^{n+1} \end{pmatrix} = \begin{bmatrix} 0 & -G_1A_1^{-1}A_{12} \\ -G_2A_2^{-1}A_{21} & 0 \end{bmatrix} \begin{pmatrix} \mathbf{u}_1^{n} \\ \mathbf{u}_2^{n} \end{pmatrix} + \begin{pmatrix} G_1A_1^{-1}\mathbf{f}_1 \\ G_2A_2^{-1}\mathbf{f}_2 \end{pmatrix}$$

Now since $A_{12}\mathbf{u}_1^n = A'_{12}G_2\mathbf{u}_2^n$ and $A_{21}\mathbf{u}_1^n = A'_{21}G_1\mathbf{u}_1^n$, we get the substructured iteration

$$\begin{pmatrix} \mathbf{g}_1^{n+1} \\ \mathbf{g}_2^{n+1} \end{pmatrix} = \begin{bmatrix} 0 & -G_1A_1^{-1}A'_{12} \\ -G_2A_2^{-1}A'_{21} & 0 \end{bmatrix} \begin{pmatrix} \mathbf{g}_1^{n} \\ \mathbf{g}_2^{n} \end{pmatrix} + \begin{pmatrix} \tilde{\mathbf{f}}_1 \\ \tilde{\mathbf{f}}_2 \end{pmatrix}$$

Solving the Substructured System

$$\begin{bmatrix} I & G_1 A_1^{-1} A'_{12} \\ G_2 A_2^{-1} A'_{21} & I \end{bmatrix} \begin{pmatrix} \mathbf{g}_1 \\ \mathbf{g}_2 \end{pmatrix} = \begin{pmatrix} \tilde{\mathbf{f}}_1 \\ \tilde{\mathbf{f}}_2 \end{pmatrix}$$

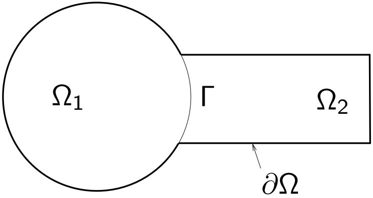


Problems of classical Schwarz: Overlap Necessary

P-L. Lions 1990:

> *However, the Schwarz method requires that the subdomains overlap, and this may be a severe restriction - without speaking of the obvious or intuitive waste of efforts in the region shared by the subdomains.*

$\mathcal{L}u = f$ in Ω



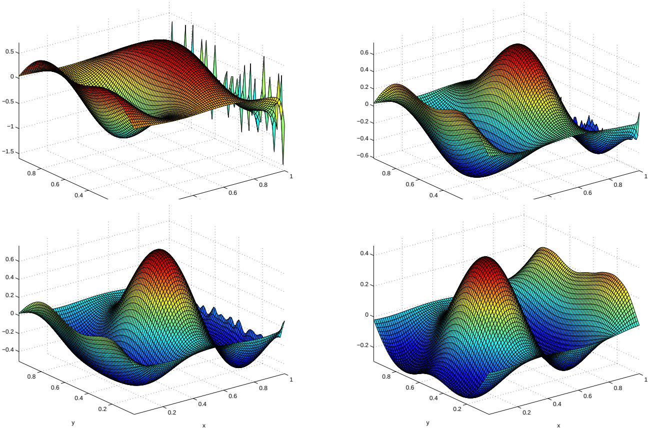
$$\begin{array}{rl} \mathcal{L}u_1^n = f & \text{in } \Omega_1 \\ (\partial_{n_1}+p_1)u_1^n = (\partial_{n_1}+p_1)u_2^{n-1} & \text{on } \Gamma \end{array} \qquad \begin{array}{rl} \mathcal{L}u_2^n = f & \text{in } \Omega_2 \\ (\partial_{n_2}+p_2)u_2^n = (\partial_{n_2}+p_2)u_1^{n} & \text{on } \Gamma \end{array}$$

P-L. Lions 1990:

> *First of all, it is possible to replace the constants in the Robin conditions by two proportional functions on the interface, or even by local or nonlocal operators.*

Other Problem: Lack of Convergence

Error of the Schwarz method on the left subdomain for the Helmholtz problem after 1,2,3, and 8 iterations:



B. Després 1990:

> *L'objectif de ce travail est, après construction d'une méthode de décomposition de domaine adaptée au problème de Helmholtz, d'en démontrer la convergence.*

Further Problem: Convergence Speed

T. Hagstrom, R. P. Tewarson and A. Jazcilevich 1988: Numerical experiments on a domain decomposition algorithm for nonlinear elliptic boundary value problems

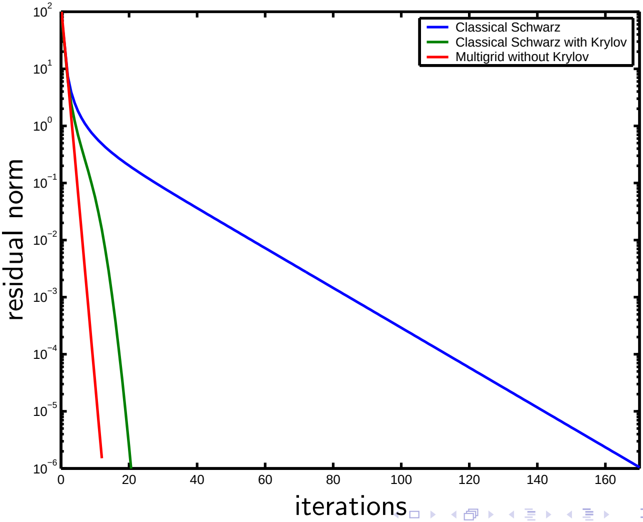
> *In general, [the coefficients in the Robin transmission conditions] may be operators in an appropriate space of function on the boundary. Indeed, we advocate the use of nonlocal conditions.*

W.-P. Tang 1992: Generalized Schwarz Splittings

> *In this paper, a new coupling between the overlap[ping] subregions is identified. If a successful coupling is chosen, a fast convergence of the alternating process can be achieved without a large overlap.*

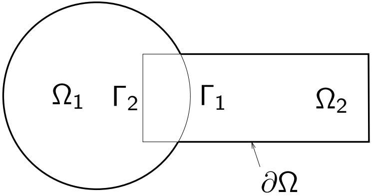
Comparison of Classical Schwarz with Multigrid

Comparison of MS with two subdomains as an iterative solver and a preconditioner for a Krylov method, with a standard multigrid solver:



Optimized Schwarz Methods

$$\mathcal{L}u = f \text{ in } \Omega$$



Instead of the classical alternating Schwarz method

$$\begin{aligned} \mathcal{L}u_1^n &= f, \text{ in } \Omega_1 \\ u_1^n &= u_2^{n-1}, \text{ on } \Gamma_1 \end{aligned} \qquad \begin{aligned} \mathcal{L}u_2^n &= f, \text{ in } \Omega_2 \\ u_2^n &= u_1^n, \text{ on } \Gamma_2 \end{aligned}$$

one uses transmission conditions adapted to the PDE,

$$\mathcal{B}_1 u_1^n = \mathcal{B}_1 u_2^{n-1}, \text{ on } \Gamma_1 \quad \mathcal{B}_2 u_2^n = \mathcal{B}_2 u_1^n, \text{ on } \Gamma_2$$

Questions:

- is there an optimal choice for the transmission operators $\mathcal{B}_j$?
- does this optimal choice lead to a practical algorithm ?

Optimal Transmission Conditions

For the model problem $\mathcal{L}u := (\eta - \Delta)u = 0$ on $\Omega = \mathbb{R}^2$, $\Omega_1 = (-\infty, L) \times \mathbb{R}$ and $\Omega_2 = (0, \infty) \times \mathbb{R}$, we choose

$$\begin{array}{rcll} (\eta - \Delta)u_1^n & = & 0 & \text{in } \Omega_1, \\ (\partial_x + \mathcal{S}_1)u_1^n & = & (\partial_x + \mathcal{S}_1)u_2^{n-1} & \text{on } x = L, \\ (\eta - \Delta)u_2^n & = & 0 & \text{in } \Omega_2, \\ (\partial_x - \mathcal{S}_2)u_2^n & = & (\partial_x - \mathcal{S}_2)u_1^n & \text{on } x = 0, \end{array}$$

After a Fourier transform in y, we obtain

$$\begin{array}{rcll} (\eta + k^2 - \partial_{xx})\hat{u}_1^n & = & 0 & \text{in } \Omega_1, \\ (\partial_x + \sigma_1)\hat{u}_1^n & = & (\partial_x + \sigma_1)\hat{u}_2^{n-1} & \text{on } x = L, \\ (\eta + k^2 - \partial_{xx})\hat{u}_2^n & = & 0 & \text{in } \Omega_2, \\ (\partial_x - \sigma_2)\hat{u}_2^n & = & (\partial_x - \sigma_2)\hat{u}_1^n & \text{on } x = 0, \end{array}$$

where σ_j is the Fourier symbol of the operator $\mathcal{S}_j$.

Convergence Result with Fourier Analysis

As before, the solution of the ordinary differential equations are

$$\hat{u}_1^n(x,k) = A_1^n e^{\sqrt{\eta+k^2}x}, \quad \hat{u}_2^n(x,k) = B_2^n e^{-\sqrt{\eta+k^2}x}.$$

To determine the constants A_j^n and B_j^n, we use the transmission conditions

$$\begin{aligned}(\partial_x + \sigma_1)\hat{u}_1^n(L,k) &= (\partial_x + \sigma_1)\hat{u}_2^{n-1}(L,k),\\ (\partial_x - \sigma_2)\hat{u}_2^n(0,k) &= (\partial_x - \sigma_2)\hat{u}_1^n(0,k),\end{aligned}$$

which give

$$A_1^n(\sqrt{\eta+k^2}+\sigma_1)e^{\sqrt{\eta+k^2}L} = B_2^{n-1}(-\sqrt{\eta+k^2}+\sigma_1)e^{-\sqrt{\eta+k^2}L}$$

and

$$B_2^{n-1}(-\sqrt{\eta+k^2}-\sigma_2) = A_1^{n-1}(\sqrt{\eta+k^2}-\sigma_2).$$

Convergence Result with Fourier Analysis

After one iteration of the optimized Schwarz method, we obtain the convergence factor

$$\rho(\eta, k, L, \sigma_1, \sigma_2) := \frac{\sqrt{\eta + k^2} - \sigma_1}{\sqrt{\eta + k^2} + \sigma_1} \frac{\sqrt{\eta + k^2} - \sigma_2}{\sqrt{\eta + k^2} + \sigma_2} e^{-2\sqrt{\eta+k^2}L}.$$

- If the symbols $\sigma_j := \sqrt{\eta + k^2}$, then the convergence factor equals 0: convergence after one double step, even without overlap $\Longrightarrow$ Optimal Schwarz Method!
- This result can be generalized to convergence after I steps for I subdomains, provided the subdomain connections have no loops.
- This choice is optimal, but expensive, since the operator associated with the symbol $\sqrt{\eta + k^2}$ is non-local (it represents the DtN operator for the equation)
- One is therefore interested in local approximations $\Longrightarrow$ Optimized Schwarz Method!

Zeroth Order Approximation

We approximate the symbols σ_j by a constant, $\sigma_j := p$, $p \in \mathbb{R}$. The transmission conditions are therefore

$$\begin{aligned}(\partial_x + p)u_1^n(L, y) &= (\partial_x + p)u_2^{n-1}(L, y),\\ (\partial_x - p)u_2^n(0, y) &= (\partial_x - p)u_1^n(0, y),\end{aligned}$$

like in Lions's algorithm.

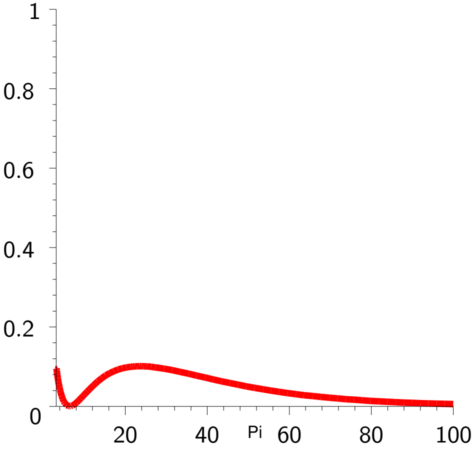
Now in order to obtain a fast method, we should choose p to make the contraction factor ρ as small as possible, i.e.

$$\min_{p\in\mathbb{R}} \max_{k\in K} \left| \left(\frac{\sqrt{\eta + k^2} - p}{\sqrt{\eta + k^2} + p} \right)^2 e^{-2\sqrt{\eta+k^2}L} \right| .$$

The set K represents Fourier modes in the computations, for example $K := (k_{\min}, k_{\max})$, with $k_{\min} = \frac{\pi}{H}$ and $k_{\max} = \frac{\pi}{h}$, and H denotes the interface length, and h the mesh size.

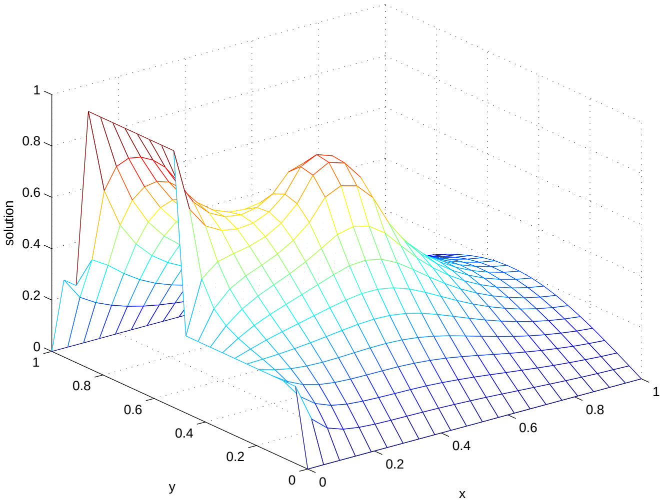
Optimized Choice in the Robin Condition

If we choose the best p, we get a contraction factor

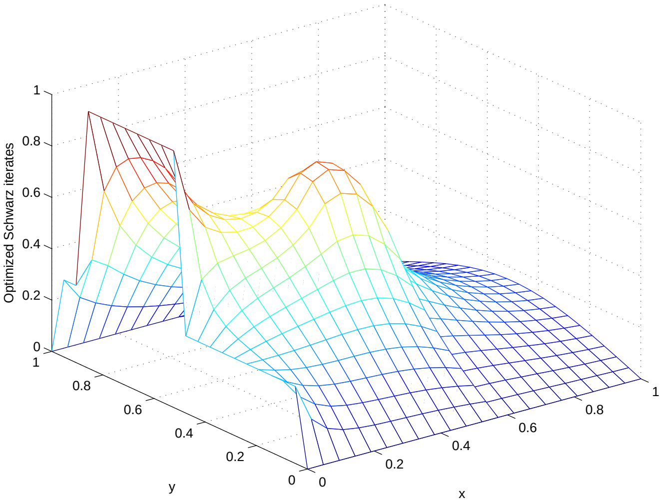


- The contraction factor is uniformly bounded by 0.1
- We observe that at the optimum, we have equioscillation

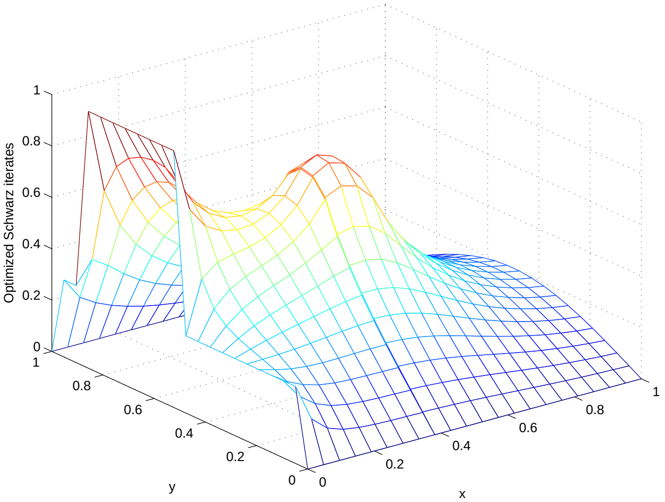
Example: Heating a Room



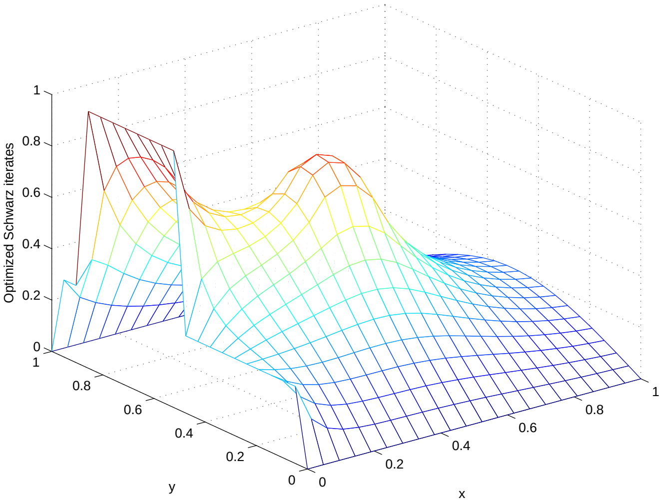
Iteration 1



Iteration 2



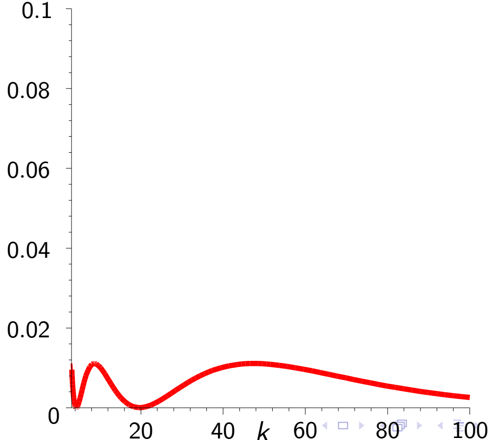
Iteration 3



Second Order Approximation

We approximate the symbols σ_j by a second degree polynomial in ik, $\sigma_j := p - qk^2$, $p, q \in \mathbb{R}$. The transmission conditions are therefore

$$\begin{aligned}(\partial_x + p + q\partial_{yy})u_1^n(L,y) &= (\partial_x + p + q\partial_{yy})u_2^{n-1}(L,y),\\ (\partial_x - p - q\partial_{yy})u_2^n(0,y) &= (\partial_x - p - q\partial_{yy})u_1^n(0,y).\end{aligned}$$



Optimized Parameters for a Model Problem

For the self adjoint coercive problem

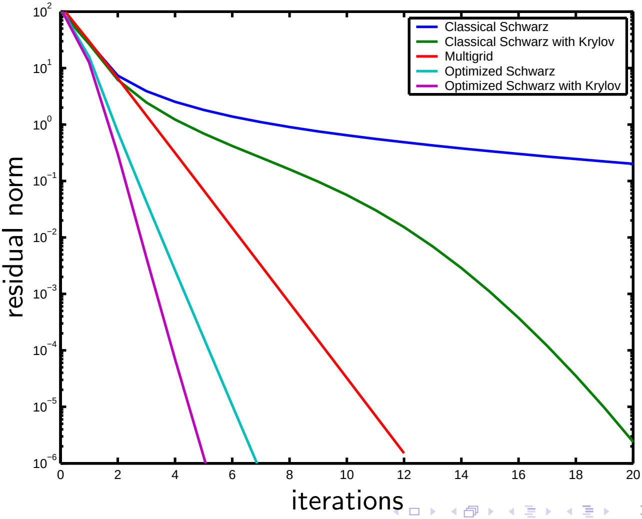
$$\mathcal{L}u = (\eta - \Delta)u = f$$

the asymptotically optimal parameters are (G 2006)

	p	q
OO0	$\frac{\sqrt{\pi}(k_{\min}^2+\eta)^{1/4}}{h^{1/2}}$	0
OO0(Ch)	$\frac{(k_{\min}^2+\eta)^{1/3}}{2^{1/3}(Ch)^{1/3}}$	0
OO2	$\frac{\pi^{1/4}(k_{\min}^2+\eta)^{3/8}}{2^{1/2}h^{1/4}}$	$\frac{h^{3/4}}{2^{1/2}\pi^{3/4}(k_{\min}^2+\eta)^{1/8}}$
OO2(Ch)	$\frac{(k_{\min}^2+\eta)^{2/5}}{2^{3/5}(Ch)^{1/5}}$	$\frac{(Ch)^{3/5}}{2^{1/5}(k_{\min}^2+\eta)^{1/5}}$
TO0	$\sqrt{\eta}$	0
TO2	$\sqrt{\eta}$	$\frac{1}{2\sqrt{\eta}}$

Comparison of Optimized Schwarz with Multigrid

Comparison of MS as an iterative solver, as a preconditioner, multigrid, and an optimized Schwarz methods used iteratively and as a preconditioner:



Schur Methods

1D model problem $(\eta - \Delta)u = f$ on $\Omega = (0,1)$
Non-overlapping subdomains $\Omega_1 = (0,\alpha)$ and $\Omega_2 = (\alpha,1)$
Finite difference discretization leads to $A\mathbf{u} = \mathbf{f}$

$$\begin{pmatrix} A_{11} & A_{1\Gamma} & 0 \\ A_{\Gamma 1} & A_{\Gamma\Gamma} & A_{\Gamma 2} \\ 0 & A_{2\Gamma} & A_{22} \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ u_\Gamma \\ \mathbf{u}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1 \\ f_\Gamma \\ \mathbf{f}_2 \end{pmatrix}$$

$$A = \left(\begin{array}{ccc|c|ccc} \frac{2}{h^2}+\eta & -\frac{1}{h^2} & & & & & \\ -\frac{1}{h^2} & \ddots & \ddots & & & & \\ & \ddots & \frac{2}{h^2}+\eta & -\frac{1}{h^2} & & & \\ \hline & & -\frac{1}{h^2} & \frac{2}{h^2}+\eta & -\frac{1}{h^2} & & \\ \hline & & & -\frac{1}{h^2} & \frac{2}{h^2}+\eta & -\frac{1}{h^2} & \\ & & & & -\frac{1}{h^2} & \ddots & \ddots \\ & & & & & \ddots & -\frac{2}{h^2}+\eta \end{array}\right)$$

Primal Schur Method

Rewriting the system by blocks yields

$$\begin{aligned} A_{11}\mathbf{u}_1 + A_{1\Gamma}u_\Gamma &= \mathbf{f}_1 \\ A_{22}\mathbf{u}_2 + A_{2\Gamma}u_\Gamma &= \mathbf{f}_2 \\ A_{\Gamma 1}\mathbf{u}_1 + A_{\Gamma 2}\mathbf{u}_2 + A_{\Gamma\Gamma}u_\Gamma &= \mathbf{f}_\Gamma \end{aligned}$$

Solving for the subdomain solutions gives

$$\mathbf{u}_1 = A_{11}^{-1}(\mathbf{f}_1 - A_{1\Gamma}u_\Gamma), \quad \mathbf{u}_2 = A_{22}^{-1}(\mathbf{f}_2 - A_{2\Gamma}u_\Gamma)$$

and introducing this into the last equation gives

$$(A_{\Gamma\Gamma} - A_{\Gamma 1}A_{11}^{-1}A_{1\Gamma} - A_{\Gamma 2}A_{22}^{-1}A_{2\Gamma})u_\Gamma = f_\Gamma - A_{\Gamma 1}A_{11}^{-1}\mathbf{f}_1 - A_{\Gamma 2}A_{22}^{-1}\mathbf{f}_2$$

the Schur complement system of Przemieniecki, based on the primal Schur complement

$$S_P = A_{\Gamma\Gamma} - A_{\Gamma 1}A_{11}^{-1}A_{1\Gamma} - A_{\Gamma 2}A_{22}^{-1}A_{2\Gamma}$$

Continuous Interpretation of Primal Schur

The interface equation $A_{\Gamma 1}\mathbf{u}_1 + A_{\Gamma 2}\mathbf{u}_2 + A_{\Gamma\Gamma} u_\Gamma = \mathbf{f}_\Gamma$ in 1D is

$$-\frac{1}{h^2}(u_1)_{a-1} + (\frac{2}{h^2} + \eta)u_\Gamma - \frac{1}{h^2}(u_2)_1 = f_\Gamma$$

and thus represents at the continuous level

$$-\frac{1}{h^2}u_1(\alpha - h) + (\frac{2}{h^2} + \eta)u_\Gamma - \frac{1}{h^2}u_2(\alpha + h) = f(\alpha) + \mathcal{O}(h^2)$$

or equivalently

$$\frac{1}{h^2}(u_1(\alpha) - u_1(\alpha - h)) - \frac{1}{h^2}(u_2(\alpha + h) - u_2(\alpha)) + \eta u_\Gamma = f(\alpha) + \mathcal{O}(h^2)$$

Using a Taylor expansion and the differential equation

$$\begin{aligned} u_1(\alpha - h) &= u_1(\alpha) - h\frac{du_1}{dx}(\alpha) + \frac{h^2}{2}\frac{d^2u_1}{dx^2}(\alpha) + o(h^2) \\ &= u_1(\alpha) - h\frac{du_1}{dx}(\alpha) + \frac{h^2}{2}(\eta u_1(\alpha) - f(\alpha)) + o(h^2) \end{aligned}$$

Hence the interface equation is a discretization of

$$\frac{du_2}{dx}(\alpha) - \frac{du_1}{dx}(\alpha) = 0$$

Continuous Interpretation of Primal Schur

The continuous formulation of

$$
\begin{aligned}
A_{11}\mathbf{u}_1 + A_{1\Gamma}u_\Gamma &= \mathbf{f}_1\\
A_{22}\mathbf{u}_2 + A_{2\Gamma}u_\Gamma &= \mathbf{f}_2\\
A_{\Gamma 1}\mathbf{u}_1 + A_{\Gamma 2}\mathbf{u}_2 + A_{\Gamma\Gamma}u_\Gamma &= \mathbf{f}_\Gamma
\end{aligned}
$$

is therefore

$$
\begin{aligned}
-\frac{d^2u_1}{dx^2} + \eta u_1 &= f \text{ in } \Omega_1\\
-\frac{d^2u_2}{dx^2} + \eta u_2 &= f \text{ in } \Omega_2,
\end{aligned}
$$

$$
u_1(\alpha) = u_2(\alpha), \qquad \frac{du_1}{dx}(\alpha) = \frac{du_2}{dx}(\alpha)
$$

where the first interface condition is explicitly enforced, i.e.

$$
u_1(\alpha) = u_2(\alpha) = u_\Gamma
$$

What is then the primal Schur formulation at the continuous level ?

Continuous Primal Schur Formulation

Assume the interface value u_Γ is given, we solve for u_i on Ω_i and evaluate at the interface $x = \alpha$ the derivative, which gives the DtN operators

$$\mathcal{S}_1^{\mathcal{DN}}(u_\Gamma, f) = \frac{du_1}{dx}(\alpha), \quad \mathcal{S}_2^{\mathcal{DN}}(u_\Gamma, f) = \frac{du_2}{dx}(\alpha).$$

Setting these derivatives equal, we obtain by linearity

$$\mathcal{S}_P\, u_\Gamma := \mathcal{S}_1^{\mathcal{DN}}(u_\Gamma, 0) - \mathcal{S}_2^{\mathcal{DN}}(u_\Gamma, 0) = -\mathcal{S}_1^{\mathcal{DN}}(0, f) + \mathcal{S}_2^{\mathcal{DN}}(0, f)$$

which is the continuous formulation of the primal Schur complement system

$$(A_{\Gamma\Gamma} - A_{\Gamma 1} A_{11}^{-1} A_{1\Gamma} - A_{\Gamma 2} A_{22}^{-1} A_{2\Gamma}) u_\Gamma = f_\Gamma - A_{\Gamma 1} A_{11}^{-1} \mathbf{f}_1 - A_{\Gamma 2} A_{22}^{-1} \mathbf{f}_2$$

Solving this system with a Krylov method, we are interested in its condition number!

Condition Number Estimate with Fourier Analysis

For the model problem $\mathcal{L}u := (\eta - \Delta)u = 0$ on $\Omega = \mathbb{R}^2$, $\Omega_1 = (-\infty, 0) \times \mathbb{R}$ and $\Omega_2 = (0, \infty) \times \mathbb{R}$,

$$\begin{aligned} (\eta - \Delta)u_1 &= 0 \quad \text{in } \Omega_1 \\ u_1 &= u_\Gamma \text{ on } x = 0 \end{aligned} \qquad \begin{aligned} (\eta - \Delta)u_2 &= 0 \quad \text{in } \Omega_2 \\ u_2 &= u_\Gamma \text{ on } x = 0 \end{aligned}$$

After a Fourier transform in y

$$(\eta + k^2 - \partial_{xx})\hat{u}_1 = 0 \text{ in } \Omega_1 \quad (\eta + k^2 - \partial_{xx})\hat{u}_2 = 0 \text{ in } \Omega_2$$

We get $\hat{u}_i(x, k) = \hat{u}_\Gamma e^{\pm\sqrt{\eta + k^2}x}$, and hence

$$\hat{\mathcal{S}}_1^{\mathcal{DN}}(\hat{u}_\Gamma, 0) = \sqrt{\eta + k^2}\hat{u}_\Gamma, \quad \hat{\mathcal{S}}_2^{\mathcal{DN}}(\hat{u}_\Gamma, 0) = -\sqrt{\eta + k^2}\hat{u}_\Gamma$$

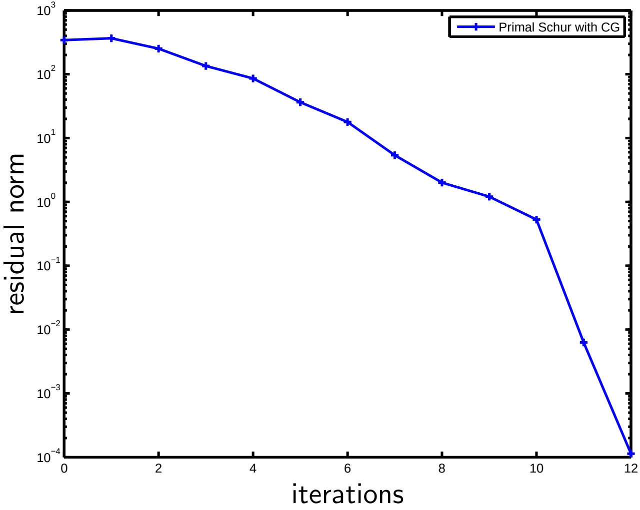
and therefore

$$\hat{\mathcal{S}}_P\, u_\Gamma = \hat{\mathcal{S}}_1^{\mathcal{DN}}(u_\Gamma, 0) - \hat{\mathcal{S}}_2^{\mathcal{DN}}(u_\Gamma, 0) = 2\sqrt{\eta + k^2}\hat{u}_\Gamma$$

The condition number of the Schur complement is thus

$$\kappa(\mathcal{S}_P) = \frac{\sqrt{\eta + k_{\max}^2}}{\sqrt{\eta + k_{\min}^2}} = \frac{\sqrt{\eta + (\frac{\pi}{h})^2}}{\sqrt{\eta + (\frac{\pi}{L})^2}} \sim O(\frac{1}{h})$$

Numerical Experiment for the Heating Problem



- Each iteration needs one subdomain solve each
- Original problem $(\eta - \Delta)u = f$ had $\kappa = O(\frac{1}{h^2})$

Dual Schur Complement Method

Starting again with the coupled problem

$$-\frac{d^2u_1}{dx^2} + \eta u_1 = f \text{ in } \Omega_1$$
$$-\frac{d^2u_2}{dx^2} + \eta u_2 = f \text{ in } \Omega_2$$

$$u_1(\alpha) = u_2(\alpha), \qquad \frac{du_1}{dx}(\alpha) = \frac{du_2}{dx}(\alpha)$$

instead of enforcing explicitly the first interface condition as in the primal Schur complement method,

$$u_1(\alpha) = u_2(\alpha) = u_\Gamma$$

in dual Schur complement methods, the second one is enforced explicitly,

$$\frac{du_1}{dx}(\alpha) = \frac{du_2}{dx}(\alpha) = u'_\Gamma$$

and then enforcing continuity gives the linear system.

Condition Number Estimate with Fourier Analysis

For the same model problem:

$$(\eta - \Delta)u_1 = 0 \quad \text{in } \Omega_1 \qquad (\eta - \Delta)u_2 = 0 \quad \text{in } \Omega_2$$
$$\frac{du_1}{dx} = u'_\Gamma \text{ on } x = 0 \qquad \frac{du_2}{dx} = u'_\Gamma \text{ on } x = 0$$

After a Fourier transform in y we get
$\hat{u}_i(x,k) = \frac{\hat{u}'_\Gamma}{\pm\sqrt{\eta+k^2}} e^{\pm\sqrt{\eta+k^2}x}$, and hence

$$\hat{\mathcal{S}}_1^{\mathcal{ND}}(\hat{u}'_\Gamma, 0) = \frac{\hat{u}'_\Gamma}{\sqrt{\eta + k^2}}, \; \hat{\mathcal{S}}_2^{\mathcal{ND}}(\hat{u}'_\Gamma, 0) = -\frac{\hat{u}'_\Gamma}{\sqrt{\eta + k^2}}$$

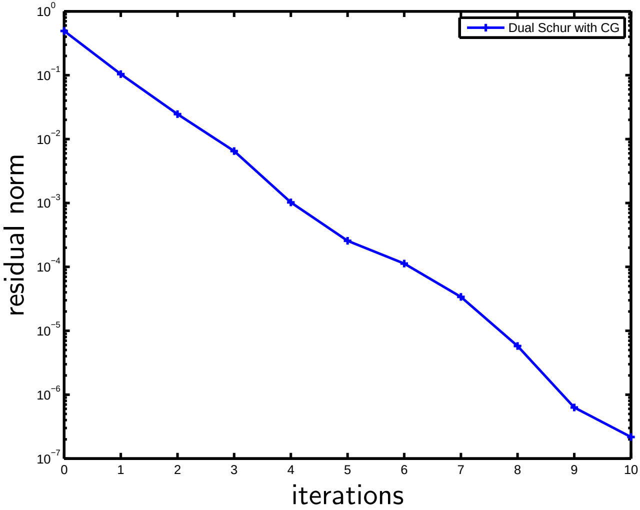
and therefore

$$\hat{\mathcal{S}}_D \, u'_\Gamma = \hat{\mathcal{S}}_1^{\mathcal{ND}}(u_\Gamma, 0) - \hat{\mathcal{S}}_2^{\mathcal{ND}}(u_\Gamma, 0) = \frac{2\hat{u}_\Gamma}{\sqrt{\eta + k^2}}$$

Condition number of the Dual Schur complement is

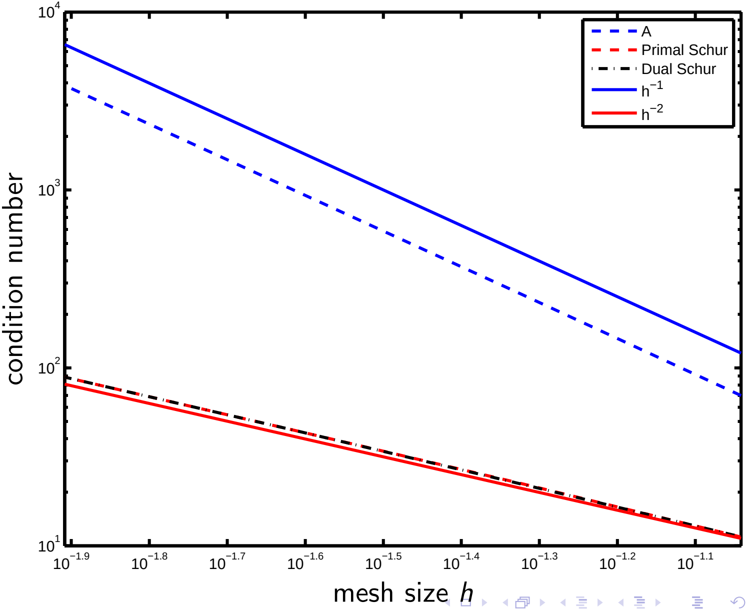
$$\kappa(\mathcal{S}_D) = \frac{\sqrt{\eta + k_{\max}^2}}{\sqrt{\eta + k_{\min}^2}} = \frac{\sqrt{\eta + (\frac{\pi}{h})^2}}{\sqrt{\eta + (\frac{\pi}{L})^2}} \sim O(\frac{1}{h})$$

Numerical Experiment for the Heating Problem



- Each iteration needs one Neumann solve per Subdomain

Condition Number Comparison



Discrete Dual Schur Complement Method

Writing the discrete derivatives as before, we get

$$u'_\Gamma = \frac{u_{1,a}-u_{1,a-1}}{h}+\frac{h}{2}(\eta u_{1,a}-f_a) = \frac{u_{2,a+1}-u_{2,a}}{h}-\frac{h}{2}(\eta u_{2,a}-f_a)$$

which gives the global, discrete coupled system

$$\begin{array}{rcll}
-\frac{u_{1,j+1}-2u_{1,j}+u_{1,j-1}}{h^2}+\eta\, u_{1,j} & = & f_{1,j}, & 1\le j\le a-1\\
-\frac{1}{h^2}u_{1,a-1}+\frac{1}{2}(\eta+\frac{2}{h^2})u_{1,a} & = & \frac{1}{2}f_a+\frac{1}{h}u'_\Gamma & \\
-\frac{u_{2,j+1}-2u_{2,j}+u_{2,j-1}}{h^2}+\eta\, u_{2,j} & = & f_{2,j}, & a+1\le j\le J\\
-\frac{1}{h^2}u_{2,a+1}+\frac{1}{2}(\eta+\frac{2}{h^2})u_{2,a} & = & \frac{1}{2}f_a-\frac{1}{h}u'_\Gamma &
\end{array}$$

or in Matrix form

$$\begin{pmatrix} A_{11} & A_{1\Gamma}\\ A_{\Gamma 1} & \frac{1}{2}A_{\Gamma\Gamma}\end{pmatrix}\begin{pmatrix}\mathbf{u}_1\\ u_{1,a}\end{pmatrix}=\begin{pmatrix}\mathbf{f}_1\\ \frac{1}{2}f_a+\frac{1}{h}u'_\Gamma\end{pmatrix}$$

$$\begin{pmatrix} \frac{1}{2}A_{\Gamma\Gamma} & A_{\Gamma 2}\\ A_{2\Gamma} & A_{22}\end{pmatrix}\begin{pmatrix}u_{2,a}\\ \mathbf{u}_2\end{pmatrix}=\begin{pmatrix}\frac{1}{2}f_a-\frac{1}{h}u'_\Gamma\\ \mathbf{f}_2\end{pmatrix}$$

Discrete Dual Schur Continued

With the discrete trace operators

$$\begin{array}{llll} \widetilde{G}_1 : \mathbb{R}^a & \to \mathbb{R}, & (u_1,\dots,u_a) & \mapsto u_a \\ \widetilde{G}_2 : \mathbb{R}^{J-a+1} & \to \mathbb{R}, & (u_a,\dots,u_J) & \mapsto u_a \end{array}$$

we extract $u_{1,a}$ and $u_{2,a}$ from the equations

$$u_{1,a} = \widetilde{G}_1 \begin{pmatrix} \mathbf{u}_1 \\ u_{1,a} \end{pmatrix} = \widetilde{G}_1 \begin{pmatrix} A_{11} & A_{1\Gamma} \\ A_{\Gamma 1} & \frac{1}{2}A_{\Gamma\Gamma} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{f}_1 \\ \frac{1}{2}f_a + \frac{1}{h}u'_\Gamma \end{pmatrix}$$

$$u_{2,a} = \widetilde{G}_2 \begin{pmatrix} u_{2,a} \\ \mathbf{u}_2 \end{pmatrix} = \widetilde{G}_2 \begin{pmatrix} \frac{1}{2}A_{\Gamma\Gamma} & A_{\Gamma 2} \\ A_{2\Gamma} & A_{22} \end{pmatrix}^{-1} \begin{pmatrix} \frac{1}{2}f_a - \frac{1}{h}u'_\Gamma \\ \mathbf{f}_2 \end{pmatrix}$$

Setting those two values equal, we obtain by linearity

$$\left(\widetilde{G}_1 \begin{pmatrix} A_{11} & A_{1\Gamma} \\ A_{\Gamma 1} & \frac{1}{2}A_{\Gamma\Gamma} \end{pmatrix}^{-1} \widetilde{G}_1^T + \widetilde{G}_2 \begin{pmatrix} \frac{1}{2}A_{\Gamma\Gamma} & A_{\Gamma 2} \\ A_{2\Gamma} & A_{22} \end{pmatrix}^{-1} \widetilde{G}_2^T \right) u'_\Gamma =$$

$$-h\,\widetilde{G}_1 \begin{pmatrix} A_{11} & A_{1\Gamma} \\ A_{\Gamma 1} & \frac{1}{2}A_{\Gamma\Gamma} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{f}_1 \\ \frac{1}{2}f_a \end{pmatrix} + h\,\widetilde{G}_2 \begin{pmatrix} \frac{1}{2}A_{\Gamma\Gamma} & A_{\Gamma 2} \\ A_{2\Gamma} & A_{22} \end{pmatrix}^{-1} \begin{pmatrix} \frac{1}{2}f_a \\ \mathbf{f}_2 \end{pmatrix}$$

The FETI Method

Finite Element Tearing and Interconnection, Farhat/Roux: solution of $-\Delta u = f$ in Ω with homogeneous bc minimizes

$$J(v) = \frac{1}{2}\int_\Omega |\nabla v|^2\,dx - \int_\Omega fv\,dx$$

Decompose J on two non-overlapping subdomains Ω_i:

$$J_1(v) = \frac{1}{2}\int_{\Omega_1}|\nabla v|^2\,dx - \int_{\Omega_1} fv\,dx,\ J_2(v) = \frac{1}{2}\int_{\Omega_2}|\nabla v|^2\,dx - \int_{\Omega_2} fv\,dx$$

minimize over (v_1, v_2) such that $v_1 = v_2$ on the interface Γ. This constraint optimization problem can be written with the Lagrangian

$$\mathcal{L}(v_1, v_2, h) = J_1(v_1) + J_2(v_2) + \int_\Gamma h(v_2 - v_1)\,ds.$$

The minimum is attained at (u_1, u_2, g) s.t.

$$\partial_{v_i}\mathcal{L}(u_1, u_2, g) = 0,\ \ i = 1, 2 \text{ and } \partial_h \mathcal{L}(u_1, u_2, g) = 0$$

FETI Derivation Continued

The derivatives are

$$\partial_{v_i}\mathcal{L}(u_1,u_2,g)\cdot v_i=\int_{\Omega_i}\nabla u_i\cdot\nabla v_i\,dx-\int_{\Omega_i}fv_i\,dx,\ \ i=1,2$$

and

$$\partial_g\mathcal{L}(u_1,u_2,g)\cdot h=\int_{\Gamma}h(u_2-u_1)\,ds$$

This can be rewritten as

$$\forall v_1\in V_1,\ \int_{\Omega_1}\nabla u_1\nabla v_1\,dx-\int_{\Omega_1}fv_1\,dx-\int_{\Gamma}gv_1\,ds=0$$

$$\forall v_2\in V_2,\ \int_{\Omega_2}\nabla u_2\nabla v_2\,dx-\int_{\Omega_2}fv_2\,dx-\int_{\Gamma}gv_2\,ds=0$$

$$\forall h\text{ on }\Gamma,\ \int_{\Gamma}h(u_2-u_1)\,ds=0$$

We recognize the weak formulation of the Dual Schur complement method, once the first two equations are solved and introduced into the last one.

Additional Ingredients of FETI

Two additional ingredients:

1. Natural coarse grid using floating subdomains
2. The condition number of FETI is $O(\frac{1}{h})$, from the Dual Schur complement operator in Fourier

$$\mathcal{S}_D \hat{u}'_\Gamma = \frac{2\hat{u}'_\Gamma}{\sqrt{\eta + k^2}}$$

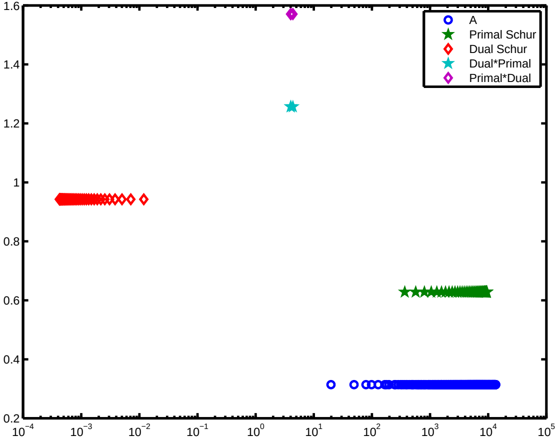
   We have also seen that the Primal Schur complement operator in Fourier is

$$\mathcal{S}_P \hat{u}_\Gamma = 2\sqrt{\eta + k^2}\,\hat{u}_\Gamma$$

   Hence Primal Schur is the ideal preconditioner for FETI!

One can also invert the approach, using a Primal Schur method preconditioned with the Dual Schur formulation, which is called (balancing) Neumann-Neumann

Spectra and Condition Numbers



J	A	Schur Primal	Schur Dual	Dual-Primal	Primal-Dual
10	48.37	6.55	7.28	1.11	1.11
20	178.06	13.04	14.31	1.10	1.10
40	680.62	25.91	28.26	1.09	1.09

Dirichlet-Neumann and Neumann-Dirichlet

Schwarz type relaxation for $(\eta - \Delta)$ on two half planes:

$$\begin{aligned} (\eta - \Delta)u_1^n &= f, \quad \text{in } \Omega_1 \\ u_1^n(0,y) &= u_2^{n-1}(0,y) \end{aligned} \qquad \begin{aligned} (\eta - \Delta)u_2^n &= f, \quad \text{in } \Omega_2 \\ \partial_x u_2^n(0,y) &= \partial_x u_1^{n-1}(0,y) \end{aligned}$$

Fourier analysis in y, $f = 0$ shows no convergence:

$$\hat{u}_1^n = \hat{u}_2^{n-1}(0)e^{\sqrt{\eta+k^2}x}, \quad \hat{u}_2^n = -\hat{u}_1^{n-1}(0)e^{-\sqrt{\eta+k^2}x} \Longrightarrow |\rho| = 1$$

Remedy: Introduce relaxation parameters γ_1 and γ_2

$$\begin{aligned} u_1^n(0,y) &= \gamma_1 u_2^{n-1}(0,y) + (1-\gamma_1)u_1^{n-1}(0,y) \\ \partial_x u_2^n(0,y) &= \gamma_2 \partial_x u_1^{n-1}(0,y) + (1-\gamma_2)\partial_x u_2^{n-1}(0,y) \end{aligned}$$

Theorem (Bjorstad, Widlund 1986): For $\gamma_2 = 1$ there exist γ_1 for which the Dirichlet-Neumann algorithm converges.

Theorem (Quarteroni, Valli 1999): For $\gamma_1 = 1$ there exist γ_2 for which the Neumann-Dirichlet algorithm converges.

Convergence Analysis for the Model Problem

Fourier transform in y, $f = 0$, parallel version

$$\begin{pmatrix} \hat{u}_1^n(0,y) \\ \partial_x \hat{u}_2^n(0,y) \end{pmatrix} = \begin{bmatrix} 1-\gamma_1 & \frac{-\gamma_1}{\sqrt{\eta+k^2}} \\ \gamma_2\sqrt{\eta+k^2} & 1-\gamma_2 \end{bmatrix} \begin{pmatrix} \hat{u}_1^{n-1}(0,y) \\ \partial_x \hat{u}_2^{n-1}(0,y) \end{pmatrix}$$

Minimizing the spectral radius using γ_1 and γ_2, $\sqrt{\eta+k^2}$ cancels:

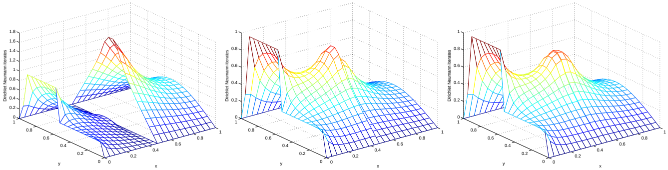
$$\gamma_1 = 1 \pm \frac{1}{\sqrt{2}},\ \gamma_2 = 1 \mp \frac{1}{\sqrt{2}}, \quad \Longrightarrow \quad \rho = 0$$

which means convergence in two iterations !

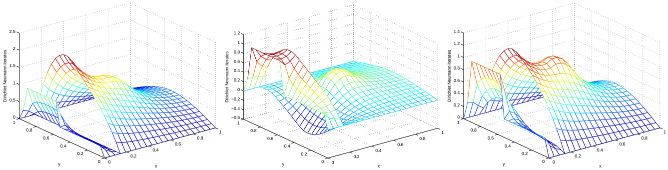
If one γ_i is fixed, then
Dirichlet-Neumann: $\gamma_2 = 1$, best $\gamma_1 = 3 \pm 2\sqrt{2}$
Neumann-Dirichlet: $\gamma_1 = 1$, best $\gamma_2 = 3 \pm 2\sqrt{2}$

In an alternating version, one can also achieve $\rho = 0$ for this symmetric case, the optimal parameter is then $\gamma_i = 1/2$.

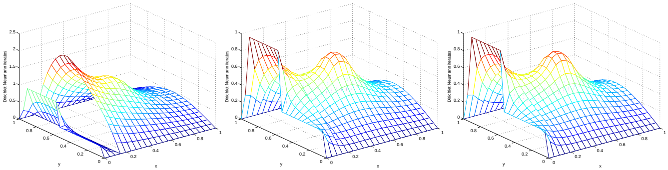
Numerical Example Heating a Room



Interface en $\alpha = 0.5$, $\theta = 0.5$



Interface en $\alpha = 0.15$, $\theta = 0.5$



Interface en $\alpha = 0.15$, $\theta = 0.3$

Interpretation of these Algorithms

The Dirichlet-Neumann algorithm in substructured form is

$$u_\Gamma^{n+1} = u_\Gamma^n + \theta\left(\mathcal{S}_2^{\mathcal{ND}}(\mathcal{S}_1^{\mathcal{DN}}(u_\Gamma^n, f), f) - u_\Gamma^n\right)$$

This is a Richardson algorithm for the preconditioned system

$$\mathcal{S}_2^{\mathcal{ND}}(\mathcal{S}_1^{\mathcal{DN}}(u_\Gamma, f), f) = u_\Gamma$$

and with $\mathcal{S}_2^{\mathcal{ND}}(\mathcal{S}_2^{\mathcal{DN}}(g, f), f) = g$ for all f, g, we get

$$\mathcal{S}_2^{\mathcal{ND}}(\mathcal{S}_1^{\mathcal{DN}}(u_\Gamma, f) - \mathcal{S}_2^{\mathcal{DN}}(u_\Gamma, f), f) = 0$$

the Primal Schur formulation preconditioned with $\mathcal{S}_2^{\mathcal{ND}}$.

Similarly, we get for the Neumann-Dirichlet algorithm

$$\mathcal{S}_2^{\mathcal{DN}}(\mathcal{S}_1^{\mathcal{ND}}(u'_\Gamma, f) - \mathcal{S}_2^{\mathcal{ND}}(u'_\Gamma, f), f) = 0$$

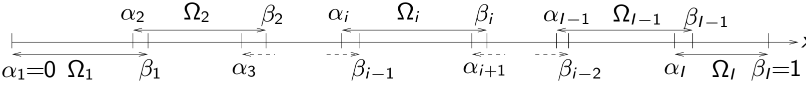
the Dual Schur formulation preconditioned with $\mathcal{S}_2^{\mathcal{DN}}$.

Coarse Grids

Strong Scalability: For a problem of fixed size, the time to solution is inversely proportional to the number of processors

Weak Scalability: The time to solution is constant, when the number of processors is increased proportionally to the problem size

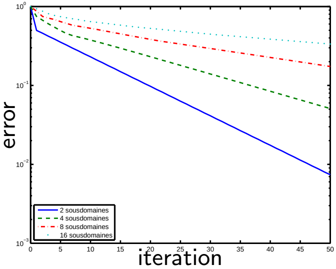
One dimensional decomposition into many subdomains:



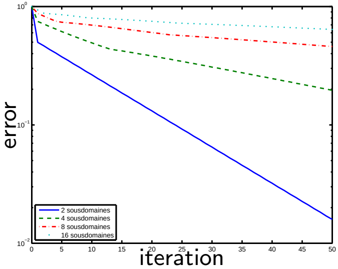
Important parameters:

- I number of subdomains
- $H_i := \beta_i - \alpha_i$ subdomain width
- $\delta_i := \beta_i - \alpha_{i+1}$ overlap

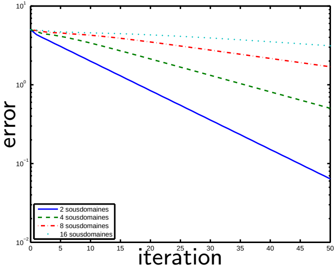
Scalability Problems of DD Methods



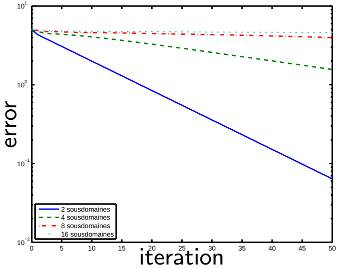
Strong: δ constant



Strong: δ diminishes with H



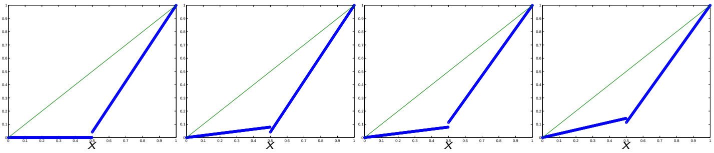
Weak: δ constant



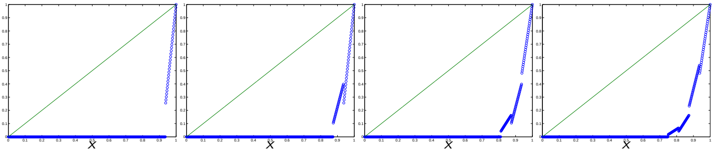
Weak: δ diminishes with H

Intuitive Explanation

Parallel Schwarz method with two subdomains



Parallel Schwarz method with sixteen subdomains



- Domain decomposition methods only communicate with neighboring subdomains
- For PDEs whose solution depends globally on data, domain decomposition methods can not be scalable without additional components

Borrow Idea from Multigrid

Need to define a global approximate solution $\mathbf{u}_n$.

Then introduce a coarse grid and compute

$$\begin{aligned} \mathbf{r}_n &= \mathbf{f} - A\mathbf{u}_n \,; \\ \mathbf{r}_c &= R\mathbf{r}_n \,; \\ \mathbf{u}_c &= A_c^{-1}\mathbf{r}_c \,; \\ \mathbf{u}_n &= \mathbf{u}_n + E\mathbf{u}_c \,; \end{aligned}$$

Standard components:

- use for the extension E interpolation
- use for the restriction R the extension transposed
- use for the coarse matrix $A_c = RAE$ (Galerkin)

Classical coarse grid choice: one (or a few) points per subdomain

Fundamental Convergence Result for AS

Theorem (M. Drjya and O. Widlund (1989))

The condition number of the additive Schwarz preconditioned system with coarse grid satisfies

$$\kappa(M_{AS}A) \leq C\left(1 + \frac{H}{\delta}\right),$$

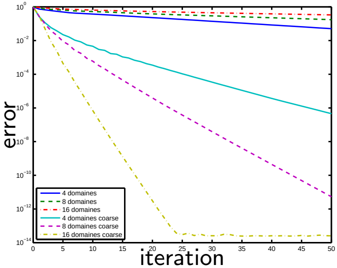
where the constant C is independent of δ and H.

Here δ is the overlap and H is the characteristic coarse mesh size of a coarse grid correction

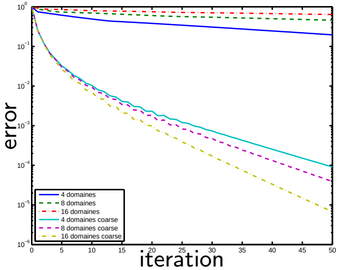
$$M_{AS} := \sum_{j=1}^{n} R_j^T A_j^{-1} R_j + R_0^T A_0^{-1} R_0$$

Hence AS can well be used as a preconditioner for a Krylov method.

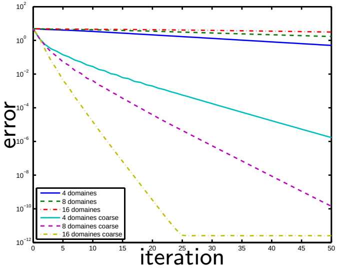
Scalability with Coarse Grid



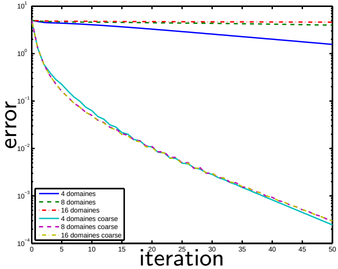
Strong: δ constant



Strong: δ diminishes with H

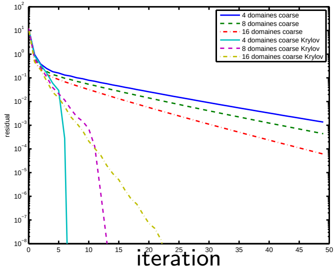


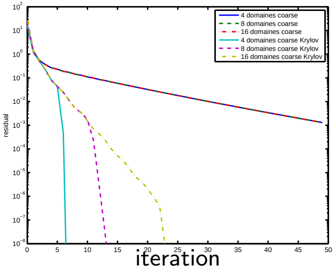
Weak: δ constant



Weak: δ diminishes with H

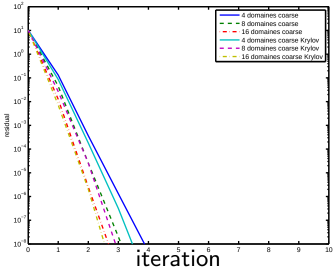
Scalability with Coarse Grid and Krylov

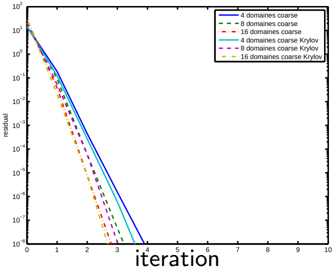




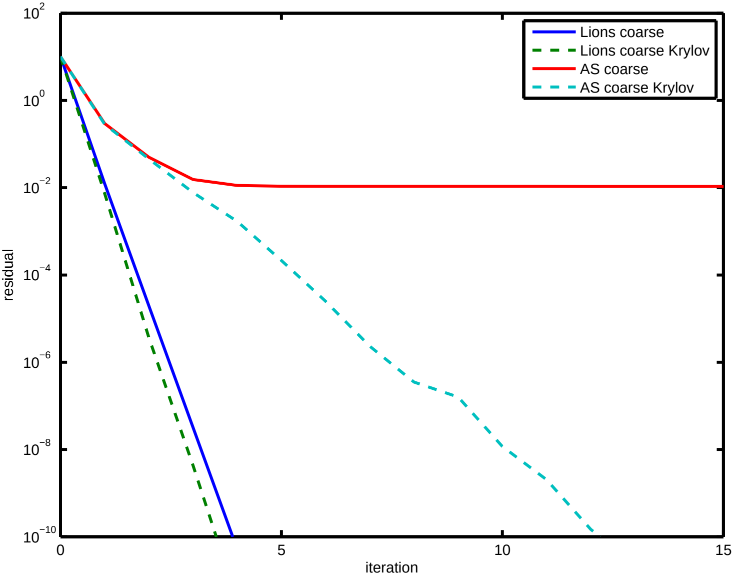
Strong: δ diminishes with H Weak: δ diminishes with H

With a coarse grid slightly different chosen with more insight:





Toward an Optimized Coarse Grid



Coarse Grid for FETI and Neumann-Neumann

As we have seen, these methods have a natural coarse grid component built in.

Theorem

The condition number of FETI (with natural coarse grid and preconditioner) or balancing Neumann-Neumann (with preconditioner) is bounded by

$$C(1+\ln(\frac{H}{h}))^2$$

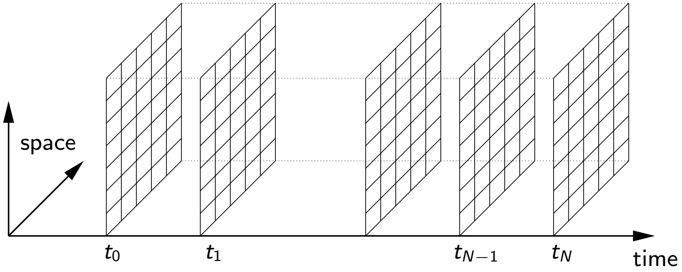
where C is a constant independent of H and h.

Proofs:

- For Neumann-Neumann see Drjya and Widlund (1995) and Mandel and Brezina (1996)
- For FETI, see Mandel and Tezaur (1996)

Solving Evolution Problems in Parallel ?

Systems of ODEs, $u' = f(u)$, or PDEs $\frac{\partial u}{\partial t} = L(u) + f$.



Time discretization, with e.g. Forward Euler for the ODE leads to

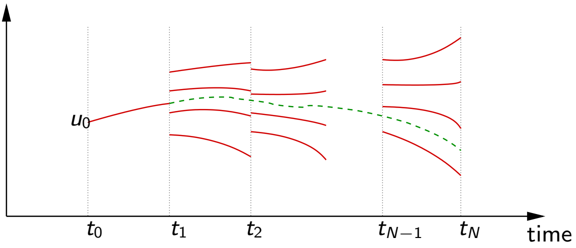
$$u_{n+1} = u_n + \Delta t f(u_n).$$

$\Longrightarrow$ **There seems to be no time parallelism in this recurrence relation**.

History of Time Parallel Algorithms

J. Nievergelt (1964): Parallel Methods for Integrating Ordinary Differential Equations

"For the last 20 years, one has tried to speed up numerical computation mainly by providing ever faster computers. **Today, as it appears that one is getting closer to the maximal speed of electronic components***, emphasis is put on allowing operations to be performed in parallel. In the near future, much of numerical analysis will have to be recast in a more "parallel" form."*



Multiple Shooting for Initial Value Problems

For the model problem

$$u' = f(u), \quad u(0) = u^0, \quad t \in [0,1]$$

one splits the time interval into subintervals $[0, \frac{1}{3}]$, $[\frac{1}{3}, \frac{2}{3}]$, $[\frac{2}{3}, 1]$, and then solves on each subinterval

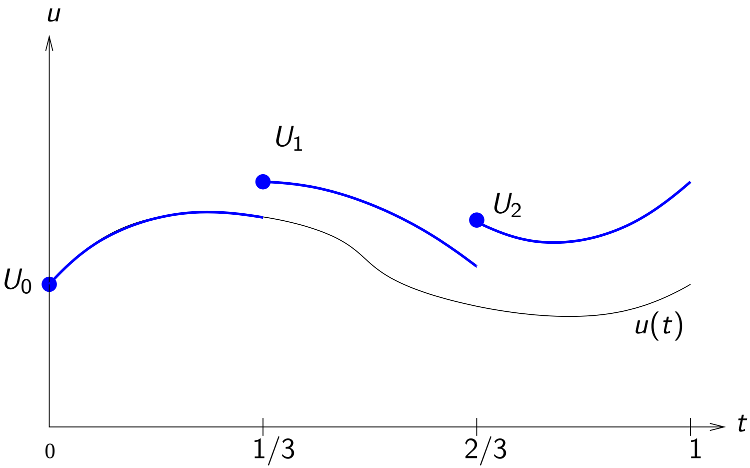
$$\begin{array}{rcl} u_0' &=& f(u_0), \\ u_0(0) &=& U_0, \end{array} \qquad \begin{array}{rcl} u_1' &=& f(u_1), \\ u_1(\frac{1}{3}) &=& U_1, \end{array} \qquad \begin{array}{rcl} u_2' &=& f(u_2), \\ u_2(\frac{2}{3}) &=& U_2, \end{array}$$

together with the matching conditions

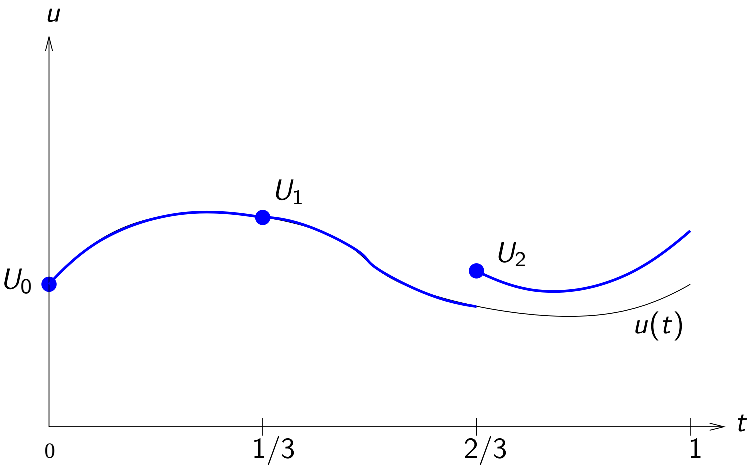
$$U_0 = u^0, \quad U_1 = u_0(\frac{1}{3}, U_0), \quad U_2 = u_1(\frac{2}{3}, U_1)$$

$$\iff \quad F(\mathbf{U}) = 0, \quad \mathbf{U} = (U_0, U_1, U_2)^T.$$

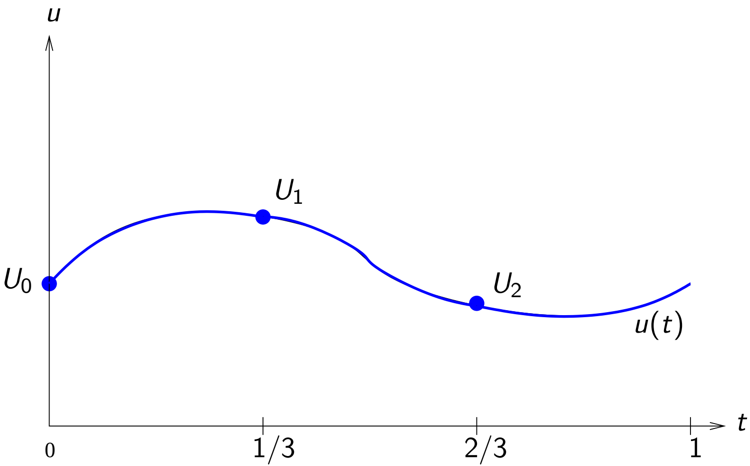
Example: first iteration



Example: second iteration



Example: third iteration



Using Newton's Method

Solving $F(\mathbf{U}) = 0$ with Newton's method leads in the general case with N intervals, $t_n = n\Delta T$, $\Delta T = 1/N$ to the time parallel shooting method

$$U_{n+1}^{k+1} = u_n(t_{n+1}, U_n^k) + \frac{\partial u_n}{\partial U_n}(t_{n+1}, U_n^k)(U_n^{k+1} - U_n^k).$$

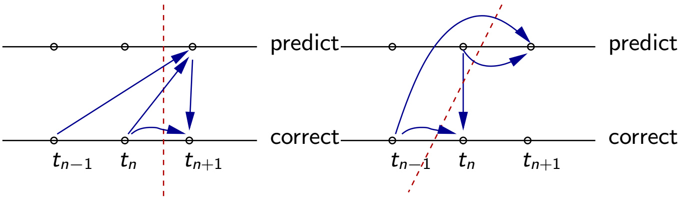
Theorem (Chartier and Philippe 1993)

If the initial guess $\mathbf{U}^0$ *is close enough to the solution, then under appropriate regularity assumptions, the multiple shooting algorithm converges quadratically.*

Parallel Time Stepping 1

W. Miranker and W. Liniger (1967): Parallel Methods for the Numerical Integration of Ordinary Differential Equations

"It appears at first sight that the sequential nature of the numerical methods do not permit a parallel computation on all of the processors to be performed. We say that **the front of computation** *is too narrow to take advantage of more than one processor... Let us consider how we might widen the computation front."*



Parallel Time Stepping 2

D. Womble (1990): A time-stepping algorithm for parallel computers.

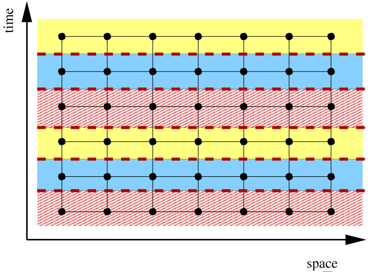
- For implicit time discretizations, e.g. Backward Euler:

$$u_{n+1} = u_n + \Delta t f(u_{n+1}) \iff F(u_{n+1}, u_n) = 0$$

- Each time step uses an iterative solver, e.g. Newton:

$$u_{n+1}^{k+1} = u_{n+1}^{k} - F'(u_{n+1}^{k}, u_n)^{-1} F'(u_{n+1}^{k}, u_n)$$

- Iteration starts at the next time step, before the previous time step result u_n is obtained accurately



A Negative Result for Parallel Time Stepping

Deshpande, Malhotra, Douglas, Schultz (1995):
Temporal Domain Parallelism: Does it Work ?

Results:

- if a good solver is used on each time step, no parallel speedup is possible.
- if a very slow solver is used on each time step, a small parallel speedup can be achieved.

Quote from the tech report (1993):

> **"We show that this approach is not normally useful".**

Schwarz Waveform Relaxation for PDEs

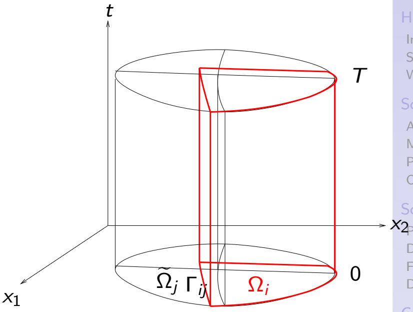
For a given evolution PDE,

$$\mathcal{L}u = f, \quad \text{in } \Omega \times (0, T),$$

with initial condition

$$u(x, 0) = u_0,$$

the Schwarz waveform relaxation algorithm is:



$$\begin{array}{rcll} \mathcal{L}u_i^n & = & f & \text{in } \Omega_i \times (0, T), \\ u_i^n(\cdot,\cdot,0) & = & u_0 & \text{in } \Omega_i, \\ u_i^n & = & u_j^{n-1} & \text{on } \Gamma_{ij} \times (0, T) \end{array}$$

The global iterate is $u^n := u_i^n$ in $\widetilde{\Omega}_i \times [0, T]$

Convergence Results for Diffusive Problems

$$\mathcal{L}u := \partial_t u + (\mathbf{a} \cdot \nabla)u - \nu\Delta u + bu = f, \quad \text{in } \Omega \times (0, T)$$

Theorem (Linear Convergence (Daoud, G 2003))

On arbitrary time intervals, the iterates u^k satisfy

$$||u^{n(m+2)} - u|| \leq (\gamma(m, L))^n \, ||u^0 - u||,$$

where $\gamma(m, L) < 1$, L measures the overlap, and m is related to the number of subdomains.

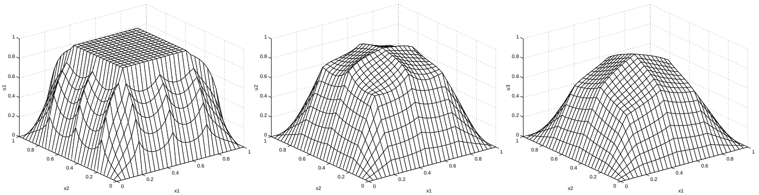
Theorem (Superlinear Convergence (Daoud, G 2003))

On bounded time intervals $t \in [0, T < \infty)$, the iterates satisfy

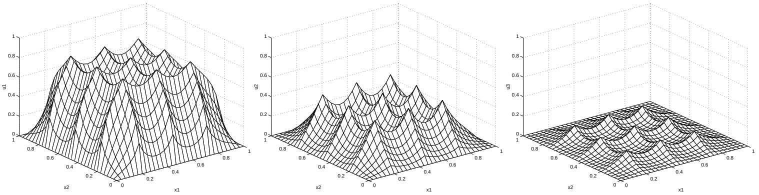
$$||u^n - u|| \leq (C(\nu, \mathbf{a}, L))^n erfc(\frac{nL}{2\sqrt{d\nu T}})||u^0 - u||.$$

Numerical Experiments

Error of 3 consecutive iterates at the end of the time interval:

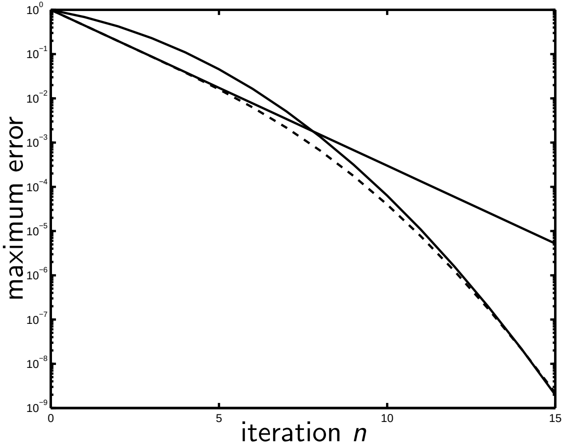


At $T = 5$, where the algorithm is in the linear convergence regime



At $T = 0.01$, algorithm in the superlinear convergence regime

Example of two Different Convergence Regimes



$\Longrightarrow$ Transition from linear to the superlinear convergence

Comparison with WR for ODEs

The superlinear convergence rate found for classical waveform relaxation algorithms is

$$\frac{(CT)^n}{n!} = \left(\frac{1}{\sqrt{2\pi}} + O(n^{-1})\right) e^{-n\ln n + (1+\ln(CT))n - \frac{1}{2}\ln n} \sim e^{-n\ln n}$$

The superlinear convergence rate for diffusive PDEs is

$$C_1^n \mathrm{erfc}\left(\frac{C_2 n}{\sqrt{T}}\right) = \left(\frac{\sqrt{T}}{C_2\sqrt{\pi}} + O(n^{-2})\right) e^{-\frac{C_2^2}{T}n^2 + \ln(C_1)n - \ln n} \sim e^{-n^2}$$

The improvement is due to the particular diffusion stemming from the heat kernel.

Convergence Result for the Wave Equation

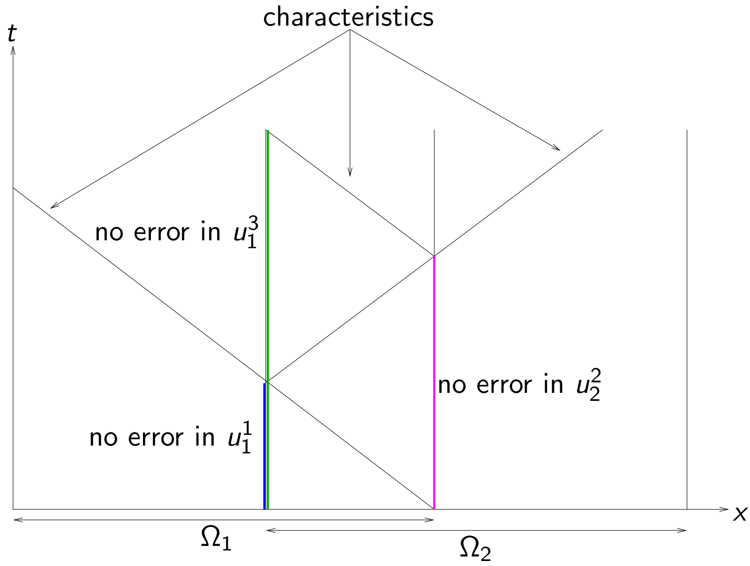
$$\begin{aligned}
\mathcal{L}u := \partial_{tt}u - c^2(x)\Delta u &= f, \quad \text{in } \Omega \times (0,T) \\
u(x,\cdot) &= u^0 \\
\partial_t u(x,\cdot) &= u_t^0 \\
u(x,t) &= g(x,t), \quad \text{on } \partial\Omega \times (0,T)
\end{aligned}$$

Theorem (Finite Step Convergence (G, Halpern 2005))

For given initial conditions $u^0 \in H^1(\Omega)$, $u_t^0 \in L^2(\Omega)$, forcing function $f \in L^2(0,T;L^2(\Omega))$, boundary condition $g \in L^2(0,T;H^{\frac{1}{2}}(\Gamma))$ and initial guess $u_0 \in L^2(0,T;H^1(\Omega))$, the classical overlapping Schwarz waveform relaxation algorithm for the wave equation has converged in $L^2(0,T;H^1(\Omega))$ as soon as the number of iterations n satisfies

$$n > \frac{T\bar{c}}{L}, \qquad \bar{c} := \sup_{x\in\Omega} c(x).$$

Graphical Convergence Proof



Convergence Speed for Waveform Relaxation

Milne (1953): "Actually this method of continuing the computation is highly inefficient and is not recommended"

Olavi Nevanlinna (1989): "Since the topic of this paper is to use Picard-Lindelöf iterations, I want to claim that the very large size of the systems solved today and the development of new machine architectures have made the approach competitive."

"In practice one is interested in knowing what subdivisions yield fast convergence for the iterations."

"The splitting into subsystems is assumed to be given. How to split in such a way that the coupling remain "weak" is an important question. The emphasis in this paper is in the superlinear effect - which allows one to iterate roughly speaking without exactly knowing how much is "weak"; if you do not see convergence even in short subintervals [...], then we can say that the couplings are not weak."

Optimized Schwarz Waveform Relaxation

Like in the case of optimized Schwarz methods:

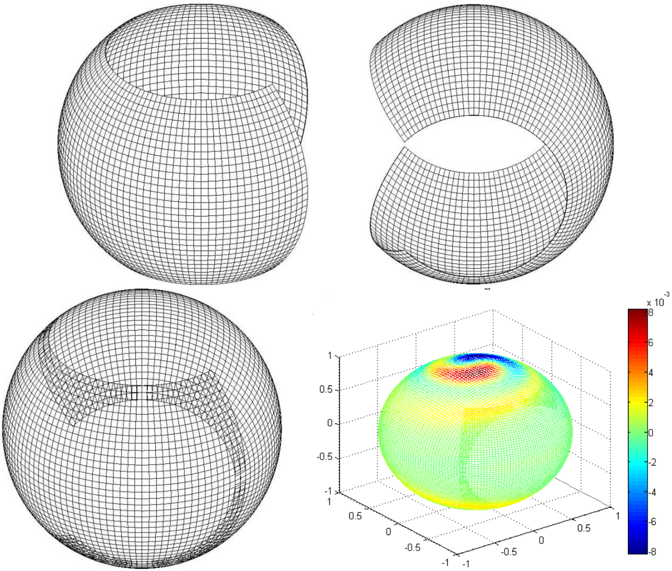
- Methods can be used with and without overlap
- Iteration cost the same as classical method

Mathematical results:

- Wave propagation problems (G, Halpern, Nataf 2003, G, Halpern 2004)
- Maxwell's equations (G, Courvoisier 2011)
- Advection reaction diffusion problems: (G, Halpern 2007, Bennequin, G, Halpern 2009)
- Circuit Simulation (Al-Khaleel, G, Ruehli, 2010/2008, G, Ruehli, 2004)

Global Weather Simulation: Cyclogenesis Test

On the Yin-Yang grid (with Côté and Qaddouri 2006)



The Parareal Algorithm

J-L. Lions, Y. Maday, G. Turinici (2001): A "Parareal" in Time Discretization of PDEs

The parareal algorithm for the model problem

$$u' = f(u)$$

is defined using two propagation operators:

1. $G(t_2, t_1, u_1)$ is a rough approximation to $u(t_2)$ with initial condition $u(t_1) = u_1$,
2. $F(t_2, t_1, u_1)$ is a more accurate approximation of the solution $u(t_2)$ with initial condition $u(t_1) = u_1$.

Starting with a coarse approximation U_n^0 at the time points $t_1, t_2, \ldots, t_N$, parareal performs for $k = 0, 1, \ldots$ the correction iteration

$$U_{n+1}^{k+1} = G(t_{n+1}, t_n, U_n^{k+1}) + F(t_{n+1}, t_n, U_n^k) - G(t_{n+1}, t_n, U_n^k).$$

Algorithmic Equivalences

Theorem (G, Vandevalle 2003)

The parareal algorithm

$$U_{n+1}^{k+1} = F(t_{n+1}, t_n, U_n^k) + G(t_{n+1}, t_n, U_n^{k+1}) - G(t_{n+1}, t_n, U_n^k),$$

is a multiple shooting method

$$U_{n+1}^{k+1} = u_n(t_{n+1}, U_n^k) + \frac{\partial u_n}{\partial U_n}(t_{n+1}, U_n^k)(U_n^{k+1} - U_n^k).$$

with an approximation of the Jacobian on a coarse time grid.

Theorem (G, Vandewalle, 2003)

The parareal algorithm is a time multigrid method with aggressive time coarsening.

A General Convergence Result for Parareal

For the non-linear IVP $u' = f(u), \quad u(t_0) = u_0$.

Theorem (G, Hairer 2005)

Let $F(t_{n+1}, t_n, U_n^k)$ denote the exact solution at t_{n+1} and $G(t_{n+1}, t_n, U_n^k)$ be a one step method with local truncation error bounded by $C_1 \Delta T^{p+1}$. If

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

then

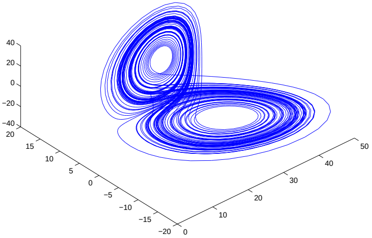
$$\max_{1\leq n\leq N} |u(t_n) - U_n^k| \leq \frac{C_1 \Delta T^{k(p+1)}}{k!}(1 + C_2\Delta T)^{N-1-k}\prod_{j=1}^{k}(N-j) \max_{1\leq n\leq N}|u(t_n) - U_n^0|$$

$$\leq \frac{(C_1 T)^k}{k!} e^{C_2(T-(k+1)\Delta T)} \Delta T^{pk} \max_{1\leq n\leq N} |u(t_n) - U_n^0|.$$

Superlinear Convergence estimate like for Waveform Relaxation

Results for the Lorenz Equations

$$\begin{aligned}\dot{x} &= -\sigma x + \sigma y\\ \dot{y} &= -xz + rx - y\\ \dot{z} &= xy - bz\end{aligned}$$



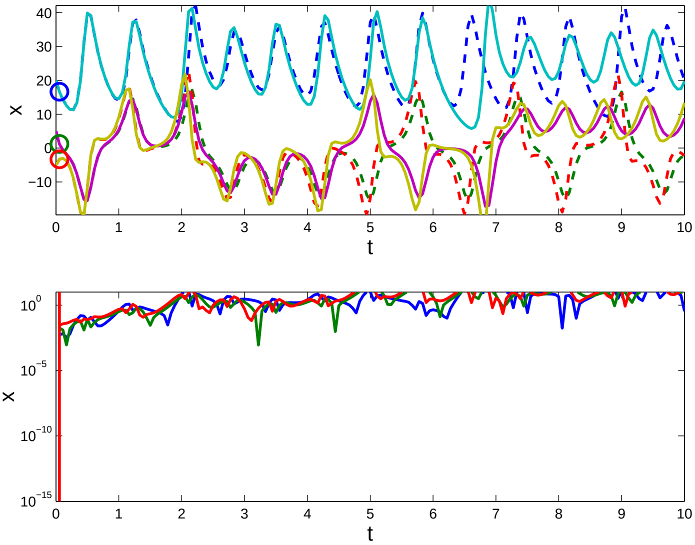
Parameters: $\sigma = 10$, $r = 28$ and $b = \frac{8}{3} \Longrightarrow$ chaotic regime.

Initial conditions: $(x, y, z)(0) = (20, 5, -5)$

Simulation time: $t \in [0, T = 10]$

Discretization: Fourth order Runge Kutta, $\Delta T = \frac{T}{180}$,

$\Delta t = \frac{T}{1800}$.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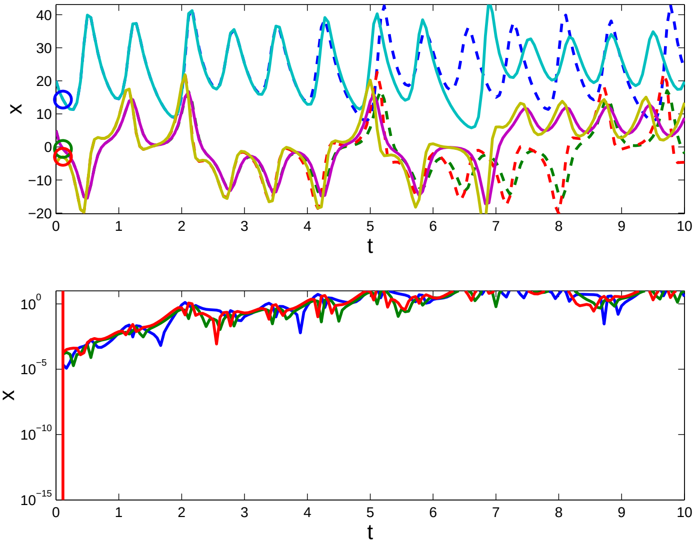
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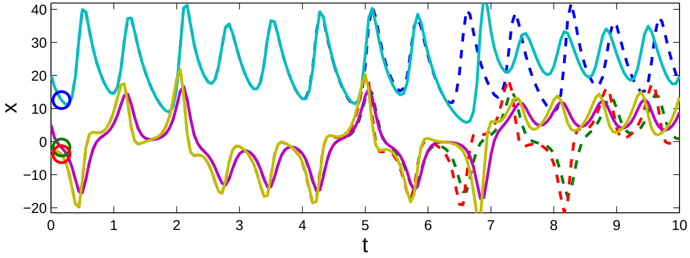

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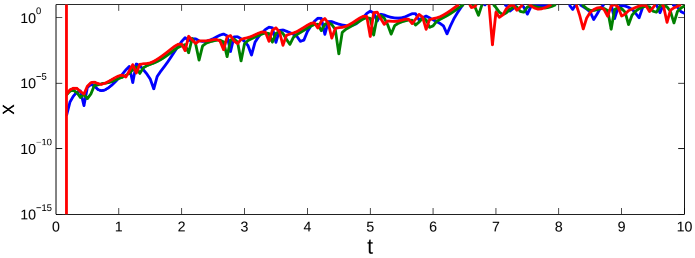

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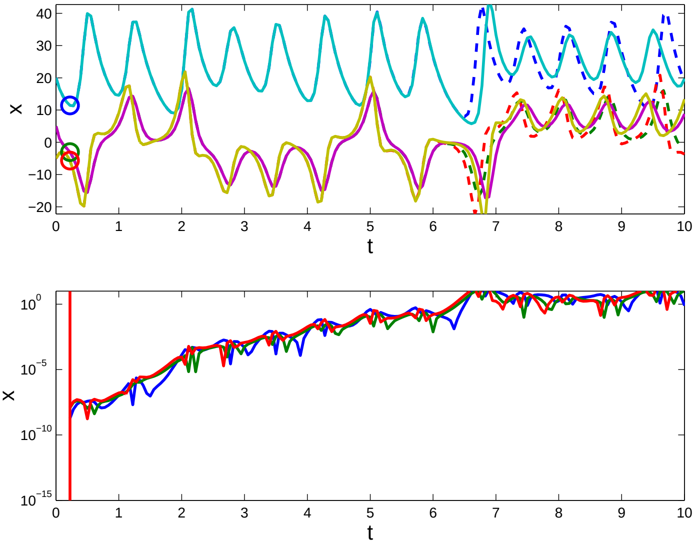
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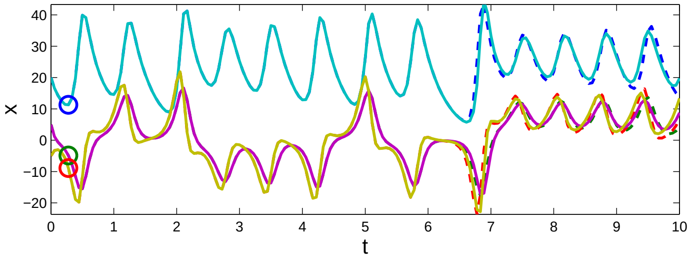

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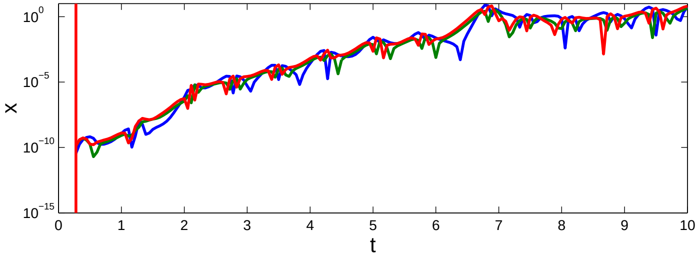

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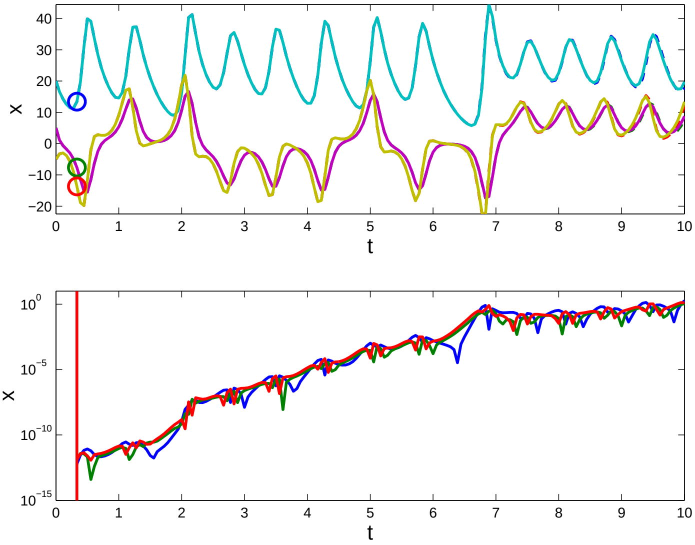
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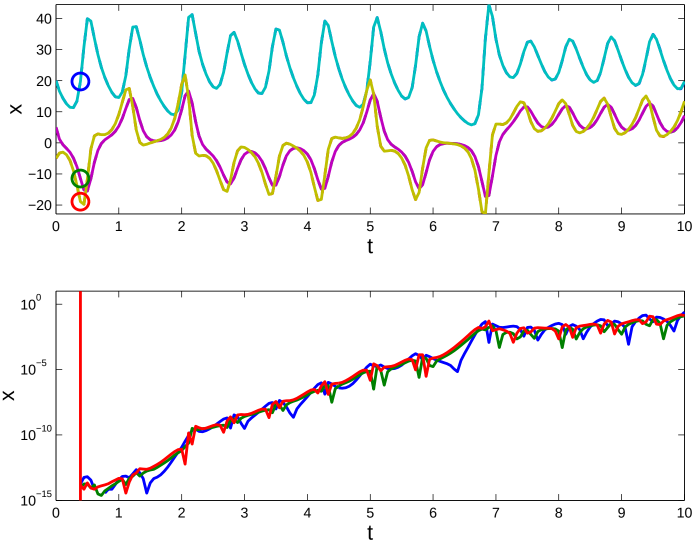

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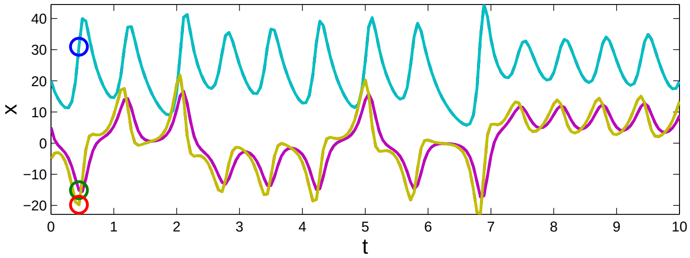

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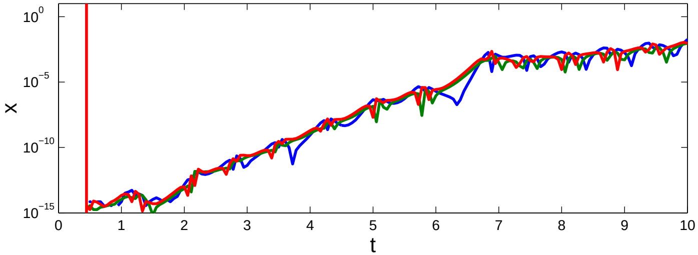

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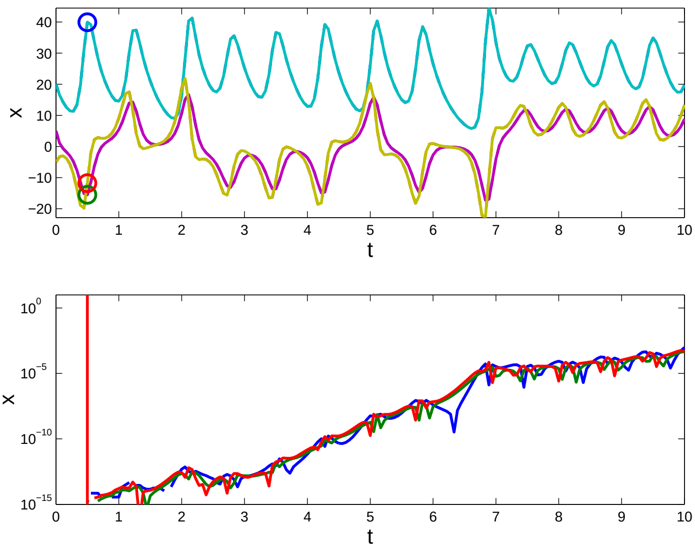
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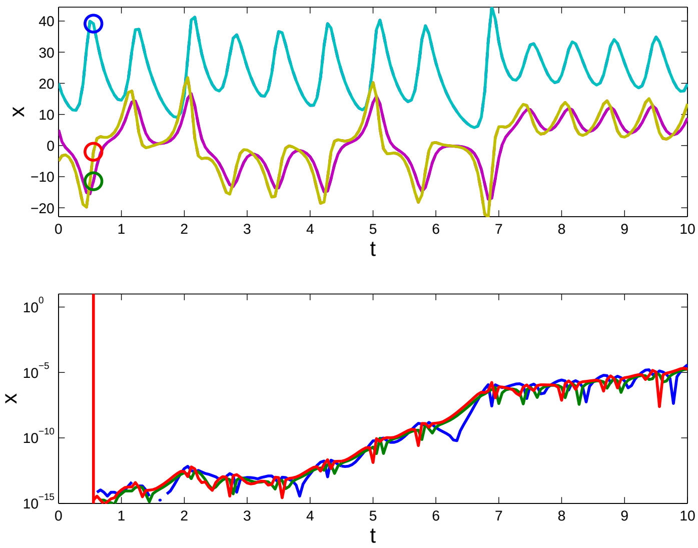
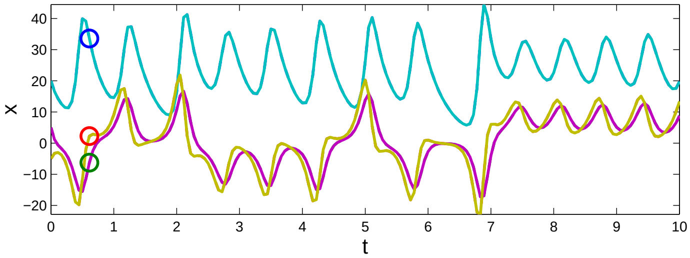
10^{-5}
10^{-10}
10^{-15}
x
0 1 2 3 4 5 6 7 8 9 10
t



x
t
x
t



40
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x
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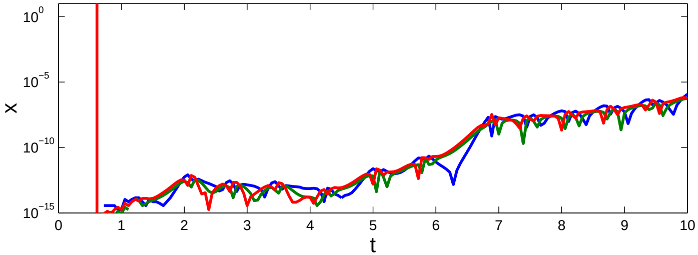

10^{0}
10^{-5}
10^{-10}
10^{-15}
x
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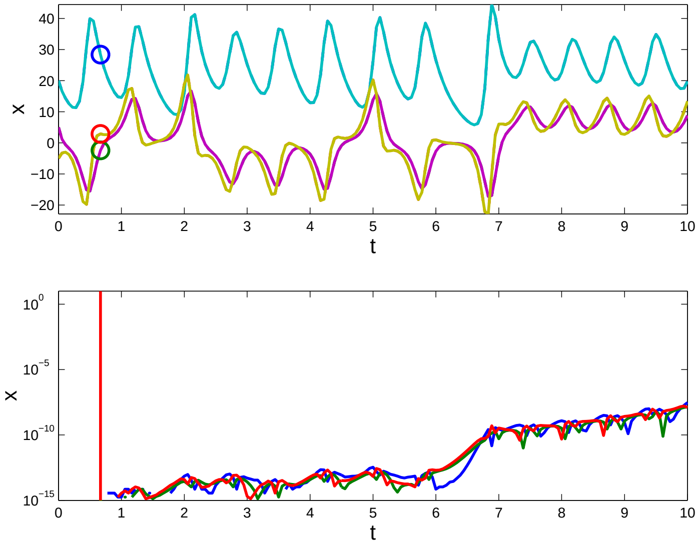
40
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t
10^0
10^−5
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10^−15
x
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7
8
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10
t

Parareal Schwarz Waveform Relaxation

Given an initial condition u_0 and boundary conditions g^- and g^+, we define $F_{in}(u_0, g^-, g^+)$ and $G_{in}(u_0, g^-, g^+)$ to be fine and coarse approximations of the solution at $t = t_{n+1}$ of

$$\begin{array}{rcll} \partial_t u &=& \partial_{xx} u, & x \in (x_i^-, x_i^+),\ t \in (t_n, t_{n+1}) \\ u(x, t_n) &=& u_0 & x \in (x_i^-, x_i^+) \\ \mathcal{B}_i^- u(x_i^-, t) &=& g^- & t \in (t_n, t_{n+1}) \\ \mathcal{B}_i^+ u(x_i^+, t) &=& g^+ & t \in (t_n, t_{n+1}) \end{array}$$

A Parareal Schwarz Waveform Relaxation Algorithm: Given initial conditions $u_{0,in}^k(x)$ and boundary conditions $\mathcal{B}_i^- u_{i-1,n}^k(t)$ and $\mathcal{B}_i^+ u_{i+1,n}^k(t)$, we compute

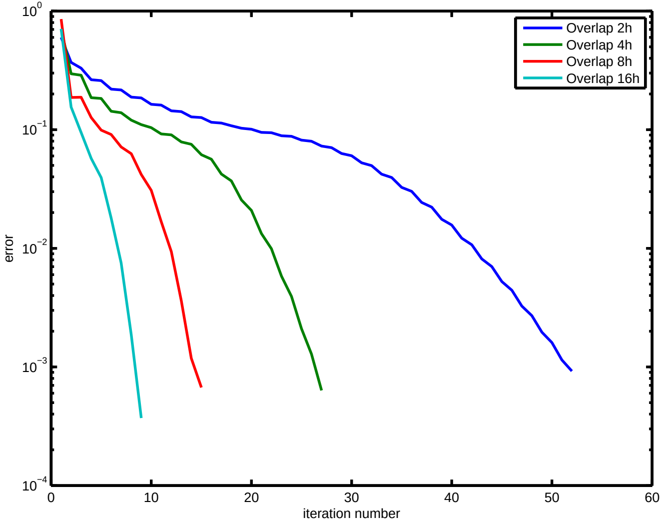
1. All $u_{in}^{k+1} := F_{in}(u_{0,in}^k, \mathcal{B}_i^- u_{i-1,n}^k, \mathcal{B}_i^+ u_{i+1,n}^k)$ in parallel
2. Compute new initial conditions using

$$u_{0,i,n+1}^{k+1} = F_{in}(u_{0,in}^k, \mathcal{B}_i^- u_{i-1,n}^k, \mathcal{B}_i^+ u_{i+1,n}^k)$$

$$+ G_{in}(u_{0,in}^{k+1}, \mathcal{B}_i^- u_{i-1,n}^{k+1}, \mathcal{B}_i^+ u_{i+1,n}^{k+1}) - G_{in}(u_{0,in}^k, \mathcal{B}_i^- u_{i-1,n}^k, \mathcal{B}_i^+ u_{i+1,n}^k)$$

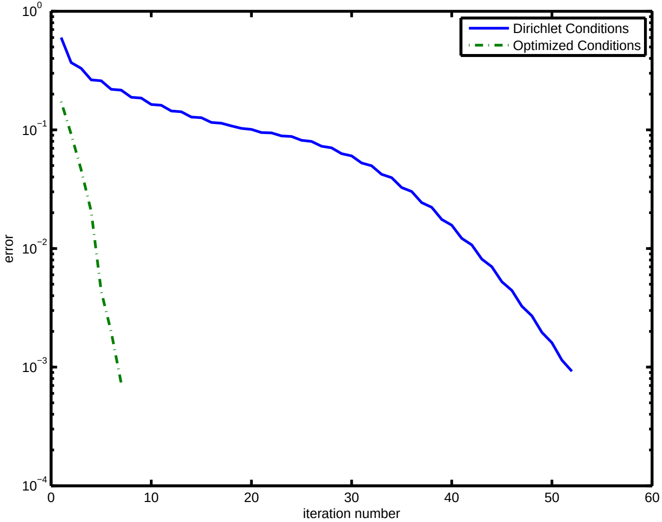
Dependence on the Overlap

$\Omega = (0, 6),\ T = 3\},\ \Delta x = \frac{1}{10},\ \Delta t = \frac{3}{100},$
$2\Delta x, 4\Delta x, 8\Delta x, 16\Delta x$ overlap, decomposition into 6 spatial subdomains, and 10 time subdomains



An Optimized Variant

$\Omega = (0, 6)$, $T = 3\}$, $\Delta x = \frac{1}{10}$, $\Delta t = \frac{3}{100}$, $2\Delta x$ overlap, decomposition into 6 spatial subdomains, and 10 time subdomains



Conclusions

- Schwarz Methods:
  - need overlap, except for optimized ones
  - easy to program and use, also algebraically
- Schur complement methods:
  - Primal and dual variants (Neumann-Neumann, FETI)
  - Have natural coarse grids
  - Need additional preconditioner
  - Dirichlet-Neumann and Neumann Dirichlet Methods are very much related to Schur complement methods
- Space-Time methods
  - Small scale parallel methods
  - Waveform Relaxation methods
  - Multiple Shooting/Parareal algorithm
  - Combinations

Reference: Méthodes de décomposition de domaines, G. and Halpern, *Encyclopédie des Techniques de l'Ingénieur*, to appear 2012.