A Schwarz Waveform Relaxation Method for Advection–Diffusion–Reaction Problems with Discontinuous Coefficients and Non-matching Grids

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Séminaire d'Analyse Numérique,
Université Paris Sud, 20 octobre 2005

Outline

1. Motivations and problem setting
2. Domain decomposition
   - First iterative algorithm
   - Improved transmission conditions
3. Some theory
   - Subdomain problem
   - Convergence of the iterative allgorithm
4. Numerical method and results
   - Description of the numerical scheme
   - Examples

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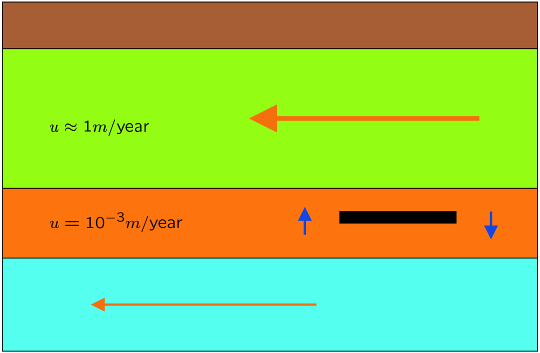
Outline

Nuclear Waste Deep Storage

Widely varying coefficients ($1 - 10^{-6}$), very long simulation times (10^6 years).
Example : COUPLEX (Comp. Geosc., 2004)



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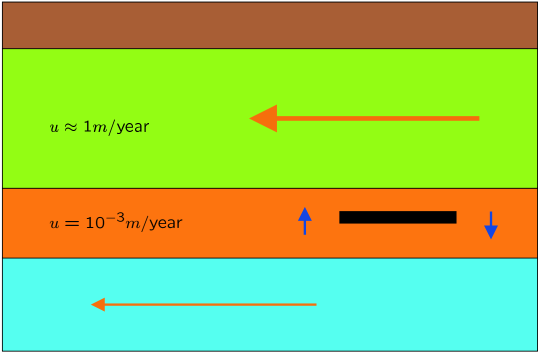

Method with different time steps in each layer ?

Mathematical Model

1D convection–diffusion–reaction equation, discontinuous coefficients

$$\begin{cases} \dfrac{\partial u}{\partial t} - \dfrac{\partial}{\partial x}\left(D\dfrac{\partial u}{\partial x} - au\right) + bu = f, \text{ on } \mathbf{R} \times [0, T] \\ u(x, 0) = u_0(x), \ x \in \mathbf{R} \end{cases}$$

- D Molecular diffusion
- a Darcy velocity
- b Radioactive decay

$$(D,\ a) = \begin{cases} (D^-,\ a^-) & x < 0 \\ (D^+,\ a^+) & x > 0 \end{cases}$$

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D Molecular diffusion

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$$(D, \; a) = \begin{cases} (D^-, \; a^-) & x < 0 \\ (D^+, \; a^+) & x > 0 \end{cases}$$

Weak solution $u \in L^\infty(0, T; L^2(\mathbf{R})) \bigcap L^2(0, T; H^1(\mathbf{R}))$ via standard variational theory

Notation: $u^- = u_{|\mathbf{R}^-}, \; u^+ = u_{|\mathbf{R}^+}$.

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Outline

Equivalent Transmission Problem

Subdomain problems

$$\frac{\partial u^-}{\partial t} - \frac{\partial}{\partial x}\left(D^- \frac{\partial u^-}{\partial x} - a^- u^-\right) + b u^- = f, \quad \text{on } \mathbf{R}^- \times [0, T]$$
$$u^-(x, 0) = u_0(x),\ x \in \mathbf{R}^-$$

$$\frac{\partial u^+}{\partial t} - \frac{\partial}{\partial x}\left(D^+ \frac{\partial u^+}{\partial x} + a^+ u^+\right) + b u^+ = f, \quad \text{on } \mathbf{R}^+ \times [0, T]$$
$$u^+(x, 0) = u_0(x),\ x \in \mathbf{R}^+$$

Equivalent Transmission Problem

Subdomain problems

$$\frac{\partial u^-}{\partial t} - \frac{\partial}{\partial x}\left(D^-\frac{\partial u^-}{\partial x} - a^- u^-\right) + bu^- = f, \quad \text{on } \mathbf{R}^- \times [0,T]$$
$$u^-(x,0) = u_0(x),\ x \in \mathbf{R}^-$$

$$\frac{\partial u^+}{\partial t} - \frac{\partial}{\partial x}\left(D^+\frac{\partial u^+}{\partial x} + a^+ u^+\right) + bu^+ = f, \quad \text{on } \mathbf{R}^+ \times [0,T]$$
$$u^+(x,0) = u_0(x),\ x \in \mathbf{R}^+$$

Transmission conditions

$$u^+(0,t) = u^-(0,t)$$
$$\left(a^+ - D^+\frac{\partial}{\partial x}\right)u^+(0,t) = \left(a^- - D^-\frac{\partial}{\partial x}\right)u^-(0,t)$$

An iterative algorithm

Algorithm with Dirichlet TC

$$\frac{\partial u_{k+1}^-}{\partial t} - \frac{\partial}{\partial x}\left(D^-\frac{\partial u_{k+1}^-}{\partial x} - a^- u_{k+1}^-\right) + b u_{k+1}^- = f, \quad \text{on } \mathbf{R}^- \times [0,T]$$

$$u_{k+1}^-(0,t) = u_k^+(0,t), \quad t \in [0,T]$$

An iterative algorithm

Algorithm with Dirichlet TC

$$\frac{\partial u_{k+1}^-}{\partial t} - \frac{\partial}{\partial x}\left(D^- \frac{\partial u_{k+1}^-}{\partial x} - a^- u_{k+1}^-\right) + b u_{k+1}^- = f, \quad \text{on } \mathbf{R}^- \times [0,T]$$

$$u_{k+1}^-(0,t) = u_k^+(0,t), \quad t \in [0,T]$$

$$\frac{\partial u_{k+1}^+}{\partial t} - \frac{\partial}{\partial x}\left(D^+ \frac{\partial u_{k+1}^+}{\partial x} + a^+ u_{k+1}^+\right) + b u_{k+1}^+ = f, \quad \text{on } \mathbf{R}^+ \times [0,T]$$

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$$u_{k+1}^+(0, t) = u_k^-(0, t), \quad t \in [0, T]$$

Dirichlet TCs: Slow convergence
Acceleration possible by using better transmission conditions

New transmission conditions

$$\left(a^- - D^- \frac{\partial}{\partial x} - \Lambda^-\right) u^-(0,t) = \left(a^+ - D^+ \frac{\partial}{\partial x} - \Lambda^-\right) u^+(0,t)$$
$$\left(a^+ - D^+ \frac{\partial}{\partial x} + \Lambda^+\right) u^+(0,t) = \left(a^- - D^- \frac{\partial}{\partial x} + \Lambda^+\right) u^-(0,t).$$

New transmission conditions

$$\left(a^- - D^- \frac{\partial}{\partial x} - \Lambda^-\right) u^-(0,t) = \left(a^+ - D^+ \frac{\partial}{\partial x} - \Lambda^-\right) u^+(0,t)$$
$$\left(a^+ - D^+ \frac{\partial}{\partial x} + \Lambda^+\right) u^+(0,t) = \left(a^- - D^- \frac{\partial}{\partial x} + \Lambda^+\right) u^-(0,t).$$

$\Lambda^{\pm}$ (pseudo–differential) operators in time, $\lambda^{\pm}$ symbol of $\Lambda^{\pm}$ ($\hat{g}$ Fourier transform of g)

$$\forall g \in L^2(\mathbf{R}),\ \widehat{\Lambda^{\pm} g}(\omega) = \lambda^{\pm}(\omega)\hat{g}(\omega)$$

New transmission conditions

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$\Lambda^\pm$ (pseudo–differential) operators in time, $\lambda^\pm$ symbol of $\Lambda^\pm$ ($\widehat{g}$ Fourier transform of g)

$$\forall g \in L^2(\mathbf{R}),\ \widehat{\Lambda^\pm g}(\omega) = \lambda^\pm(\omega)\widehat{g}(\omega)$$

Still equivalent to original problem (if $\Lambda^+ \neq \Lambda^-$)

New iterative algorithm

Left subdomain

$$\frac{\partial u^-_{k+1}}{\partial t} - \frac{\partial}{\partial x}\left(D^- \frac{\partial u^-_{k+1}}{\partial x} - a^- u^-_{k+1}\right) + b u^-_{k+1} = f, \quad \text{on } \mathbf{R}^- \times [0,T]$$

$$u^-(x,0) = u_0(x),\ x \in \mathbf{R}^-$$

$$\left(a^- - D^- \frac{\partial}{\partial x} - \Lambda^-\right) u^-_{k+1}(0,t) = \left(a^+ - D^+ \frac{\partial}{\partial x} - \Lambda^-\right) u^+_k(0,t)$$

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New iterative algorithm

Left subdomain

$$\frac{\partial u_{k+1}^-}{\partial t} - \frac{\partial}{\partial x}\left(D^- \frac{\partial u_{k+1}^-}{\partial x} - a^- u_{k+1}^-\right) + b u_{k+1}^- = f, \quad \text{on } \mathbf{R}^- \times [0, T]$$

$$u^-(x, 0) = u_0(x), \ x \in \mathbf{R}^-$$

$$\left(a^- - D^- \frac{\partial}{\partial x} - \Lambda^-\right) u_{k+1}^-(0, t) = \left(a^+ - D^+ \frac{\partial}{\partial x} - \Lambda^-\right) u_k^+(0, t)$$

Right subdomain

$$\frac{\partial u_{k+1}^+}{\partial t} - \frac{\partial}{\partial x}\left(D^+ \frac{\partial u_{k+1}^+}{\partial x} + a^+ u_{k+1}^+\right) + b u_{k+1}^+ = f, \quad \text{on } \mathbf{R}^+ \times [0, T]$$

$$u^+(x, 0) = u_0(x), \ x \in \mathbf{R}^+$$

$$\left(a^+ - D^+ \frac{\partial}{\partial x} + \Lambda^+\right) u_{k+1}^+(0, t) = \left(a^- - D^- \frac{\partial}{\partial x} + \Lambda^+\right) u_k^-(0, t)$$

Properties of iterative algorithm

- Use outgoing BC on each subdomain
- If convergence, limit is solution to original problem

Equation for error $e_k^{\pm} = u_k^{\pm} - u^{\pm}$

$$\frac{\partial e_{k+1}^{\pm}}{\partial t} - \frac{\partial}{\partial x}\left(D^{\pm}\frac{\partial e_{k+1}^{\pm}}{\partial x} - a^{\pm}e_{k+1}^{\pm}\right) + be_{k+1}^{-} = 0, \quad \text{on } \mathbf{R}^{\pm} \times [0,T]$$

$$e^{\pm}(x,0) = 0, \; x \in \mathbf{R}^{\pm}$$

$$\left(a^{-} - D^{-}\frac{\partial}{\partial x} - \Lambda^{-}\right)e_{k+1}^{-}(0,t) = \left(a^{+} - D^{+}\frac{\partial}{\partial x} - \Lambda^{-}\right)e_{k}^{+}(0,t)$$

$$\left(a^{+} - D^{+}\frac{\partial}{\partial x} + \Lambda^{+}\right)e_{k+1}^{+}(0,t) = \left(a^{-} - D^{-}\frac{\partial}{\partial x} + \Lambda^{+}\right)e_{k}^{-}(0,t)$$

Optimal transmission conditions

Equation for error, Fourier transform in time:

$$i\omega\widehat{e}^{\pm} - D^{\pm}\frac{d^2\widehat{e}^{\pm}}{dx^2} + a^{\pm}\frac{d\widehat{e}^{\pm}}{dx} + b\widehat{e}^{\pm} = 0,\ x \in \mathbf{R}^{\pm}$$

Characteristic equation

$$Dr^2 - ar - (b + i\omega) = 0$$

$r^+(a, D, \omega)$ (resp. $r^-(a, D, \omega)$) is root with positive (resp. negative) real part

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Characteristic equation

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$r^+(a, D, \omega)$ (resp. $r^-(a, D, \omega)$) is root with positive (resp. negative) real part

$$\begin{cases} \hat{e}_k^- = \alpha_k^-(\omega)e^{r^+(a^-, D^-, \omega)x}, & x < 0 \\ \hat{e}_k^+ = \alpha_k^+(\omega)e^{r^-(a^+, D^+, \omega)x}, & x > 0 \end{cases}$$

Convergence rate

Transmission conditions give

$$\alpha_k^+(a^+ - D^+ r^-(a^+, D^+, \omega) + \lambda^+) = \alpha_{k-1}^-(a^- - D^- r^+(a^-, D^-, \omega) + \lambda^+)$$
$$\alpha_k^-(a^- - D^- r^+(a^-, D^-, \omega) - \lambda^-) = \alpha_{k-1}^+(a^+ - D^+ r^-(a^+, D^+, \omega) - \lambda^-).$$

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Convergence rate

$$\rho(\omega) = \left(\frac{a^- - D^- r^+(a^-, D^-, \omega) + \lambda^+}{a^+ - D^+ r^-(a^+, D^+, \omega) + \lambda^+}\right)\left(\frac{a^+ - D^+ r^-(a^+, D^+, \omega) - \lambda^-}{a^- - D^- r^+(a^-, D^-, \omega) - \lambda^-}\right)$$

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Convergence rate

Transmission conditions give

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Convergence rate

$$\rho(\omega) = \left(\frac{a^- - D^-r^+(a^-,D^-,\omega)+\lambda^+}{a^+ - D^+r^-(a^+,D^+,\omega)+\lambda^+}\right)\left(\frac{a^+ - D^+r^-(a^+,D^+,\omega)-\lambda^-}{a^- - D^-r^+(a^-,D^-,\omega)-\lambda^-}\right)$$

Choose λ^+, λ^- to minimize convergence rate.

Optimal and approximate transmission conditions

Optimal choice

For

$$\lambda^-(\omega) = \quad a^+ - D^+ r^-(a^+, D^+, \omega) = \frac{\sqrt{\Delta(a^+, D^+)} + a^+}{2}$$

$$\lambda^+(\omega) = -a^- + D^- r^+(a^-, D^-, \omega) = \frac{\sqrt{\Delta(a^-, D^-)} - a^-}{2}$$

the algorithm converges in 2 iterations.

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Operators non–local in time : need approximations
Approximate $\sqrt{\Delta(a, D)} = \sqrt{a^2 + 4D(b + i\omega)}$ by local operators.

Optimal and approximate transmission conditions

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Operators non–local in time : need approximations
Approximate $\sqrt{\Delta(a, D)} = \sqrt{a^2 + 4D(b + i\omega)}$ by local operators.

- Robin TC: Take $\sqrt{\Delta^\pm} \approx p^\pm$ (constant)
- First order TC: Take $\sqrt{\Delta^\pm} \approx p^\pm + iq^\pm\omega$ (cf Absorbing Boundary Conditions)

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Robin transmission conditions

Gander, Halpern, Japhet, Martin, Nataf.

$$\left(D^-\frac{\partial}{\partial x} - a^- + \lambda^+\right)u_{k+1}^-(0,t) = \left(D^+\frac{\partial}{\partial x} - a^+ + \lambda^+\right)u_k^+(0,t),$$
$$\left(D^+\frac{\partial}{\partial x} - a^+ - \lambda^-\right)u_{k+1}^+(0,t) = \left(D^-\frac{\partial}{\partial x} - a^- - \lambda^-\right)u_k^-(0,t)$$

$$\lambda^- = \frac{p^+ + a^+}{2}, \quad \lambda^+ = \frac{p^- - a^-}{2}$$

Robin transmission conditions

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$$\lambda^- = \frac{p^+ + a^+}{2}, \quad \lambda^+ = \frac{p^- - a^-}{2}$$

- Low frequency approximation : $p^\pm = \sqrt{a^{\mp 2} + 4 b^\mp D^\mp}$
- Optimized coefficients : take $p^\pm$ to minimize convergence rate

Iterative algorithm with Robin transmission conditions

Iterative algorithm: given $g_0^{\pm}$ on $[0, T]$

$$\frac{\partial u_{k+1}^-}{\partial t} - \frac{\partial}{\partial x}\left(D^- \frac{\partial u_{k+1}^-}{\partial x} - a^- u_{k+1}^-\right) + b u_{k+1}^- = f, \quad \text{on } \mathbf{R}^- \times [0, T]$$

$$\left(a^- - D^- \frac{\partial}{\partial x} - \lambda^-\right) u_{k+1}^-(0, t) = g_k^+(t)$$

$$\frac{\partial u_{k+1}^+}{\partial t} + \frac{\partial}{\partial x}\left(D^+ \frac{\partial u_{k+1}^+}{\partial x} + a^+ u_{k+1}^+\right) + b u_{k+1}^+ = f, \quad \text{on } \mathbf{R}^+ \times [0, T]$$

$$\left(a^+ - D^+ \frac{\partial}{\partial x} + \lambda^+\right) u_{k+1}^+(0, t) = g_k^-(t)$$

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$$\left(a^+ - D^+ \frac{\partial}{\partial x} + \lambda^+\right) u_{k+1}^+(0, t) = g_k^-(t)$$

$$g_{k+1}^-(t) = \left(a^- - D^- \frac{\partial}{\partial x} + \lambda^+\right) u_{k+1}^-(0, t)$$

$$g_{k+1}^+(t) = \left(a^+ - D^+ \frac{\partial}{\partial x} - \lambda^-\right) u_{k+1}^+(0, t)$$

Outline

Interlude : Anisotropic Sobolev spaces

Needed for boundary regularity (Lions–Magenes, vol. 2)

Definition

$$H^{r,s}(\Omega \times (0,T)) = L^2(0,T;H^r(\Omega)) \bigcap H^s(0,T;L^2(\Omega))$$

For $u \in H^{2,1}(\Omega \times (0,T))$, ($j = 0,1,2$, $k = 0,1$):

$$\frac{\partial^j}{\partial x^j}\frac{\partial^k}{\partial t^k} u \in H^{2\nu,\nu}(\Omega \times (0,T)), \quad \nu = 1 - \left(j/2 + k\right)$$

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Theorem

Trace space For $u \in H^{2,1}(\Omega \times (0,T))$

$$u(x,0) \in H^1(\Omega), \quad \frac{\partial^j u}{\partial x^j}(0,t) \in H^{3/4-j/2}(0,T),\ j = 0,1$$

(+ compatibility conditions)

Well-posedness of subdomain problem

Subdomain problem

$$\frac{\partial v}{\partial t} - \frac{\partial}{\partial x}\left(D^- \frac{\partial v}{\partial x} - a^- v\right) + bv = f, \quad \text{on } \mathbf{R}^- \times [0, T]$$

$$v(x, 0) = u_0(x), \quad \text{on } \mathbf{R}^-$$

$$\left(D^- \frac{\partial}{\partial x} - a^- + \lambda^-\right) v(0, t) = g^-(t), \quad t \in [0, T]$$

Energy identity

$$\frac{1}{2}\frac{d}{dt}\|v\|^2 + D\left\|\frac{\partial v}{\partial x}\right\|^2 + b\|v\|^2 - \left(D^- \frac{\partial v}{\partial x} - \frac{a^-}{2} v\right)(0) v(0) = (f, v)$$

Existence and uniqueness

Theorem

If $u_0 \in H^1(\mathbf{R}^-)$, $f \in L^2((0,T), L^2(\mathbf{R}^-))$, $g^- \in H^{1/4}(0,T)$, $\lambda^- + a^- > 0$
The subdomain problem has a unique solution $u \in H^{2,1}((0,T) \times \mathbf{R}^-)$

Existence and uniqueness

Theorem

If $u_0 \in H^1(\mathbf{R}^-)$, $f \in L^2((0,T), L^2(\mathbf{R}^-))$, $g^- \in H^{1/4}(0,T)$, $\lambda^- + a^- > 0$
The subdomain problem has a unique solution $u \in H^{2,1}((0,T) \times \mathbf{R}^-)$

Proof (Bennequin, Gander, Halpern (04)).

1. Lifting, trace theorem : reduce to $u_0 = 0, g = 0$;
2. Standard estimates : $u \in L^\infty(0,T; L^2(\mathbf{R}^-)) \cap L^2(0,T; H^1(\mathbf{R}^-))$;
3. Non-standard estimates (multiply by $\frac{\partial^2 v}{\partial x^2}$) give more smoothness.

□

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Algorithm with Robin TC is well–defined

Smoothness needed for transmissions conditions

Theorem

Under same hypotheses as above, the algorithm is well defined : given $(g_0^-, g_0^-) \in H^{1/4}(0,T)^2$, *the algorithm generates* $(u_k^+, u_k^-) \in H^{2,1}(\mathbf{R}^- \times (0,T))$.

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Under same hypotheses as above, the algorithm is well defined : given $(g_0^-, g_0^-) \in H^{1/4}(0,T)^2$, *the algorithm generates* $(u_k^+, u_k^-) \in H^{2,1}(\mathbf{R}^- \times (0,T))$.

Proof.

By trace theorem, $t \to au(0,.) - D\dfrac{\partial u}{\partial x}(0,.) \in H^{1/4}(0,T)$

If initial guesses $(g_0^+, g_0^-) \in H^{1/4}(\mathbf{R}^-) \times H^{1/4}(\mathbf{R}^+)$, then still true for all iterates : (g_k^+, g_k^-), $k \geq 1$. □

Convergence of iterative algorithm

Theorem

- *Same assumptions as above*
- $\lambda^+ + \lambda^- \geq 0$, $\lambda^+ - \lambda^- + a^- > 0$, $-\lambda^+ + \lambda^- + a^+ > 0$

The sequence (u_k^+, u_k^-) *converges to* (u^+, u^-) *in* $L^\infty(0, T; L^2(\mathbf{R}^-)) \cap L^2(0, T; H^1(\mathbf{R}^-)) \times L^\infty(0, T; L^2(\mathbf{R}^+)) \cap L^2(0, T; H^1(\mathbf{R}^+))$.

Proof.

By energy estimates (Despres (95), Lions (87), Bennequin, Gander, Halpern (04)).

Define $\mathcal{E}_k^\pm = \frac{1}{2}\frac{d}{dt}\left\|e_k^\pm\right\|^2 + D^+\left\|\frac{\partial e_k^\pm}{\partial x}\right\|^2 + b\left\|e_k^\pm\right\|^2$

Also denote $B^\pm v = D^\pm \frac{\partial v}{\partial x} - a^\pm v$

□

Proof of convergence theorem (ctd).

Energy estimate with transmission conditions

$$\mathcal{E}_k^- + \frac{1}{2(\lambda^+ + \lambda^-)}\left(B^- e_k^- - \lambda^+ e_k^-\right)^2 + (\lambda^+ - \lambda^- + a^-)\left|e_k^-(0)\right|^2 = \frac{1}{2(\lambda^+ + \lambda^-)}(B^+ e_{k-1}^+ - \lambda^- e_{k-1}^+)^2$$

$$\mathcal{E}_k^+ + \frac{1}{2(\lambda^+ + \lambda^-)}\left(B^+ e_k^+ - \lambda^- e_k^+\right)^2 + (-\lambda^+ + \lambda^- + a^+)\left|e_k^+(0)\right|^2 = \frac{1}{2(\lambda^+ + \lambda^-)}(B^- e_{k-1}^- - \lambda^+ e_{k-1}^-)^2$$

Add over k : telescopic sum.

Proof of convergence theorem (ctd).

Energy estimate with transmission conditions

$$\mathcal{E}_k^- + \frac{1}{2(\lambda^+ + \lambda^-)}\left(B^- e_k^- - \lambda^+ e_k^-\right)^2 + (\lambda^+ - \lambda^- + a^-)\left|e_k^-(0)\right|^2 = \frac{1}{2(\lambda^+ + \lambda^-)}(B^+ e_{k-1}^+ - \lambda^- e_{k-1}^+)^2$$

$$\mathcal{E}_k^+ + \frac{1}{2(\lambda^+ + \lambda^-)}\left(B^+ e_k^+ - \lambda^- e_k^+\right)^2 + (-\lambda^+ + \lambda^- + a^+)\left|e_k^+(0)\right|^2 = \frac{1}{2(\lambda^+ + \lambda^-)}(B^- e_{k-1}^- - \lambda^+ e_{k-1}^-)^2$$

Add over k : telescopic sum.

Proof of convergence theorem (ctd).

Energy estimate with transmission conditions

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Optimization of convergence rate

Choose $\lambda^{\pm}$ to minimize $\max_{\omega \in [0,\omega_{\max}]} |\rho(\omega)|$.
Numerical scheme : $\omega_{\max} = \pi / \Delta t$.

Optimization of convergence rate

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Numerical scheme : $\omega_{\max} = \pi/\Delta t$.
Investigate how convergence rate depends on time step
Assume $a^+, a^- > 0$, Δt "small".

Theorem (Asymptotic convergence rate)

If $p^+ = p^- = p$, then solution of the min-max problem is

$$p \approx \frac{\left(2^3\pi(D^+D^-)\left(a^+ - a^- + \sqrt{(a^+)^2 + 4D^+b} + \sqrt{(a^-)^2 + 4D^-b}\right)^2\right)^{\frac{1}{4}}}{\left(\sqrt{D^+} + \sqrt{D^-}\right)^{1/2}} \Delta t^{-\frac{1}{4}},$$

Asymptotic bound on convergence rate

$$|\rho| \leq 1 - \left(\frac{2^5\left(\sqrt{D^+} + \sqrt{D^-}\right)^2\left(a^+ - a^- + \sqrt{(a^+)^2 + 4D^+b} + \sqrt{(a^-)^2 + 4D^-b}\right)^2}{D^+D^-\pi}\right)^{\frac{1}{4}} \Delta t^{\frac{1}{4}}.$$

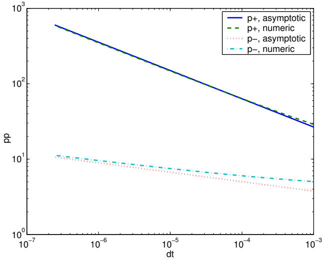
Theorem

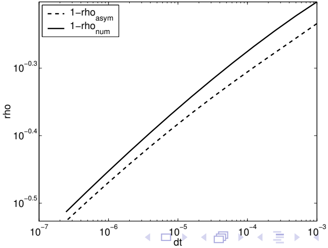
If $D^+ = D^- = D$, then the solution of the min-max problem is

$$
\begin{aligned}
p^+ &\approx \left(2^9\pi^3 D^3\left(a^+ - a^- + \sqrt{(a^+)^2 + 4Db} + \sqrt{(a^-)^2 + 4Db}\right)^2\right)^{\frac{1}{8}} \Delta t^{-\frac{3}{8}},\\
p^- &\approx \left(2^{-5}\pi D\left(a^+ - a^- + \sqrt{(a^+)^2 + 4Db} + \sqrt{(a^-)^2 + 4Db}\right)^6\right)^{\frac{1}{8}} \Delta t^{-\frac{1}{8}},
\end{aligned}
$$

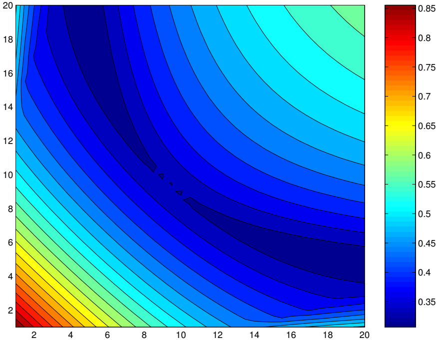
Asymptotic bound on the convergence rate

$$
|\rho| \leq 1 - \left(\frac{2^{13}\left(a^+ - a^- + \sqrt{(a^+)^2 + 4Db} + \sqrt{(a^-)^2 + 4Db}\right)^2}{D\pi}\right)^{\frac{1}{8}} \Delta t^{\frac{1}{8}}.
$$

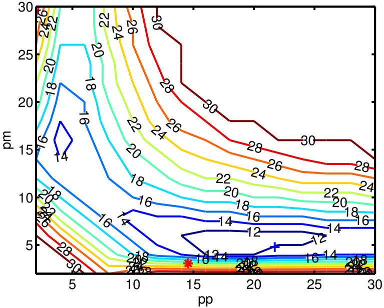




Theoretical and numerical convergence rate



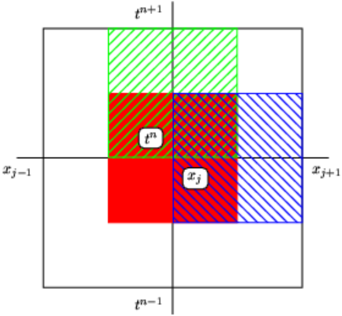
Theoretical convergence rate



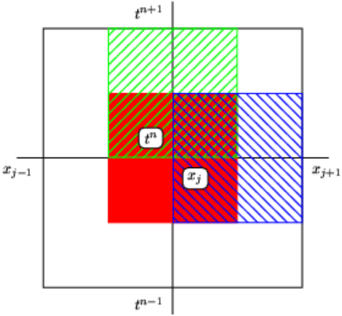
Experimental convergence rate
(blue cross: “optimal parameters”,
red cross: aymptotic parameters)

Outline

A Space–Time Finite Volume scheme



- Function constant on square;
- space and time derivatives defined by difference quotient on staggered grids, ;
- Implicit upwind scheme, finite difference in interior



- Function constant on square;
- space and time derivatives defined by difference quotient on staggered grids, ;
- Implicit upwind scheme, finite difference in interior

Green's formula : $I_L + I_R + I_T + I_B = \int_{\text{square}} f$ with

$$I_{\text{side}} = \int_{\text{side}} \left(-(D \frac{\partial u}{\partial x} - au) \right) \cdot \begin{pmatrix} n_t \\ n_x \end{pmatrix} ds$$

Interior scheme

3 points difference formula ($u_j^{n+1/2} = \dfrac{u_j^n + u_j^{n=1}}{2}$)

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} - D\frac{u_{j+1}^{n+1/2} - 2u_j^{n+1/2} + u_{j-1}^{n+1/2}}{\Delta x^2} + a\frac{u_{j+1}^{n+1/2} - u_{j-1}^{n+1/2}}{2\Delta x}$$
$$- \frac{\gamma \Delta x}{2} |a| \frac{u_{j+1}^{n+1/2} - 2u_j^{n+1/2} + u_{j-1}^{n+1/2}}{\Delta x^2} + bu_j^{n+1/2} = f_j^{n+1/2}$$

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γ controls upwinding ($\gamma = 0$: centered, $\gamma = 1$: upwind)
Implicit scheme, unconditionally stable, order 1 for $\gamma \neq 0$, order 2 for $\gamma = 0$

Fourier analysis

Look for solution $u_j^n = g(k)^n e^{ijk\Delta x}$

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$$g(k) = \frac{1 - \frac{b\Delta t}{2} - \Delta t\left(\frac{2D}{\Delta x^2} + \frac{\gamma\,|a|}{\Delta x}\right)\sin^2\frac{k\Delta x}{2} - ia\frac{\Delta t}{2\Delta x}\sin k\Delta x}{1 + \frac{b\Delta t}{2} - \Delta t\left(\frac{2D}{\Delta x^2} + \frac{\gamma\,|a|}{\Delta x}\right)\sin^2\frac{k\Delta x}{2} + ia\frac{\Delta t}{2\Delta x}\sin k\Delta x}$$

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Can show that

$$|g(k)|^2 = 1 - \frac{4\alpha}{(1+\alpha)^2 + \beta^2}.$$

with

$$\alpha = \frac{b\Delta t}{2} + \Delta t\left(\frac{2D}{\Delta x^2} + \frac{\gamma\,|a|}{\Delta x}\right)\sin^2\frac{k\Delta x}{2} \geq 0, \quad \beta = a\frac{\Delta t}{2\Delta x}\sin k\Delta x.$$

Interior scheme : examples

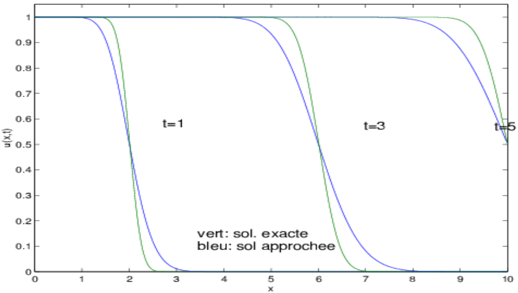
Solution on half-line, with Dirichlet left BC ($\xi = \sqrt{a^2 + 4bD}$)

$$u(x,t) = \frac{u_L}{2} \exp\left(\frac{ax}{2D}\right) \left\{ \exp\left(-\frac{x}{2D}\xi\right) \operatorname{erfc}\left(\frac{x - \sqrt{a^2+4bD}t}{2\sqrt{Dt}}\right) + \exp\left(\frac{x}{2D}\xi\right) \operatorname{erfc}\left(\frac{x + \sqrt{a^2+4bD}t}{2\sqrt{Dt}}\right) \right\},$$

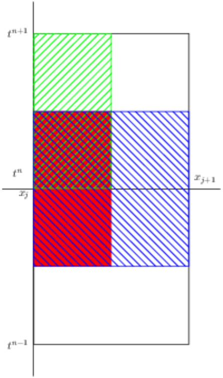
$D = 0.02$

$a = 2$

$b = 0$



Numerical transmission conditions

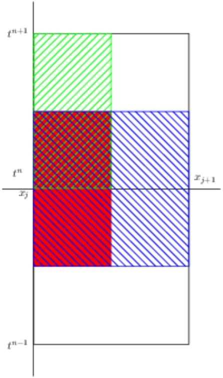


Integrate on $]0, x_{1/2}[\times]t^n, t^{n+1}[$, use TC to close system

On right subdomain ($\gamma = 1$: upwind scheme),

$$g^{+,n+1/2} = \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} g^+(t)\, dt$$

Numerical transmission conditions



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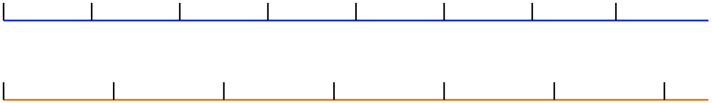
$$\boxed{\frac{\Delta x}{2}\frac{u_0^{+,n+1} - u_0^{+,n}}{\Delta t}} - D^+\frac{u_1^{+,n+1/2} - u_0^{+,n+1/2}}{\Delta x} + a^+ u_0^{+,n+1/2} + \boxed{\frac{\Delta x}{2} b u_0^{+,n+1/2}} + \lambda^+ u_0^{+,n+1/2} = g^{+,n+1/2}$$

Numerical transmission conditions (contd.)

$$g^{+,n+1/2} = \boxed{-\frac{\Delta x}{2}\frac{u_0^{-,n+1} - u_0^{-,n}}{\Delta t}} - D^- \frac{u_0^{-,n+1/2} - u_{-1}^{-,n+1/2}}{\Delta x}$$

$$+ a^- u_{-1}^{-,n+1/2} + \boxed{\frac{\Delta x}{2} b u_0^{-,n+1/2}} + \lambda^- u_0^{-,n+1/2}$$

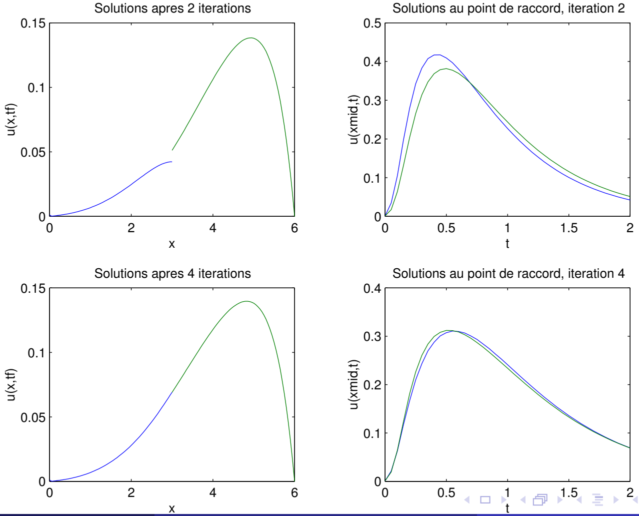
Consistent with interior scheme.
If different time steps, project g^+ on left grid (recompute integral on other grid)



Matlab code (M. Gander)

Homogeneous example

Homogeneous medium, with $a = 2$, $D = 1$, $b = 0.1$, $u_0(x) = e^{(-3(3/2-x)^2)}$, $0 < x < 6$. Interface at $x = 3$.



Heterogeneous example

Left subdomain $[0, 1]$

$D^- = 4\,10^{-2}$, $a^- = 4$,
$\Delta x^- = 10^{-2}$, $\Delta t^- = 4\,10^{-3}$

Right subdomain $[1, 1.8]$

$D^- = 12\,10^{-2}$, $a^- = 2$,
$\Delta x^- = 8\,10^{-2}$, $\Delta t^- = 10^{-2}$

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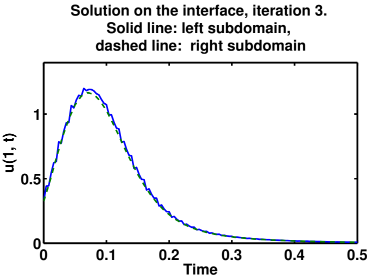
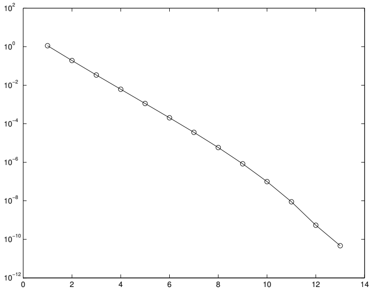


Solutions on the interface



Convergence history

INRIA

Heterogeneous example (ctd.)

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$D^- = 4\,10^{-2}$, $a^- = 4$,
$\Delta x^- = 10^{-2}$, $\Delta t^- = 10^{-3}$

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$D^- = 12\,10^{-2}$, $a^- = 2$,
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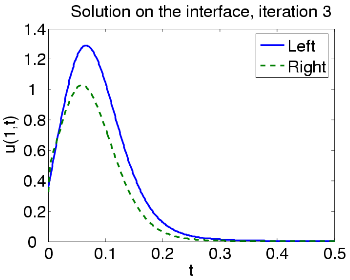
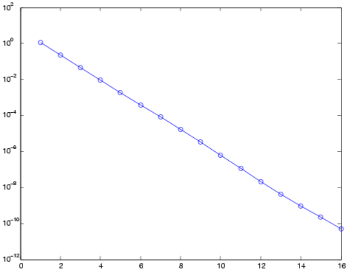


Solutions on the interface
Sol. after 2 iterations
Sol. at convergence



Convergence history

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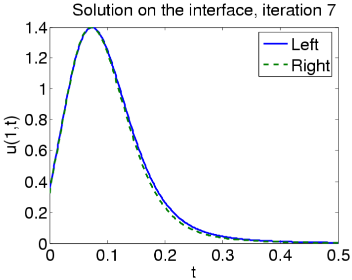

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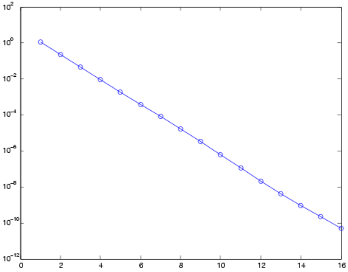

Convergence history

Conclusions – perspectives

Conclusions

- Method for CDR problems, discontinuous coefficients, different grids
- Optimized transmission conditions
- Satisfactory behavior on simple examples

Further work

- More challenging test cases
- More subdomains, 2D
- Substructuring