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

L. Halpern[1] M. Gander[2] M. Kern[3] H. Sickout–Mavoungou[3]

[1]Université Paris 13
France

[2]Université de Genève
Switzerland

[3]INRIA Rocquencourt
France

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Outline

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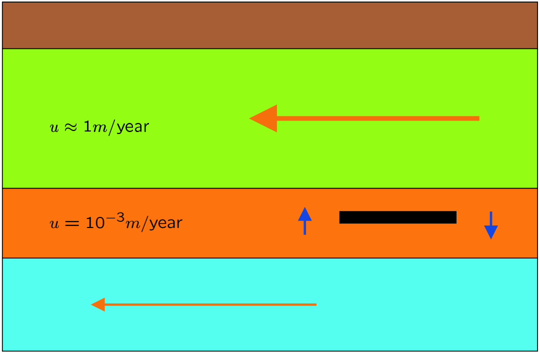
Nuclear Waste Deep Storage

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



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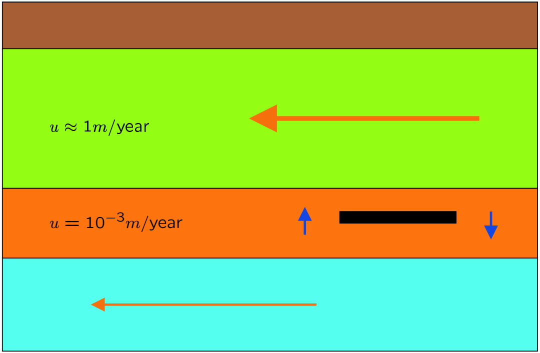

Method with different time steps in each layer ?

Mathematical Model

1D convection–diffusion–reaction equation, discontinuous coefficients

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

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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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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

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Equivalent Transmission Problem

Subdomain problems

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

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

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

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Transmission conditions

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

Iterative algorithm with Robin transmission conditions

Dirichlet TCs lead to slow algorithm. Acceleration possible by using other transmission conditions (Gander, Halpern, Japhet, Martin, Nataf).

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

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

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

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

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

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

Properties of iterative algorithm

- Subdomain problem well posed ($\lambda^{\pm} > 0$)
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Convergence rate

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

$r^{\pm}(a, D, \omega)$ root with positive (resp. negative) real part of characteristic equation : $Dr^2 - ar + (b + i\omega) = 0$

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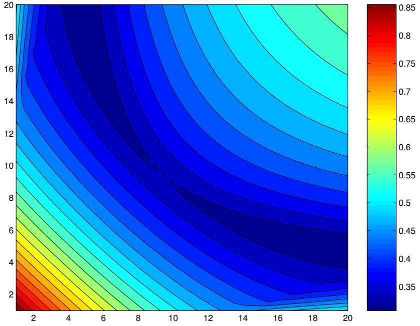
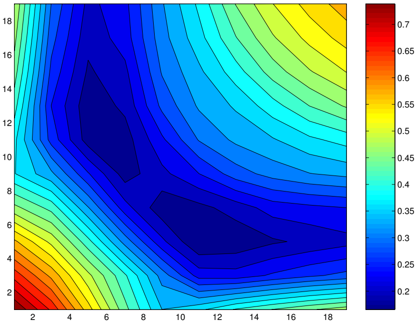
Convergence proof ?

Optimization of convergence rate

Choose $\lambda^{\pm}$ to minimize $\max_{\omega\in[0,\omega_{\max}]} |\rho(\omega)|$.



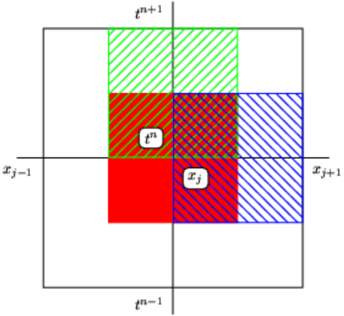
Theoretical convergence rate



Experimental convergence rate

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

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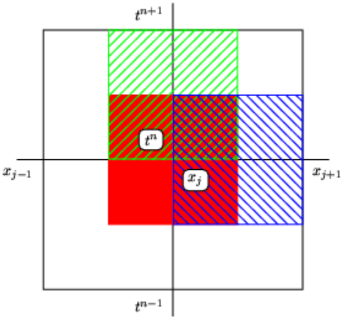

- Function constant on square;
- space and time derivatives defined by difference quotient on staggered grids, ;
- Implicit upwind scheme, finite difference in interior

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

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

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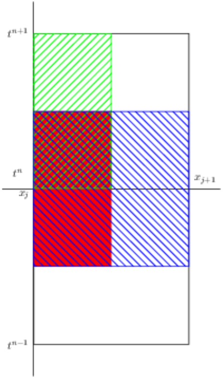
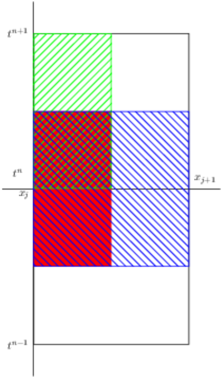
γ controls upwinding ($\gamma = 0$: centered, $\gamma = 1$: upwind)
Implicit scheme, unconditionally stable, order 1 for $\gamma \neq 0$, order 2 for $\gamma = 0$

Numerical transmission conditions



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



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

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

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

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

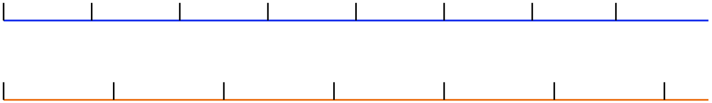
$$+ a^+ u_0^{+,n+1/2} + \boxed{\frac{\Delta x}{2} b u_0^{+,n+1/2}} + \lambda^+ u_0^{+,n+1/2} = g^{+,n+1/2}$$

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.

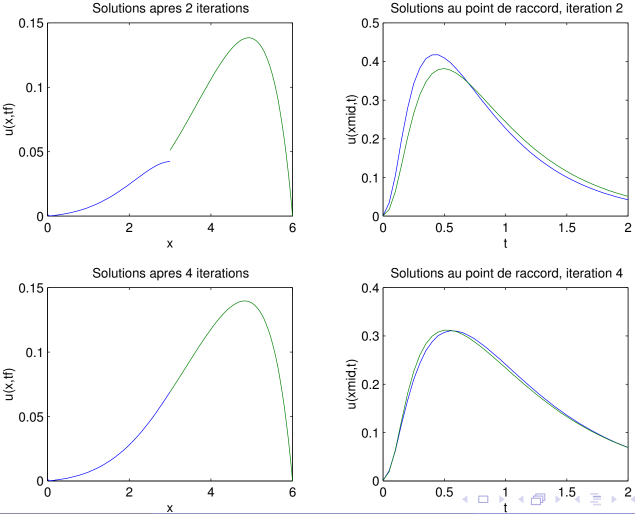
If different time steps, project g^+ on left grid (recompute integral on other grid)



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 $[1,1.8]$

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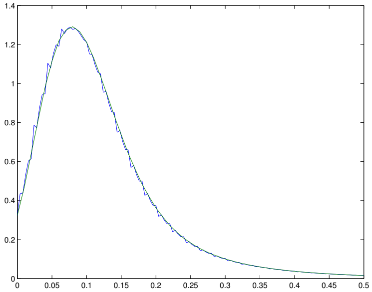
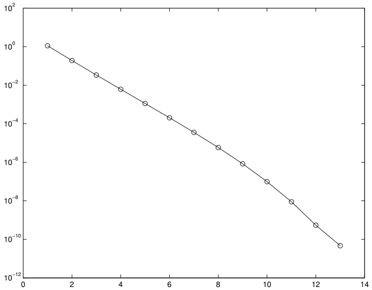


Solutions on the interface



Convergence history

Heterogeneous example (ctd.)

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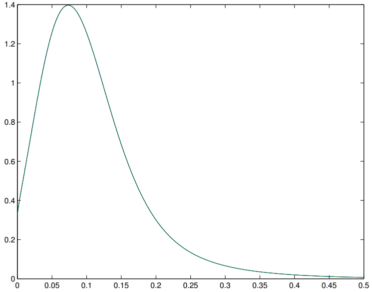
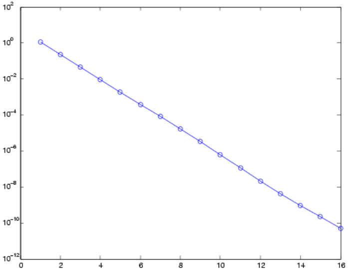


Solutions on the interface
Sol. after 2 iterations
Sol. at convergence



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