Nonconforming time discretization methods for coupling advection-diffusion problems with discontinuous coefficients

Caroline Japhet
japhet@math.univ-paris13.fr
avec Laurence Halpern, Jérôme Jaffré, Michel Kern et Jean Roberts

LAGA, Université Paris 13 et Inria (Projet ESTIME)

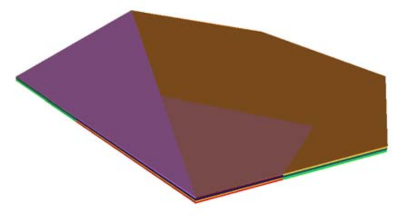
Outline

Outline

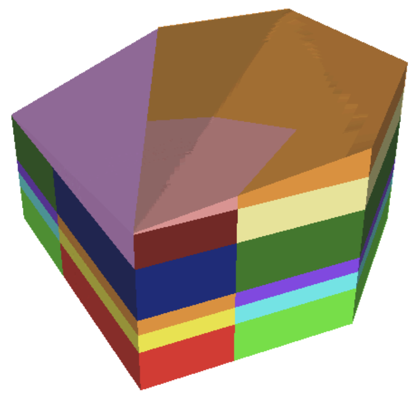
1. Application for nuclear waste disposal
2. The numerical model
3. Subdomain time stepping with nonconforming time grids
4. Conclusions

Far field 3D : The calculation domain

Actual dimensions:
$40km \times 40km \times 500m$



A blow-up in the vertical direction (30 times)



The repository is located in the red part of the bottom layer.

Hydrogeological data

Hydrogeologic layers	Thickness [m]	Porosity [%]	Permeability [m/s]		Effective diffusion coefficient [m^2/s]	Dispersivity Coefficients [m]
			Regional	Local		
Tithonian	Variable	10	3.10^{-5}	3.10^{-5}	10^{-9}	6.0, 0.6
Kimmeridgian when it outcrops	Variable	10	3.10^{-4}	3.10^{-4}	10^{-9}	6.0, 0.6
Kimmeridgian under cover			10^{-11}	10^{-12}		
Oxfordian L2a-L2b	165	6	$2\ 10^{-7}$	10^{-9}	10^{-9}	6.0, 0.6
Oxfordian Hp1-Hp4	50	18	$6\ 10^{-7}$	$8\ 10^{-9}$	10^{-9}	1600, 30
Oxfordian C3a-C3b	60	1	10^{-10}	10^{-12}	4.10^{-12}	6.0, 0.6
Callovo-Oxfordian Cox	135	1	$K_v=10^{-14}$ $K_h=10^{-12}$		4.10^{-12}	6.0, 0.6

Equations

Contaminant transport

$$\omega R \frac{\partial c}{\partial t} + \mathrm{div}(-\mathbf{D}\nabla c + c\mathbf{u}) + \omega R \lambda c = 0,$$

with the diffusion-dispersion tensor

$$\mathbf{D} = d_e \mathbf{I} + |\mathbf{u}|[\alpha_l \mathbf{E}(\mathbf{u}) + \alpha_t (I - \mathbf{E}(\mathbf{u}))], \quad E_{ij}(\mathbf{u}) = \frac{u_i u_j}{|\mathbf{u}|^2}.$$

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Spatial discretization

based on the mixed formulation

$$\omega \frac{\partial c}{\partial t} + \mathrm{div}(\mathbf{r} + c\mathbf{u}) = 0$$
$$\mathbf{r} = -\mathbf{D}\nabla c$$

with

$\mathcal{T}_h -$ a grid of hexahedral and/or tetrahedral elements K.

$\mathcal{F}_h -$ the set of faces F of elements K of $\mathcal{T}_h$.

use mixed finite elements with the approximation spaces

$\mathcal{M}_h -$ the space of functions constant on each element of $\mathcal{T}_h$.

$\mathcal{W}_h -$ Raviart-Thomas-Nedelec spaces or Kuznetsov-Repin spaces.

Spatial discretization with mixed finite elements

Look for $c_h \in \mathcal{M}_h$ and $\mathbf{r}_h \in \mathcal{W}_h$ such that

$$\int_K \omega \, \frac{\partial c_h}{\partial t} + \int_K \operatorname{div} \mathbf{r}_h + \int_{\partial K} c_h^* \mathbf{u} \cdot \mathbf{n}_K = 0, \quad K \in \mathcal{T}_h$$

$$\int_{\Omega_i} \mathbf{D}^{-1} \mathbf{r}_h \cdot \mathbf{v} - \int_{\Omega_i} c_h \operatorname{div} \mathbf{v} = -\int_{\partial\Omega} c_d \, \mathbf{v} \cdot \mathbf{n}_{\Omega_i}, \quad \mathbf{v} \in \mathcal{W}_h$$

where c_h^* is the upstream value on ∂K.

Time discretization

First order Euler

- Diffusion: implicit
- Advection: explicit with upstream weighting

$$\int_K \omega \frac{c_h^{n+1} - c_h^n}{\Delta t} + \int_K \operatorname{div} \mathbf{r}_h^{n+1} + \int_{\partial K} c_h^{n*} \mathbf{u} \cdot \mathbf{n}_K = 0, \quad K \in \mathcal{T}_h$$

$$\int_\Omega \mathbf{D}^{-1} \mathbf{r}_h^{n+1} \cdot \mathbf{v} - \int_\Omega c_h^{n+1} \operatorname{div} \mathbf{v} = -\int_{\partial\Omega} c_d \, \mathbf{v} \cdot \mathbf{n}_\Omega, \quad \mathbf{v} \in \mathcal{W}_h$$

with c_h^{n*} the upstream concentration.

Outline

The objective

- Strong heterogeneities

$\Downarrow$

- Different time scales

$\Downarrow$

- Subdomain time discretization

- To improve precision
- To decrease computing time

Related work

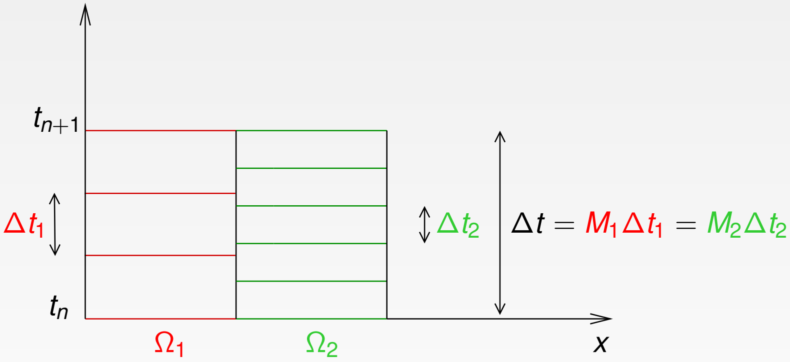
- J.-L. Lions, Y. Maday, G. Turinici (2001): Parareal algorithms

- M. F. Wheeler, I. Yotov: Mortar mixed finite elements

- C. Japhet, Y. Maday, F. Nataf (2004): A new cement to glue nonconforming grids with Robin interface conditions

- M. J. Gander, L. Halpern, C. Japhet, M. Kern, F. Nataf (2002-2005): Optimized Schwarz wavefrom relaxation for nonconforming time discretization

Subdomain time stepping with nonconforming time grids



Spatial discretization

Division of Ω into subdomains Ω_i, $\quad (i = 1, 2)$

$\mathcal{T}_{hi}$ a finite element grid on Ω_i (suppose matching grids)

$\mathcal{F}_{hi}$ the set of faces of elements of $\mathcal{T}_{hi}$

with associated approximation spaces $\mathcal{M}_{hi}$ and $\mathcal{W}_{hi}$

Denote by γ the interface between Ω_1 and Ω_2, $\qquad \gamma = \bar{\Omega}_1 \cap \bar{\Omega}_2$

$\mathcal{G}_h$ the set of faces of elements of $\mathcal{T}_{hi}$ that lie on γ

with associated approximation space

Λ_h - the space of functions constant on each face of $\mathcal{G}_h$

For one hyper time step Δt in Ω_i (without advection)

For $m_i = 0, \cdots, M_i - 1$, with $c_i^{n,0} = c_i^n$ and $\mathbf{r}_i^{n,0} = \mathbf{r}_i^n$, look for

$$c_i^{n,m_i+1} \in \mathcal{M}_{hi}, \quad \mathbf{r}_i^{n,m_i+1} \in \mathcal{W}_{hi}, \qquad \lambda_i^{n,m_i+1} \in \Lambda_h$$

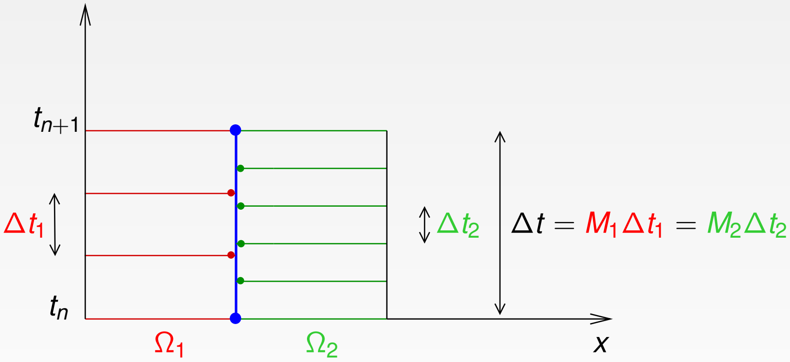
such that

$$\int_K \omega \, \frac{c_i^{n,m_i+1} - c_i^{n,m_i}}{\Delta t_i} + \int_K \operatorname{div} \mathbf{r}_i^{n,m_i+1} = 0, \quad K \in \mathcal{T}_{hi}$$

$$\int_{\Omega_i} \mathbf{D}^{-1} \mathbf{r}_i^{n,m_i+1} \cdot \mathbf{v} - \int_{\Omega_i} c_i^{n,m_i+1} \operatorname{div} \mathbf{v} = - \int_{\partial\Omega_i \cap \partial\Omega} c_d \, \mathbf{v} \cdot \mathbf{n}_{\Omega_i} - \int_\gamma \lambda_i^{n,m_i+1} \mathbf{v} \cdot \mathbf{n}_{\Omega_i}, \; \mathbf{v} \in \mathcal{W}_{hi}$$

Transmission conditions on the interface γ

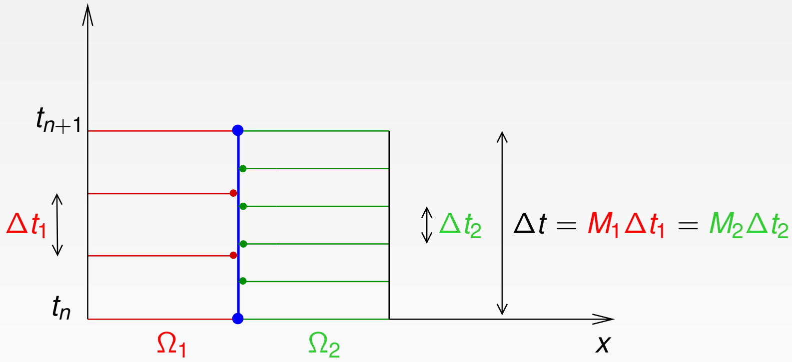
- Continuity of the concentration at t_{n+1}
- Conservation over the interval (t_n, t_{n+1})



A projection operator

Knowing $\lambda^n = \lambda_1^n = \lambda_2^n$, determine $\lambda^{n+1} = \lambda_1^{n+1} = \lambda_2^{n+1}$ as follows:

Define $\quad \pi_i : \Lambda_h \longrightarrow \Lambda_h^{M_i},\ i = 1, 2, \quad$ by $\quad \pi_i(\lambda)^{m_i} = \lambda,$



Dirichlet-to-Neumann operators in $\Omega_i \times (t^n, t^{n+1})$

Solve for $c_i^{m_i+1} = c_i^{n,m_i+1}(\lambda) \in \mathcal{M}_{hi}$, $\mathbf{r}_i^{m_i+1} = \mathbf{r}_i^{n,m_i+1}(\lambda) \in \mathcal{W}_{hi}$,

$$\int_K \omega \frac{c_i^{m_i+1} - c_i^{m_i}}{\Delta t_i} + \int_K \operatorname{div} \mathbf{r}_i^{m_i+1} = 0, \quad K \in \mathcal{T}_{hi}$$

$$\int_{\Omega_i} \mathbf{D}^{-1} \mathbf{r}_i^{m_i+1} \cdot \mathbf{v} - \int_{\Omega_i} c_i^{m_i+1} \operatorname{div} \mathbf{v} = -\int_{\partial\Omega_i \cap \partial\Omega} c_d \, \mathbf{v} \cdot \mathbf{n}_{\Omega_i} - \int_\gamma (\pi_i(\lambda))^{m_i+1} \mathbf{v} \cdot \mathbf{n}_{\Omega_i}, \; \mathbf{v} \in \mathcal{W}_{hi}$$

and calculate $\mathbf{r}_i^{n,m_i+1}(\lambda) \cdot \mathbf{n}_{\Omega_i}$.

Let $\quad \mathcal{S}_i(\lambda) = \pi_i^*(\mathbf{r}_i^{n,m_i+1}(\lambda) \cdot \mathbf{n}_{\Omega_i}) = \Delta t_i \sum_{m=0}^{M_i-1} \mathbf{r}_1^{n,m_1+1} \cdot \mathbf{n}_{\Omega_1}.$

Domain decomposition formulation

Find $\lambda \in \Lambda_h$ such that

$$\mathcal{S}_1(\lambda) + \mathcal{S}_2(\lambda) = 0.$$

This linear system has a unique solution.

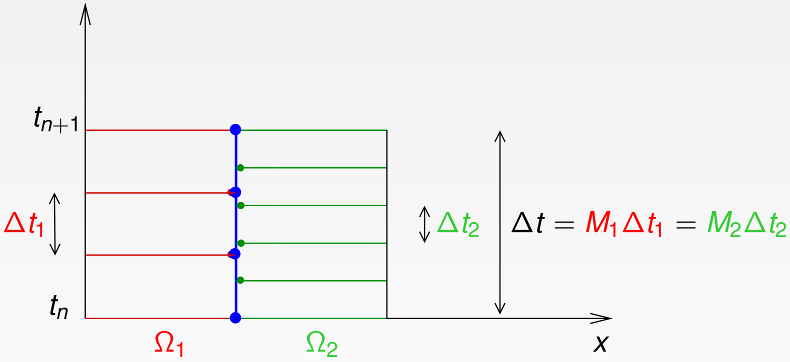
It is nonsymmetric and needs to be solved iteratively.

Set $\lambda^{n+1} = \lambda$.

- One interface unknown ($\lambda \in \Lambda_h$) per time step.

Transmission conditions - a more expensive scheme

- Weak continuity of concentration over (t_n, t_{n+1})
- Conservation over the interval $I_{n,m_1} = (t_{n,m_1}, t_{n,m_1+1}),\ m_1 = 1, \cdots, M_1$



Domain decomposition formulation

Find λ such that

$$\mathcal{S}_1(\lambda) + \mathcal{S}_2(\lambda) = 0$$

(A nonsymmetric linear system to be solved iteratively.)

Set $\lambda^{n,m_i} = \lambda^{m_i}, \quad m_i = 1, \cdots M_1$ and then set $\lambda^{n+1} = \lambda^{n,M_1}$

- M_1 interface unknowns $(\lambda^1, \cdots, \lambda^{M_1} \in \Lambda_h)$ per time step.

Robin transmission conditions : fast and robust solver

Problem : transmission conditions on the concentration and the flux lead to slow convergence $\Rightarrow$ preconditioning

An efficient preconditioning way: Optimized transmission conditions

$$\mathbf{r}_1 \cdot \mathbf{n}_{\Omega_1} + \alpha_1 c_1 = \pi_{1,2}(-\mathbf{r}_2 \cdot \mathbf{n}_{\Omega_2} + \alpha_1 c_2),$$
$$\mathbf{r}_2 \cdot \mathbf{n}_{\Omega_2} + \alpha_2 c_2 = \pi_{2,1}(-\mathbf{r}_1 \cdot \mathbf{n}_{\Omega_1} + \alpha_2 c_1).$$

where $\alpha_1,\ \alpha_2$ optimize the convergence rate

$\Rightarrow$ Optimized Schwarz waveform relaxation
Gander/Halpern/Nataf (2002), Martin (2003),
Gander/Halpern/Bennequin (2004), Gander/Halpern/Kern (2004)

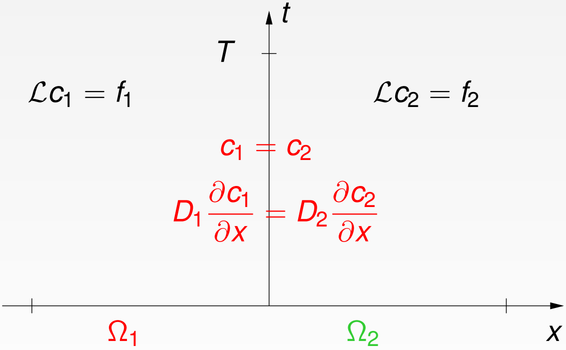
with discontinous Galerkin in time for nonconforming time discretization Blayo/Halpern/Japhet (2004), Halpern/Japhet (2005)

Advection-diffusion problems with discontinuous coefficients

$$\mathcal{L}c = \frac{\partial c}{\partial t} + \frac{\partial}{\partial x}(cu) - \frac{\partial}{\partial x}(D(x)\frac{\partial c}{\partial x}) = f \text{ in }]z_1, z_2[\times[0, T]$$

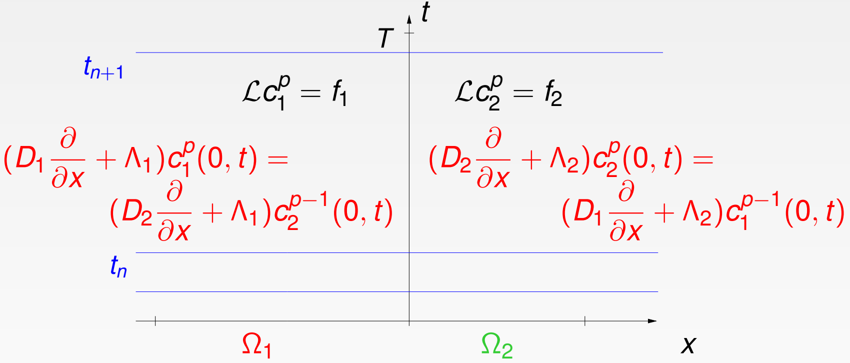
$$c(z_1, t) = c(z_2, t) = 0 \text{ , } t \in [0, T], \quad c(x, 0) = c_0(x), x \in [z_1, z_2]$$

with $D(x) = D_i$ in Ω_i, $u \geq 0$, $D_i > 0$, $i = 1, 2$



$$\Lambda_1 = \alpha_1 + \beta_1 \frac{\partial}{\partial t}, \quad \Lambda_2 = \alpha_2 + \beta_2 \frac{\partial}{\partial t}$$

where $\alpha_1, \alpha_2, \beta_1, \beta_2$ optimize the convergence rate



How to discretize these conditions with nonmatching grids in time ?

Time Discontinuous Galerkin Method

(Eriksson-Johnson-Thomée, 1985)

Subdomain problem in $\Omega_j = [x_{j-1}, x_j]$,
in one time window $I_n = (t_n, t_{n+1})$

$$\left\{ \begin{array}{rcll} \mathcal{L}c & = & f & \text{in } \Omega_j \times I_n, \\ c(\cdot, t_n) & = & c_0 & \text{in } \Omega_j, \\ (-D\dfrac{\partial}{\partial x} + \beta^- Id + \gamma^- \dfrac{\partial}{\partial t})\, c(x_{j-1}, \cdot) & = & g^- & \text{on } I_n, \\ (D\dfrac{\partial}{\partial x} + \beta^+ Id + \gamma^+ \dfrac{\partial}{\partial t})\, c(x_j, \cdot) & = & g^+ & \text{on } I_n. \end{array} \right.$$

Weak formulation

Let $V_j = H^1(\Omega_j)$,
Find $c \in \mathcal{C}^0(0, T; L^2(\Omega_j)) \cap L^2(0, T; H^1(\Omega_j))$ such that $c(\cdot, t_n) = c_0$,

$$(\!(\frac{dc}{dt}(t), \varphi)\!) + b(c(t), \varphi) = (f(t), \varphi) + g^-(t)\varphi(x_{j-1}) + g^+(t)\varphi(x_j), \quad \forall \varphi \in V_j,$$

where, for φ, ψ in V_j:

$$\left\{ \begin{array}{l} (\!(\varphi, \psi)\!) = (\varphi, \psi) + \gamma^-\varphi(x_{j-1})\psi(x_{j-1}) + \gamma^+\varphi(x_j)\psi(x_j), \\ b(\varphi, \psi) = (D(x)\frac{\partial \varphi}{\partial x}, \frac{\partial \psi}{\partial x}) + (u(x)\varphi, \frac{\partial \psi}{\partial x}) + \beta^-\varphi(x_{j-1})\psi(x_{j-1}) + \beta^+\varphi(x_j)\psi(x_j). \end{array} \right.$$

Discontinuous Galerkin Method

Let $\mathcal{T}$ be a decomposition of $I_n = \cup_{k=1}^{K} I_n^k$ with $I_n^k = [t_{n,k-1}, t_{n,k}]$. Defined

$$\begin{aligned} \mathbf{P}_q(V) &= \{\varphi : \ \varphi(t) = \sum_{i=0}^{q} \varphi_i t^i, \ \varphi_i \in V\} \\ \mathcal{P}_q(V, \mathcal{T}) &= \{\varphi : I \to V, \ \varphi_{|I_n^k} \in \mathbf{P}_q(V), \ 1 \leq k \leq K\}. \end{aligned}$$

Let $\varphi^{k,\pm} = \varphi(t_{n,k} \pm 0)$
The Discontinouous Galerkin method defines recursively on I_n^k, an approximate solution C in $\mathcal{P}_q(V_j, \mathcal{T})$ by

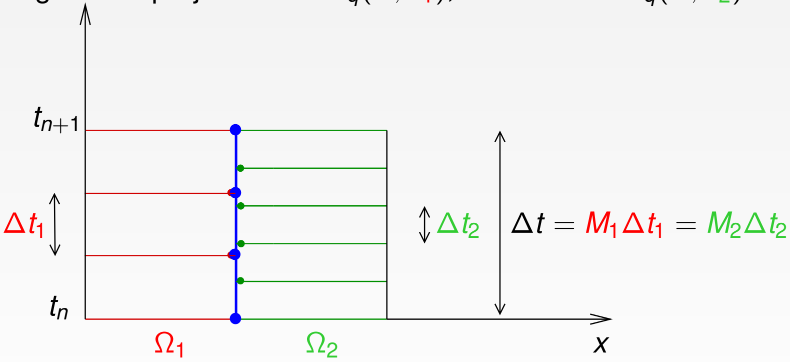
$$\begin{cases} C^{0,-} = c_0, \\ \forall \varphi \in \mathbf{P}_q(V_j) : \quad \displaystyle\int_{I_n^k} [((\frac{dC}{dt}, \varphi)) + b(C, \varphi)] \, dt + ((C^{k-1,+}, \varphi^{k-1,+})) = \\ \qquad \displaystyle\int_{I_n^k} [(f(t), \varphi(t)) + g^-(t)\varphi(x_{j-1}) + g^+(t)\varphi(x_j)] dt + ((C^{k-1,-}, \varphi^{k-1,+})). \end{cases}$$

Projections between time grids (in one time window)

generalization of the method developed in Gander/Halpern/Nataf(2003)

$\mathcal{T}_i$ a partition of the time window I_n in Ω_i, $i = 1, 2$

$\pi_{2,1}$ orthogonal L^2 projection on $\mathcal{P}_q(\mathbb{R}, \mathcal{T}_2)$, restricted to $\mathcal{P}_q(\mathbb{R}, \mathcal{T}_1)$.
$\pi_{1,2}$ orthogonal L^2 projection on $\mathcal{P}_q(\mathbb{R}, \mathcal{T}_1)$, restricted to $\mathcal{P}_q(\mathbb{R}, \mathcal{T}_2)$.



Projections between time grids (in one time window)

Continuous transmission conditions

$$\begin{aligned} f_1(t) &= g_2(t), \quad \forall t \in I \\ f_2(t) &= g_1(t), \quad \forall t \in I \end{aligned}$$

$$\begin{aligned} f_1(t) &= (D_1 \tfrac{\partial}{\partial x} + \alpha_1 + \beta_1 \tfrac{\partial}{\partial t}) c_1(0,t), \quad & g_2(t) &= (D_2 \tfrac{\partial}{\partial x} + \alpha_1 + \beta_1 \tfrac{\partial}{\partial t}) c_2(0,t) \\ f_2(t) &= (D_2 \tfrac{\partial}{\partial x} + \alpha_2 + \beta_2 \tfrac{\partial}{\partial t}) c_2(0,t), \quad & g_1(t) &= (D_1 \tfrac{\partial}{\partial x} + \alpha_2 + \beta_2 \tfrac{\partial}{\partial t}) c_1(0,t) \end{aligned}$$

Nonconforming discrete transmission conditions

The discrete approximations F_1, G_1 of f_1, g_1 in $\mathcal{P}_q(\mathbb{R}, \mathcal{T}_1)$, and F_2, G_2 of f_2, g_2 in $\mathcal{P}_q(\mathbb{R}, \mathcal{T}_2)$ verify the nonconforming matching conditions

$$\int_{I_n} [F_1 - G_2]\, V_1 = 0, \quad \forall V_1 \in \mathcal{P}_q(\mathbb{R}, \mathcal{T}_1)$$

$$\int_{I_n} [F_2 - G_1]\, V_2 = 0, \quad \forall V_2 \in \mathcal{P}_q(\mathbb{R}, \mathcal{T}_2)$$

An efficient way to perform the projections between time grids

Based on the method in Gander/Halpern/Nataf (2003)

Let $\{V_k^1\}$ (resp. $\{V_\ell^2\}$) the shape functions of $\mathcal{P}_q(\mathbb{R}, \mathcal{T}_1)$ (resp. $\mathcal{P}_q(\mathbb{R}, \mathcal{T}_2)$)

How to compute $M_{k,\ell} = \int_I V_k^1 V_\ell^2$?

$\Rightarrow$ **1D interface : Linear complexity algorithm without an additional grid**

$\Rightarrow$ **extensions to 2D and 3D interfaces** (C.J, M.J. Gander, 2007)

(see *http://www.unige.ch/~gander*)

Theoretical results : convergence, error estimates

based on the theorical results in Eriksson/Johnson/Larsson (1998)

Convergence: if $D_1 \neq D_2,\ \alpha_1 \neq \alpha_2,\ \beta_1 = \beta_2$ the continuous algorithm converges.

The coupling time discrete problem has a unique solution and the Schwarz discrete algorithm converges.

Error estimates: actually in the monodomain case

$$\|u(t) - U(t)\|_{L^\infty(I;L^2(\Omega_j))} = \mathcal{O}(\Delta t^{q+1})$$

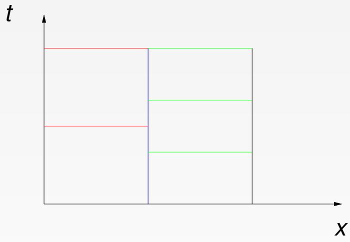
$$\|u(t_N) - U(t_N)\|_{L^2(\Omega_j)} = \mathcal{O}(\Delta t^{2q+1})$$

with $\Delta t = sup_k \Delta t_k$

Numerical Results

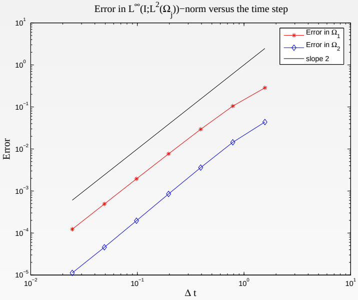
Replace V_j with V_j^h (P_1 finite element space)

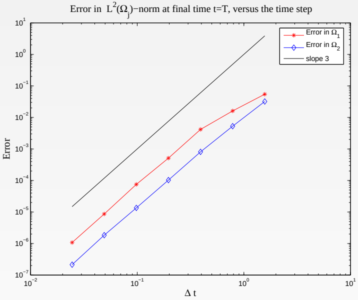
Exact solution $u(x,t) = cos(x)cos(t)$, in $[-\frac{\pi}{2}, \frac{\pi}{2}] \times [0, 2\pi]$
$u = 1$, $D_1 = D_2 = 1$
Interface : x=0.5, $\Delta x = 10^{-4}$
Stopping criterion : the jump of interface conditions is smaller than 10^{-6}



Initial nonconforming time grids

Error in $L^\infty(I; L^2(\Omega_j))$ norm (left part)
Error in $L^2(\Omega_j)$ norm at final time $t = T$ (right part)





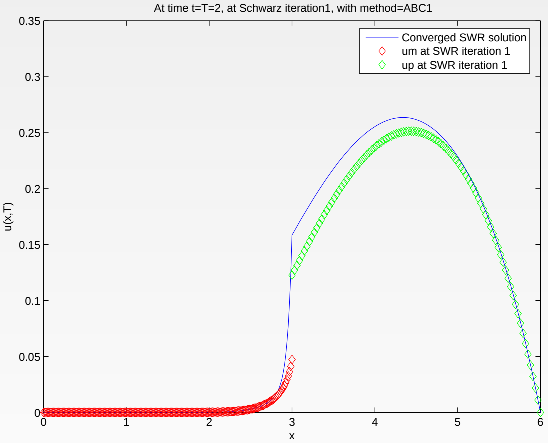
An example of computed solution in one time window

$$\mathcal{L}c = \frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} - \frac{\partial}{\partial x}(D(x)\frac{\partial c}{\partial x}) = 0 \text{ dans }]0,6[\times[0,2]$$

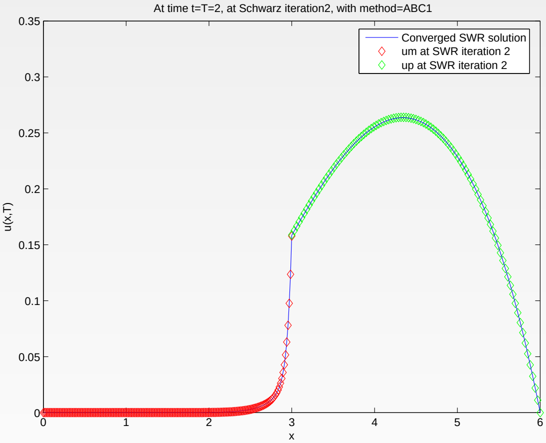
$$c(0,t) = c(6,t) = 0 \text{ , } t \in [0,2], \quad c(x,0) = e^{-3(2.5-x).^2}, x \in [0,6]$$

$D_1 = 0.05, \ \Delta t_1 = 0.016, \ \Delta x_1 = 0.015$
$D_2 = 1, \ \Delta t_2 = 0.04, \ \Delta x_2 = 0.03$

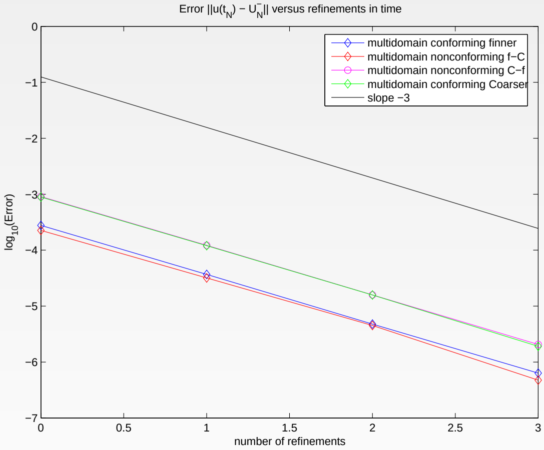
Optimized Order 1 transmission conditions iteration 1



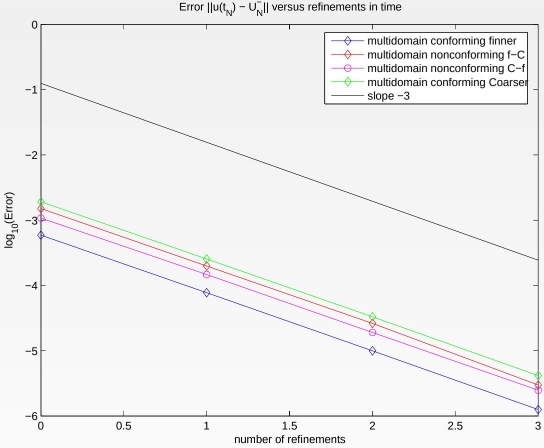
Optimized Order 1 transmission conditions iteration 2



Discontinuous coefficients / time nonmatching grids
Error $\|u(t_N) - U_N^-\|_{L^2(\Omega_1)}$ at $t_N = T$



Discontinuous coefficients / time nonmatching grids
Erreur $\|u(t_N) - U_N^-\|_{L^2(\Omega_1)}$ at $t_N = T$



Outline

Conclusions

- Time discontinuous Galerkin method with Optimized Schwarz Waveform Relaxation

  $\Rightarrow$ a simple and efficient algorithm to perform projection between nonmatching time grids, convergence proof

  $\Rightarrow$ lead to physical transmission conditions in very few iterations (2 iterations is sufficient)

  $\Rightarrow$ independant time steps with preservation of the scheme global order in time in the subdomains

- Perspectives

  - Extension to the Mixte Finite Element and Splitting approach
  - implementation in the 3D code
  - space-time nonmatching grids (based on C.J., Y. Maday et F. Nataf, 2004)