Accuracy and Stability of a Predictor-Corrector Crank–Nicolson Method with Many Subdomains

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Model Problem

Suppose we want to solve

$$\begin{aligned} \frac{\partial u}{\partial t} &= \mathcal{L}u + f \qquad && \text{on } \Omega \subset \mathbb{R}^d, \\ u &= g && \text{on } \partial\Omega, \end{aligned}$$

where

$$\mathcal{L}u = \sum_{i,j} \frac{\partial}{\partial x_i}\left(a_{ij}(x)\frac{\partial u}{\partial x_j}\right) - c(x)u$$

is uniformly elliptic, i.e., $[a_{ij}]$ is uniformly s.p.d. and $c(x) \geq 0$.

Method of Lines

- Assume the spatial discretization

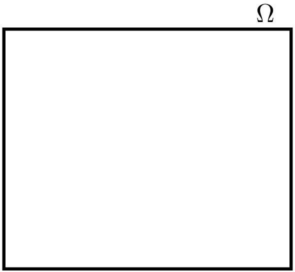
$$\mathcal{L}u \approx -\frac{1}{h^2}A\mathbf{u} + O(h^2),$$

where

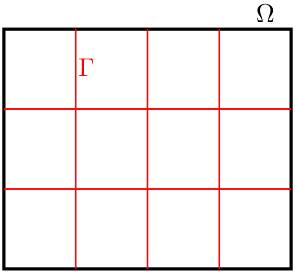
  - A is large and sparse
  - A is symmetric positive definite (due to Dirichlet boundary)
  - $\|A\|_2$ is independent of h (due to $\frac{1}{h^2}$ factor)

- If the time discretization is implicit, one must solve a large sparse linear system involving A at *every* time step

Domain Decomposition

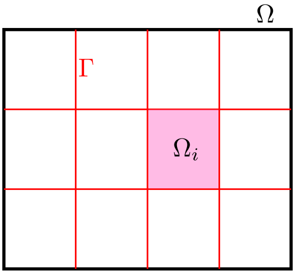


Domain Decomposition



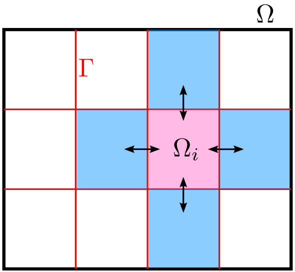
- Decompose Ω into several *subdomains* Ω_i

Domain Decomposition



- Decompose Ω into several *subdomains* Ω_i
- Define subdomain problems that can be solved in parallel

Domain Decomposition



- Decompose Ω into several *subdomains* Ω_i
- Define subdomain problems that can be solved in parallel
- Exchange interface data between subdomains
- Iterate to get consistent solution across subdomains

Types of DD algorithms

Example : Backward Euler

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = -\frac{1}{h^2} A \mathbf{u}^{n+1} + \mathbf{f}$$

1. Domain decomposition in space : at each time step, solve

$$(I + \tfrac{\Delta t}{h^2} A)\mathbf{u}^{n+1} = F(\mathbf{u}^n, \mathbf{f}^n)$$

using domain decomposition in space only

Types of DD algorithms

Example : Backward Euler

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = -\frac{1}{h^2} A\mathbf{u}^{n+1} + \mathbf{f}$$

2. Schwarz waveform relaxation : solve

$$(I + \tfrac{\Delta t}{h^2} A)\mathbf{u}_i^{n+1} = F_i(\mathbf{u}_i^n, \mathbf{u}_{i\pm 1}^n, \mathbf{f}^n)$$

on each Ω_i independently over *many time steps* and exchange interface data over the *entire time window*

- Must iterate to convergence

Types of DD algorithms

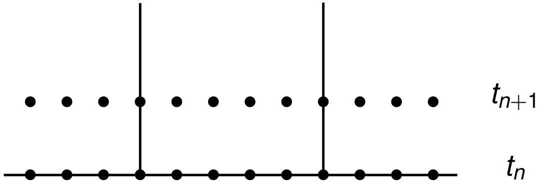
Example : Backward Euler

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^{n}}{\Delta t} = -\frac{1}{h^2} A\mathbf{u}^{n+1} + \mathbf{f}$$

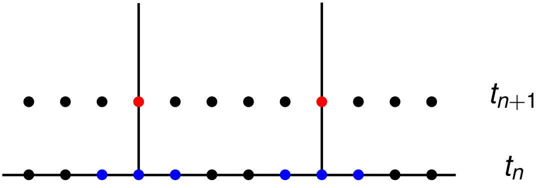
3. Predictor-corrector method : for each time step,
   - *Predict* interface values explicitly (Forward Euler)
   - Solve subdomain problems (Backward Euler) using predicted values
   - *Correct* interface values (Backward Euler) using interior values

- *Advantage :* No need to iterate to convergence !

Predictor-Corrector Euler



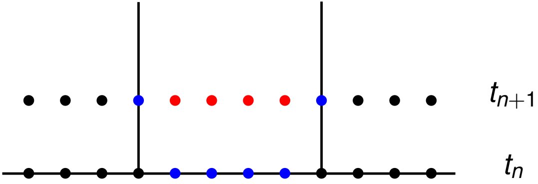
Predictor-Corrector Euler



1. *Predict* interface values $\mathbf{u}_\Gamma^*$ explicitly (Forward Euler)

$$\frac{\mathbf{u}_\Gamma^* - \mathbf{u}_\Gamma^n}{\Delta t} = -\frac{1}{h^2}\left(A_\Gamma \mathbf{u}_\Gamma^n + A_{\Gamma I}\mathbf{u}_I^n\right) + R_\Gamma \mathbf{f}$$

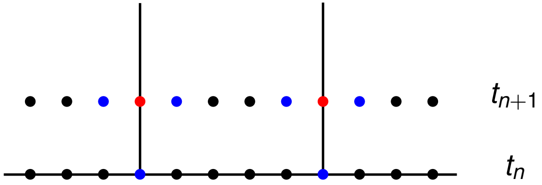
Predictor-Corrector Euler



2. Solve *independent* problems over Ω_i using $\mathbf{u}_\Gamma^*$

$$\frac{\mathbf{u}_I^{n+1/2} - \mathbf{u}_I^n}{\Delta t} = -\frac{1}{h^2}(A_I \mathbf{u}_I^{n+1/2} + A_{I\Gamma}\mathbf{u}_\Gamma^*) + R_I \mathbf{f}$$

Predictor-Corrector Euler



3. *Correct* $\mathbf{u}_\Gamma$ implicitly (Backward Euler) using interior values

$$\frac{\mathbf{u}_\Gamma^{n+1} - \mathbf{u}_\Gamma^n}{\Delta t} = -\frac{1}{h^2}(A_\Gamma \mathbf{u}_\Gamma^{n+1} + A_{\Gamma I}\mathbf{u}_I^{n+1/2}) + R_\Gamma \mathbf{f}$$

Predictor-Corrector Crank–Nicolson

- To derive Crank–Nicolson, make a time step to $t_{n+1/2}$ using backward Euler, then extrapolate :

$$\frac{\mathbf{u}^{n+1/2} - \mathbf{u}^{n}}{\Delta t/2} = -\frac{1}{h^2} A\mathbf{u}^{n+1/2} + \mathbf{f}$$

$$\mathbf{u}^{n+1} = 2\mathbf{u}^{n+1/2} - \mathbf{u}^{n}$$

Predictor-Corrector Crank–Nicolson

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(where $k = \Delta t/h^2$)

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$$(I + \frac{k}{2}A)\mathbf{u}^{n+1} = (I - \frac{k}{2}A)\mathbf{u}^n + \Delta t \cdot \mathbf{f}$$

(where $k = \Delta t/h^2$)

Predictor-Corrector Crank–Nicolson

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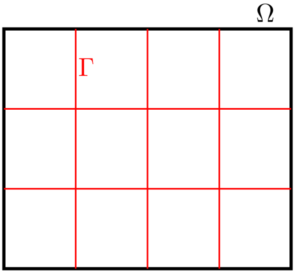
(where $k = \Delta t/h^2$)

- Do the same for the predictor-corrector version :

$$(I+\frac{k}{2}X_2A)(I+\frac{k}{2}X_1A)\mathbf{u}^{n+1} = (I-\frac{k}{2}X_2A)(I-\frac{k}{2}X_1A)\mathbf{u}^n+\Delta t\cdot\mathbf{f}$$

Predictor-Corrector Crank–Nicolson



$$(I + \frac{k}{2} X_2 A)(I + \frac{k}{2} X_1 A)\mathbf{u}^{n+1} = (I - \frac{k}{2} X_2 A)(I - \frac{k}{2} X_1 A)\mathbf{u}^{n} + \Delta t \cdot \mathbf{f}$$

- X_1 = projection onto Γ
- $X_2 = I - X_1$ = projection onto $\Omega \setminus \Gamma$

Predictor-Corrector Crank–Nicolson

- Introduced by Rempe and Chopp (SISC 2006)
- Used to simulate neural activity in branched structures
- Shown experimentally to have formal second order in time and in space
- What about simultaneous refinement ? Must analyze :
  - Stability
  - Accuracy

Stability

$$\underbrace{(I + \frac{k}{2}X_2A)(I + \frac{k}{2}X_1A)}_{B}\,\mathbf{u}^{n+1} = \underbrace{(I - \frac{k}{2}X_2A)(I - \frac{k}{2}X_1A)}_{C}\,\mathbf{u}^{n} + \Delta t \cdot \mathbf{f}$$

- Stability matrix :

$$B^{-1}C = (I + \frac{k}{2}X_1A)^{-1}(I + \frac{k}{2}X_2A)^{-1}(I - \frac{k}{2}X_2A)(I - \frac{k}{2}X_1A)$$

Stability

$$\underbrace{(I+\frac{k}{2}X_2A)(I+\frac{k}{2}X_1A)}_{B}\mathbf{u}^{n+1}=\underbrace{(I-\frac{k}{2}X_2A)(I-\frac{k}{2}X_1A)}_{C}\mathbf{u}^{n}+\Delta t\cdot\mathbf{f}$$

- Stability matrix :

$$B^{-1}C=(I+\frac{k}{2}X_1A)^{-1}(I+\frac{k}{2}X_2A)^{-1}(I-\frac{k}{2}X_2A)(I-\frac{k}{2}X_1A)$$

- Expect unconditional stability, but
  - Factors are non-symmetric
  - Factors do not commute

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Stability

$$B^{-1}C = (I + \frac{k}{2}X_1A)^{-1}(I + \frac{k}{2}X_2A)^{-1}(I - \frac{k}{2}X_2A)(I - \frac{k}{2}X_1A)$$

Stability

$$A^{1/2}B^{-1}CA^{-1/2} = (I + \frac{k}{2}A^{1/2}X_1A^{1/2})^{-1}(I + \frac{k}{2}A^{1/2}X_2A^{1/2})^{-1} \cdot (I - \frac{k}{2}A^{1/2}X_2A^{1/2})(I - \frac{k}{2}A^{1/2}X_1A^{1/2})$$

- Symmetrize the factors

Stability

$$A^{1/2}B^{-1}CA^{-1/2} = (I+\frac{k}{2}M_1)^{-1}(I+\frac{k}{2}M_2)^{-1}(I-\frac{k}{2}M_2)(I-\frac{k}{2}M_1)$$

- Symmetrize the factors

Stability

$$\overbrace{A^{1/2}(I+\frac{k}{2}M_1)B^{-1}}^{S}\,\overbrace{C(I+\frac{k}{2}M_1)^{-1}A^{-1/2}}^{S^{-1}} =$$
$$(I+\frac{k}{2}M_2)^{-1}(I-\frac{k}{2}M_2)(I-\frac{k}{2}M_1)(I+\frac{k}{2}M_1)^{-1}$$

- Symmetrize the factors
- Move the first factor to the back

Stability

$$\|SB^{-1}CS^{-1}\|_2 = \|(I + \frac{k}{2}M_2)^{-1}(I - \frac{k}{2}M_2)\|_2 \cdot \|(I - \frac{k}{2}M_1)(I + \frac{k}{2}M_1)^{-1}\|_2$$

- Symmetrize the factors
- Move the first factor to the back
- Bound each piece by the 2-norm

Stability

$$\|SB^{-1}CS^{-1}\|_2 = \|(I + \frac{k}{2}M_2)^{-1}(I - \frac{k}{2}M_2)\|_2 \cdot \|(I - \frac{k}{2}M_1)(I + \frac{k}{2}M_1)^{-1}\|_2$$

- Each $M_i = A^{1/2}X_iA^{1/2}$ is symmetric, with eigenvalues ≥ 0
- $(I + \frac{k}{2}M_i)^{-1}(I - \frac{k}{2}M_i)$ is symmetric and has eigenvalues

$$\left|\frac{1 - k\lambda_i/2}{1 + k\lambda_i/2}\right| \leq 1$$

for all $k > 0 \implies$ unconditional stablity !

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Local Truncation Error

- Would like to pick $\Delta t = h$ like in classical Crank–Nicolson

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- The exact solution $u(\cdot, t_n)$ satisfies

$$Bu(\cdot, t_{n+1}) = Cu(\cdot, t_n) + \Delta t \cdot f(\cdot, t_{n+1/2}) + \rho_n$$

where

$$\rho_n = \Delta t \left[\frac{\Delta t^2}{4h^2} X_2 A X_1 \cdot \mathcal{L} u_t(\cdot, t_{n+1/2}) + O(\Delta t^2) + O(h^2) \right]$$

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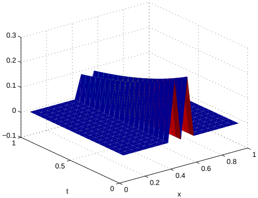
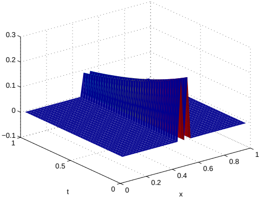
- If $\Delta t = h$, method is inconsistent !

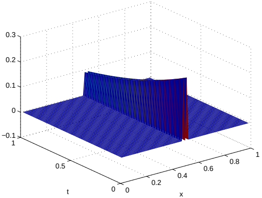
Local Truncation Error



$n = 20$



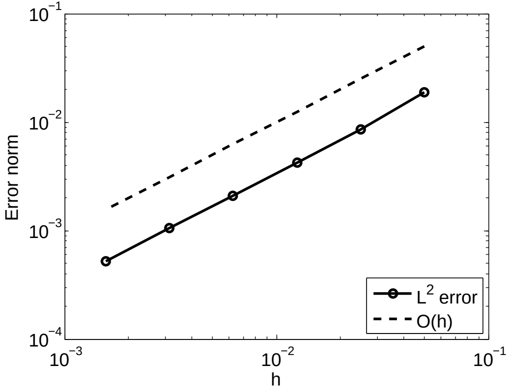
$n = 40$



$n = 80$

- Local truncation error does not decrease !

Global Error, $\Delta t = h$



- But, L^2 error shows first-order convergence !

Convergence Analysis

- Global error ε_n satisfies

$$\varepsilon_n = \sum_{j=1}^{n} (B^{-1}C)^{n-j} B^{-1} \rho_{j-1}$$

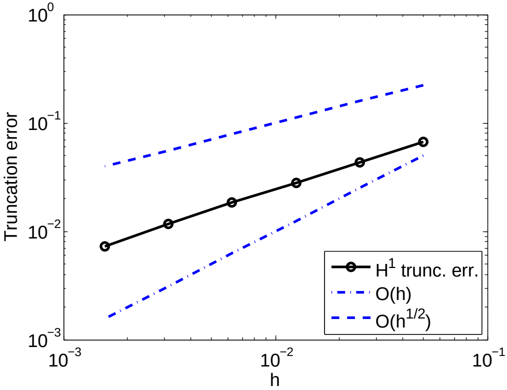
- Want to bound the discrete H^1 seminorm of ε_n :

$$C_1 h^{d-2} \|\varepsilon_n\|_A^2 \leq |\varepsilon_n|_{H^1(\Omega)}^2 \leq C_2 h^{d-2} \|\varepsilon_n\|_A^2$$

- Standard argument using stability shows

$$\|\varepsilon_n\|_A \leq \sum_{j=1}^{n} \|(I + \frac{k}{2} X_2 A)^{-1} \rho_{j-1}\|_A$$

Convergence Analysis



- A-norm of $(I + \frac{k}{2}X_2 A)^{-1}\rho_0$ decays to zero, but not fast enough !

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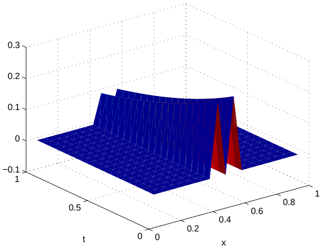
Another Approach



Observations :

- Local truncation error is a *smooth* function in time (but not in space !)
- The geometric series $\sum_{j=0}^{\infty}(B^{-1}C)^j$ converges

Another Approach

- Define $\delta_n = \rho_n - \rho_{n-1}$:

$$\rho_n = \tau\left[\frac{\tau^2}{4h^2} X_2 A X_1 \cdot \mathcal{L} u_t(\cdot, t_{n+1/2})\right]$$

$$\delta_n = \tau^{2}\left[\frac{\tau^2}{4h^2} X_2 A X_1 \cdot \mathcal{L} u_{tt}(\cdot, t_n)\right]$$

- Exchange the order of summation

$$\varepsilon_n = \sum_{j=1}^{n} (B^{-1}C)^{n-j} B^{-1} \underbrace{\sum_{l=0}^{j-1} \delta_l}_{\rho_{j-1}}$$

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$$\varepsilon_n = \sum_{l=0}^{n-1} \sum_{j=l+1}^{n} (B^{-1}C)^{n-j} B^{-1} \delta_l$$

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$$\varepsilon_n = \sum_{l=0}^{n-1} (I - (B^{-1}C)^{n-l})(I - B^{-1}C)^{-1} B^{-1} \delta_l$$

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- Exchange the order of summation

$$\varepsilon_n = \sum_{l=0}^{n-1} (I - (B^{-1}C)^{n-l})(\underbrace{B - C}_{=kA})^{-1} \delta_l$$

Another Approach

- Define $\delta_n = \rho_n - \rho_{n-1}$:

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- Exchange the order of summation

$$\varepsilon_n = \frac{1}{k} \sum_{l=0}^{n-1} \underbrace{(I - (B^{-1}C)^{n-l})}_{\|\cdot\| \leq 2} A^{-1} \delta_l$$

Convergence

- After some more manipulations, we get

$$\|A^{1/2}\varepsilon_n\|_2^2 \leq C\kappa(\mathcal{S}_\Gamma)h^{-(d-1)} \max_{0\leq j<n} \left(\tau^2 \|\mathcal{L}u_{tt}(\cdot, t_j)\|_\infty\right)^2$$

  where $\mathcal{S}_\Gamma$ is the Schur complement of A onto the interface Γ
- Under fairly general conditions,

$$\kappa(\mathcal{S}_\Gamma) = O(1/h)$$

- Thus, if $\Delta t = O(h^\alpha)$, then

$$|\varepsilon_n|_{H^1(\Omega)} \leq C\frac{\tau^2}{h} = O(h^{2\alpha-1}).$$

- Same estimate in $\|\cdot\|_{L^2}$ (using Poincaré inequality)

Convergence

$$|\varepsilon_n|_{H^1(\Omega)} \leq C\frac{\tau^2}{h} = O(h^{2\alpha-1})$$

- $\Delta t = h \ (\alpha = 1) \implies$ first order convergence
- $\Delta t = h^{3/2} \ (\alpha = 3/2) \implies$ second order convergence !
- Cannot go beyond second order due to $O(\Delta t^2 + h^2)$ terms away from the interface

1D Example

- Solve

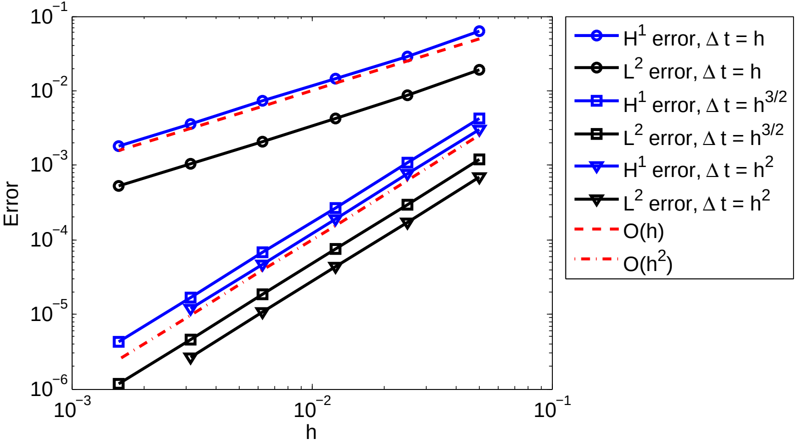
$$u_t = u_{xx} + f(x,t), \qquad u(x,0) = g(x)$$

  over $(x,t) \in (0,1) \times (0,1]$
- Choose $f(x,t)$ and $g(x)$ to have exact solution

$$u(x,t) = x\sin(\pi x)\sin(t)$$

- Two subdomains with interface at $x = 0.5$
- Choose $\Delta t = h^{\alpha}$ with $\alpha = 1, 1.5, 2$
- Measure error in L^2 norm and H^1 semi-norm

1D Example



$(n = 20, 40, 80, 160, 320, 640)$

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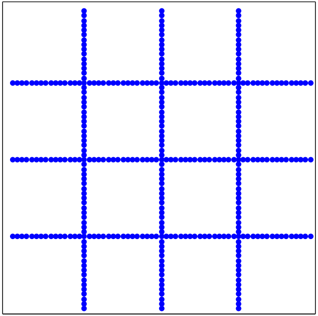
2D Example



- Solve $u_t = \Delta u + f(x, t)$ on unit square, $t \in (0, 1]$
- Exact solution :

$$u(x, y, t) = sin(3\pi x)(1 - e^{2y})(1 - e^{y-1})\sqrt{1 + t}$$

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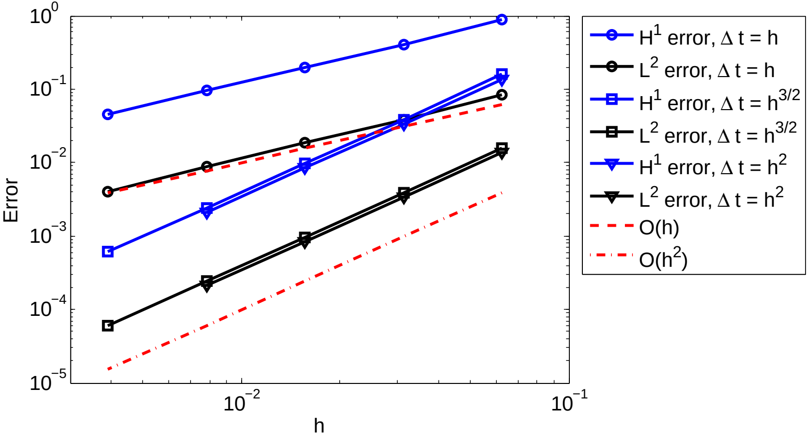
2D Example



$(n = 16, 32, 64, 128, 256)$

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Conclusion

- The Crank–Nicolson predictor-corrector method is
  - Unconditionally stable
  - Low order (or even inconsistent) near the interface
  - Converges with order $\min\{2\alpha - 1, 2\}$ for $\Delta t = O(h^{\alpha})$
- Ongoing work :
  - Influence of number of subdomains on convergence
  - Singular A (e.g., Neumann boundary)
  - Non-symmetric A (e.g., advection-diffusion equations)