A hybrid parareal Monte-Carlo algorithm for parabolic problems

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Seminar CEA-DAM, November 22nd 2021

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informatics mathematics
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Outline

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Simplified model for neutron transport in nuclear reactors.

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Boltzmann equation $$\frac{1}{|v|}\frac{\partial \psi}{\partial t}(\boldsymbol{r}, E, \boldsymbol{\Omega}, t) + (\mathcal{A} - \mathcal{S} - \mathcal{F})\,\psi(\boldsymbol{r}, E, \boldsymbol{\Omega}, t) = Q(\boldsymbol{r}, \boldsymbol{\Omega}, E, t)$$

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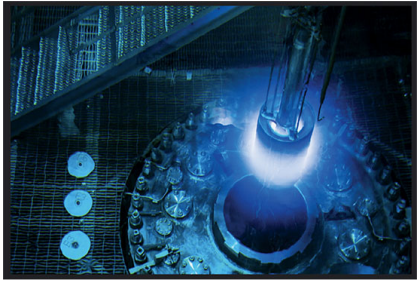
Can we speed-up a Monte Carlo resolution?

$\rightarrow$ time parallelization

Very complicated model: Start with a diffusion problem to understand the involved underlying mechanisms.



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Model problem

Time-dependent diffusion equation with dirichlet boundary conditions:

$$\begin{cases} \partial_t u - \mathcal{D}\Delta u = 0 & \text{in} \quad \Omega \times [0,T], \\ u(\cdot,0) = u^0 & \text{in} \quad \Omega, \\ u = 0 & \text{on} \quad \partial\Omega \times [0,T]. \end{cases}$$

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Weak formulation: Find $u \in H_0^1(\Omega)$ such that

$$\langle \partial_t u, v \rangle_{H^{-1}(\Omega), H_0^1(\Omega)} + \mathcal{D} \int_\Omega \boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v \, \mathrm{dx} = 0 \quad \forall v \in H_0^1(\Omega)$$ Well-posed problem

Lions (1969), Dautrey & Lions (1985), Brezis (2011)

Parareal algorithm

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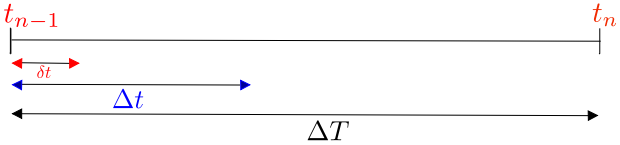

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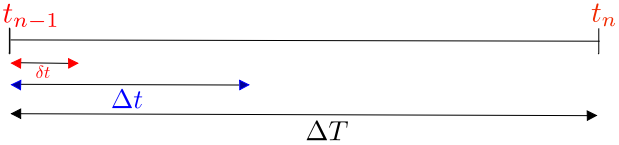

- Initialization : Compute a coarse solution at each time step n

$$\boldsymbol{U}^{n+1}_{k=0} := \mathcal{G}_{\Delta T}(\boldsymbol{U}^{n}_{k=0}), \quad \text{with} \quad \boldsymbol{U}^{0}_{k=0} = \boldsymbol{U}^{0} \qquad k : \text{ parareal iteration}$$

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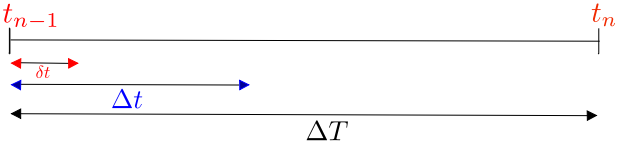

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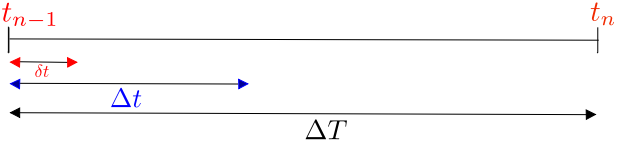

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- Parareal updates

$$\boxed{\boldsymbol{U}^{n}_{k} \approx u(t_n)} \qquad \boldsymbol{U}^{n+1}_{k+1} := \underbrace{\mathcal{G}_{\Delta T}(\boldsymbol{U}^{n}_{k+1})}_{\text{prediction}} + \underbrace{\mathcal{F}_{\Delta T}(\boldsymbol{U}^{n}_{k}) - \mathcal{G}_{\Delta T}(\boldsymbol{U}^{n}_{k})}_{\text{correction}} \quad \text{with} \quad \boldsymbol{U}^{0}_{k+1} := \boldsymbol{U}^{0}$$

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Some remarks on parareal

1. In general the two solvers are deterministic
2. Parareal converges for parabolic problems Gander, Vandewalle (2007)
3. Instability observed for hyperbolic problems Gander (2008)

Goal: Construct a hybrid parareal Monte Carlo algorithm for parabolic problems

Outline

Coarse propagator

$\mathcal{T}_h$: mesh of the domain Ω

$\mathcal{V}_h$: Lagrange nodes, $\mathcal{V}_h^{\text{int}}$: interior nodes,

$\mathcal{N}_h^{\text{int}}$: number of internal Lagrange nodes, N_e : number of elements

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The finite element propagator

$$X_h^p := \left\{ v_h \in \mathcal{C}^0(\Omega);\, v_h|_K \in \mathbb{P}_p(K)\ \forall K \in \mathcal{T}_h \right\} \subset H^1(\Omega)$$

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The discrete vector of unknowns : $\boldsymbol{U}_h^n \in \mathbb{R}^{\mathcal{N}_h^{\text{int}}}$ satisfies $\boldsymbol{U}_h^n = \mathcal{G}_{\Delta t}(\boldsymbol{U}_h^{n-1})$ with

$$\mathcal{G}_{\Delta t}(\boldsymbol{U}_h^{n-1}) = [\mathbb{A}^n]^{-1} \times \boldsymbol{F}^{n-1}, \qquad \underbrace{[\mathbb{A}^n]^{-1}}_{\text{Stiffness matrix+mass matrix}} \in \mathbb{R}^{\mathcal{N}_h^{\text{int}}, \mathcal{N}_h^{\text{int}}}, \quad \boldsymbol{F}^{n-1} \in \mathbb{R}^{\mathcal{N}_h^{\text{int}}}$$

The cell centered finite volume propagator

$$\boldsymbol{U}_h^n := (\boldsymbol{U}_K^n)_{K\in\mathcal{T}_h}, \quad \textbf{one value per cell and time step}$$

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$$\mathcal{G}_{\Delta t}(\boldsymbol{U}_h^{n-1}) = [\mathbb{A}^n]^{-1} \times \boldsymbol{F}^{n-1}, \quad \underbrace{[\mathbb{A}^n]^{-1}}_{\text{Sparse}} \in \mathbb{R}^{N_e,N_e}, \quad \boldsymbol{F}^{n-1} \in \mathbb{R}^{N_e}$$

The discontinuous Galerkin propagator

$\mathcal{N}_h^{\text{int}}$: total number of local internal degrees of freedom.

Discontinuous Galerkin space:

$$X_h^p := \left\{ v_h \in L^2(\Omega);\, v_h|_K \in \mathbb{P}_p(K)\ \forall K \in \mathcal{T}_h \right\} \not\subset H^1(\Omega),$$
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local matrix $[\mathbb{A}^n]_K^{-1}$ = stiffness matrix + mass matrix + consistency and stability terms.

Fine propagator : Monte-Carlo

Principle: It gives an approximation of

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Consider M particles and sample a collection $X_1, X_2, \cdots, X_M$ of M points from the PDF f. Denote by $\omega_i \in \mathbb{R}_+$ their statistical weight.

Compute $g(X_1)$,...,$g(X_M)$.

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Central limit Theorem:

$$\text{error} \approx 1/\sqrt{M}.$$

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The table lookup method:

Probability each element: $\mathbb{P}([x_{i-1}, x_i]) = \int_{[x_{i-1},x_i]} f(x)\,\mathrm{d}x$,

Cumulative function: $F_i : \Omega \to [0,1],\ F_i = \sum_{j \le i} \mathbb{P}([x_{j-1}, x_j])$

Let $\xi_1 \sim \mathcal{U}([0,1])$. Identify the two intervals such that $F_{i-1} \le \xi_1 \le F_i$.

Position of the particle: $X_i = \dfrac{(x_i - x_{i-1})\,\xi_1 - x_i F_{i-1} + x_{i-1} F_i}{F_i - F_{i-1}}$.

Repeat M times the procedure.

Kernel Transport

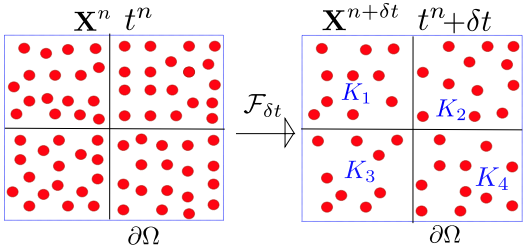
$(\boldsymbol{x}, t)$: position of the particle $\boldsymbol{x}$ at time t, $(\boldsymbol{x}', t')$: position of the particle $\boldsymbol{x}'$ at time t'

Density transition kernel:

$$T(\boldsymbol{x}', t' \to \boldsymbol{x}, t) := \frac{1}{\sqrt{2\pi\mathcal{D}\,(t - t')}} \exp\left(-\frac{(\boldsymbol{x} - \boldsymbol{x}')^2}{2\mathcal{D}\,(t - t')}\right).$$

Pratical formula for the brownian motion:

$$T(\boldsymbol{X}^{n+\delta t}, t^n + \delta t) = T(\boldsymbol{X}^n, t^n) + \sqrt{2\mathcal{D}\delta t}\,\mathcal{S}_n \quad \text{where} \quad \mathcal{S}_n \sim \mathcal{N}(0, 1)$$



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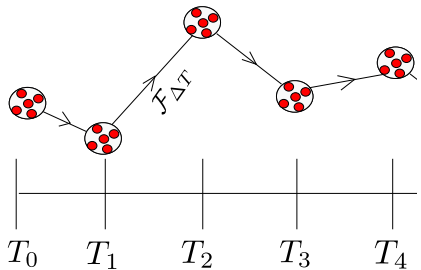
Hybrid parareal algorithm

Philosophy of the present work

Assume that 1000 processors are available.

Monte Carlo : We simulate 10^6 particules per processor. Precision : $1/\sqrt{10^9}$

1 replica = 1 processor



Required time for the propagation over a window ΔT: $\mathcal{F}_{\Delta T} = T/4$ seconds.

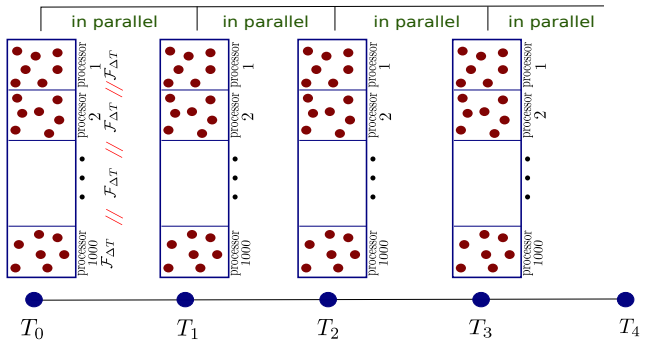
Total required time for each replica $= T$ seconds $\Rightarrow$ total time $\approx T$ secondes.

Assume now that 4000 processors are available.

precision: $1/\sqrt{4 \times 10^9}$ but statistical precision was already achieved...

Parareal : We employ the excess processors to parallelize the time variable !

- 4 **processors allocated to the time parallelization**
- For each time observable we have 1000 processors. For each of these processors we simulate 10^6 particles.



Precision :

$$\frac{1}{\sqrt{10^9}}$$

CPU cost :

$$\widetilde{T} = \frac{T}{4} \times \overline{k} \quad \text{with} \quad \overline{k} < 4$$

Other possibility: simulate a Borwnian motion on an interval $\left[0, \frac{4}{\overline{k}} T\right]$.

The hybrid algorithm

- **Coarse propagator :** Deterministic solver
- **Fine propagator:** Monte-Carlo solver: deterministic data + sampling + average

The numerical solution obtained for a replica $j \in [1, p]$ at parareal iteration k is denoted by $\boldsymbol{U}_{k,j}^{n+1}$

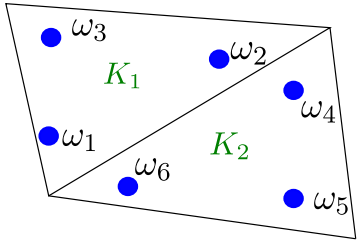
$$\boldsymbol{U}_{k}^{n+1} := \frac{1}{p} \sum_{j=1}^{p} \boldsymbol{U}_{k,j}^{n+1}$$

When $\boldsymbol{U}_{k,j}^{n+1}$ is computed, we need its statistical version for the computation of $\boldsymbol{U}_{k+1,j}^{n+2} = \mathcal{G}_{\Delta T}(\boldsymbol{U}_{k+1,j}^{n+1}) \times \dfrac{\mathcal{F}_{\Delta T}(\boldsymbol{U}_{k,j}^{n+1})}{\mathcal{G}_{\Delta T}(\boldsymbol{U}_{k,j}^{n+1})}$. Introduce bias in the Monte-Carlo solver.

Updating the statistical weights

Example: How avoid sampling $\boldsymbol{U}^3_{k=2} = \mathcal{G}_{\Delta T}(U^2_{k=2}) \times \frac{\mathcal{F}_{\Delta T}(\boldsymbol{U}^2_{k=1})}{\mathcal{G}_{\Delta T}(\boldsymbol{U}^2_{k=1})}$? We consider the statistical representation $\widetilde{\mathcal{F}_{\Delta T}(\boldsymbol{U}^2_{k=1})}$ before the average and we modify each of its particle weigths.

$$[\omega^3_{k=2}]_{i\in K} = [\omega_{\widetilde{\mathcal{F}_{\Delta T}(\boldsymbol{U}^2_{k=1})}}]_{i\in K} \times \left(\frac{\boldsymbol{U}^3_{k=2}}{\mathcal{F}_{\Delta T}(\boldsymbol{U}^2_{k=1})} \right) |_K$$



$$\omega_{1,2,3} \leftarrow \alpha_{K_1} \times \omega_{1,2,3} \qquad \alpha_{K_1} = \frac{[\mathbf{U}^2_{k=2}]|_{K_1}}{[\mathcal{F}_{\Delta T}(\mathbf{U}^1_{k=1})]|_{K_1}}$$

$$\omega_{4,5,6} \leftarrow \alpha_{K_2} \times \omega_{4,5,6} \qquad \alpha_{K_2} = \frac{[\mathbf{U}^2_{k=2}]|_{K_2}}{[\mathcal{F}_{\Delta T}(\mathbf{U}^1_{k=1})]|_{K_2}}$$

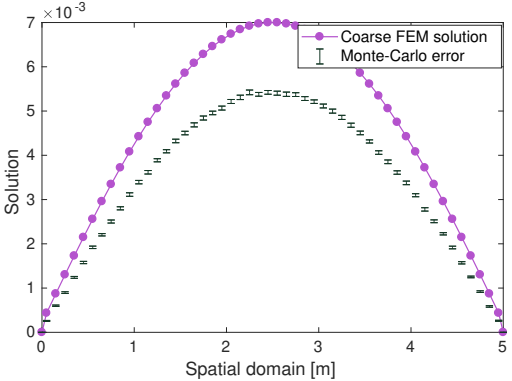
Outline

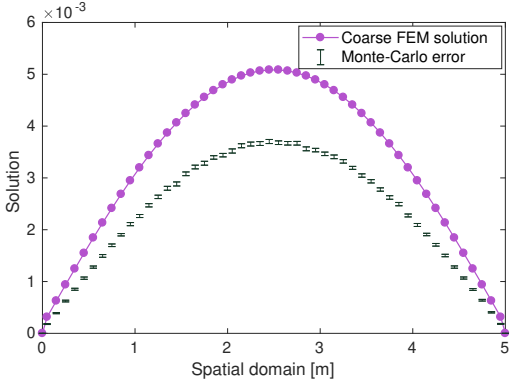
Numerical experiments

Final simulation time: $T = 10s$. **Diffusion coefficient:** $\mathcal{D} = 0.5m^2 \cdot s^{-1}$.

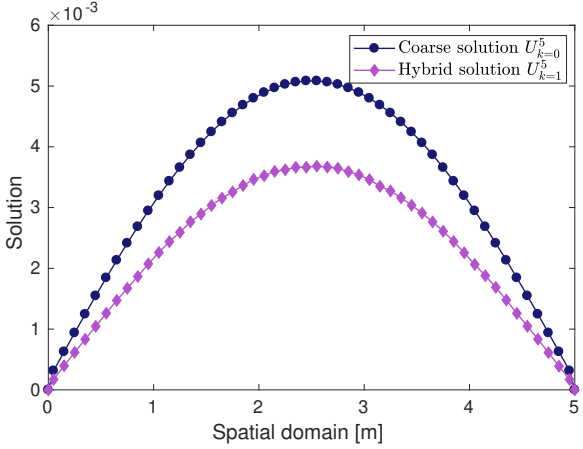
Coarse propagator: $\mathbb{P}_1$ FEM, $\Delta t = 2s$, **Fine propagator:** Monte-Carlo, $\delta t = 2 \times 10^{-4} s$.

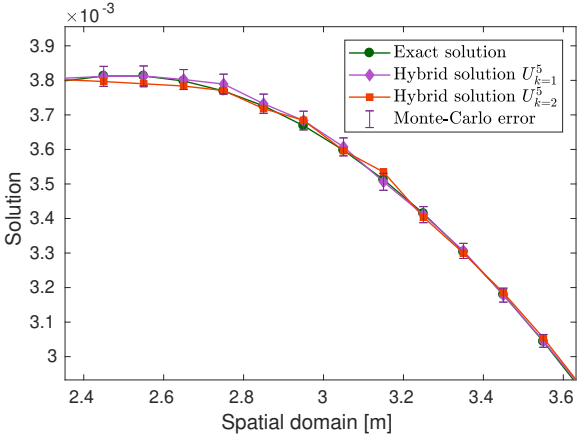
Initial condition: $u_0(x) = \frac{1}{L}$, **Number of particles:** 10^4, **Number of replicas:** 10^3





Hybrid solution





CPU time and convergence

Hybrid parareal resolution						
Number of processors time parallelization	Number of replicas for each parallel-in-time propagation	Number of particles for one replica j	CPU time $k=1$	CPU time $k=2$	Gain factor $k=1$	Gain factor $k=2$
5	10^2	10^5	335.76 s	537.16 s	4.92	3.04
5	10^3	10^4	33.05 s	53.1 s	4.96	3.09
5	10^4	10^3	3.39 s	5.49 s	4.97	3.07
5	10^5	10^2	0.35 s	0.58 s	5.08	3.02

A second test case

Final simulation time: $T = 14s$.

Deterministic propagator: $\mathbb{P}_1$ finite element, $\Delta t = 2s$.

Fine propagator: Monte-Carlo, $\delta t = 2 \times 10^{-4} s$.

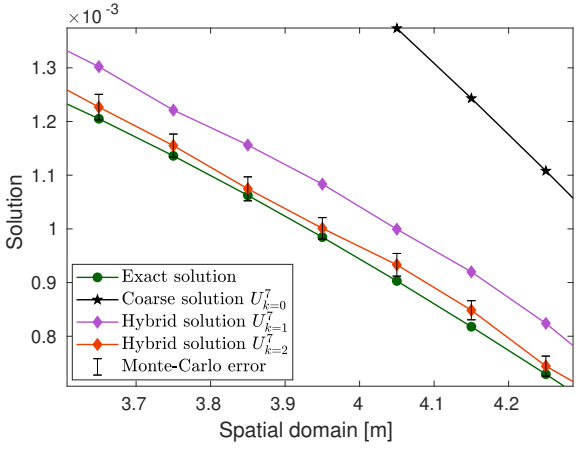
Diffusion coefficient MC: $\mathcal{D} = 0.5 m^2 \cdot s^{-1}$

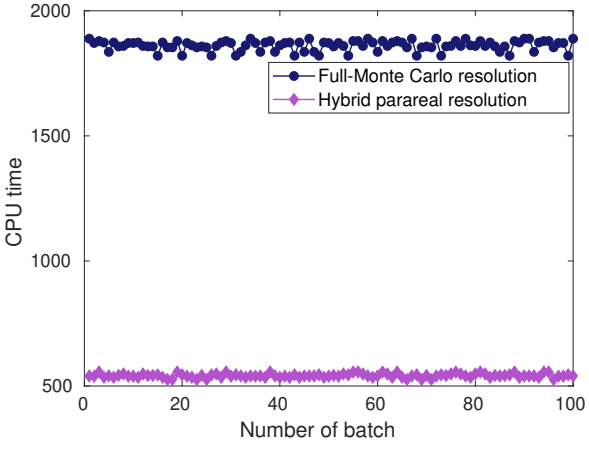
Diffusion coefficient FEM: $\mathcal{D} = 0.48 m^2 \cdot s^{-1}$

Initial condition: $u_0(x) = \frac{1}{L}\left(1 + \cos(\frac{\pi x}{L})\right)$.

Number of particles: 10^5, **Number of replicas:** 10^2

CPU time and convergence





A third test case

Final simulation time: $T = 50s$.

Deterministic propagator: $\mathbb{P}_1$ finite element, $\Delta t = 2s$.

Fine propagator: Monte-Carlo, $\delta t = 2 \times 10^{-3} s$.

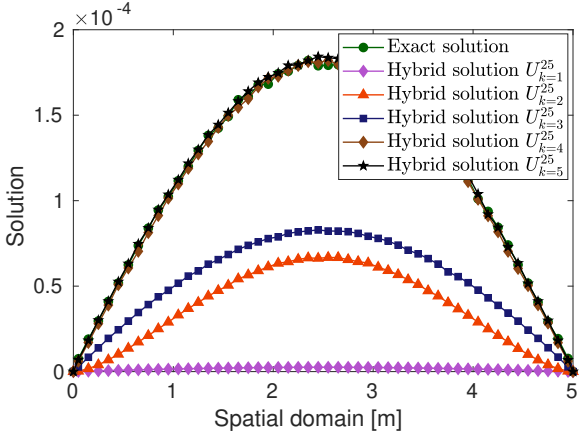
Diffusion coefficient MC: $\mathcal{D} = 0.25 m^2 \cdot s^{-1}$

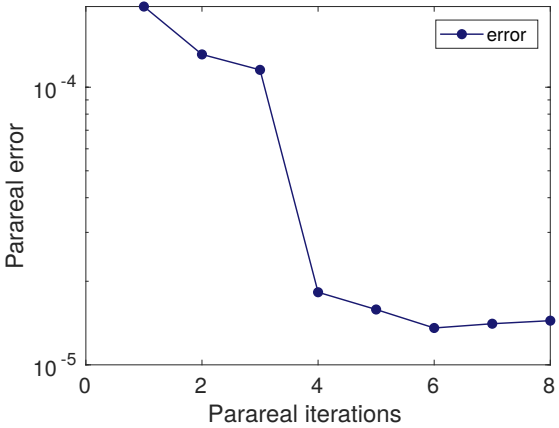
Diffusion coefficient FEM: $\mathcal{D} = 0.25 m^2 \cdot s^{-1}$

Initial condition: $u_0(x) = \dfrac{1}{L}$.

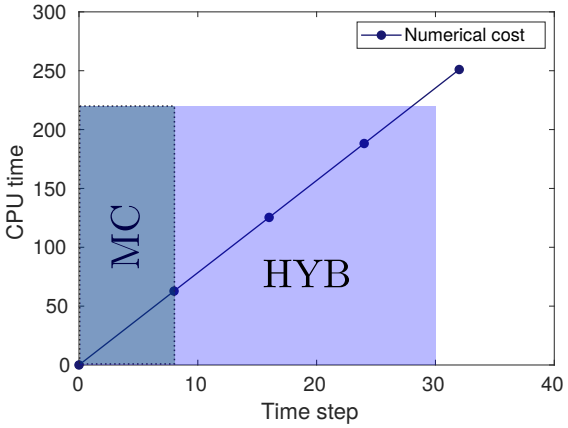
Number of particles: 10^5, **Number of replicas:** 10^3

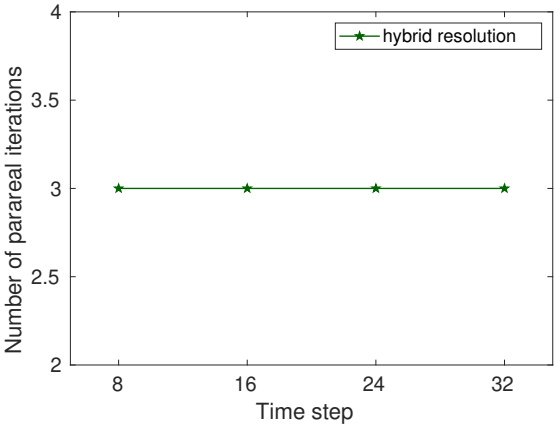
Convergence





Simulate longer times





J. DABAGHI, Y. MADAY, A. ZOIA, *A hybrid parareal Monte-Carlo algorithm for parabolic problems*. IN REVISION (2021)

Outline

Model problem

monokinetic 1D Boltzmann model

$$\frac{\partial \psi_+}{\partial t}(x,t) + \frac{\partial \psi_+}{\partial x}(x,t) + \Sigma_t \psi_+(x,t) = \left(\frac{\Sigma_s}{2} + \nu\frac{\Sigma_f}{2}\right)(\psi_+(x,t) + \psi_-(x,t))$$
$$\frac{\partial \psi_-}{\partial t}(x,t) - \frac{\partial \psi_-}{\partial x}(x,t) + \Sigma_t \psi_-(x,t) = \left(\frac{\Sigma_s}{2} + \nu\frac{\Sigma_f}{2}\right)(\psi_+(x,t) + \psi_-(x,t)).$$

- unknowns : ψ_+ and ψ_- : angular fluxes in direction $+1$ and -1
- $\Sigma_t = \Sigma_s + \Sigma_a + \Sigma_f$ (cross sections)
- ν : average number of neutrons emitted per fission

Fine propagator : The Monte Carlo algorithm

Fine propagator : The Monte Carlo algorithm

1. **Sampling the initial guess**

   → Position of particles (direct inversion of cumulative, table lookup, rejection...)

   → direction of particles. Select $\xi \sim \mathcal{U}([0,1])$. If $\xi \leq p^+$, $\omega_i = +1$. Otherwise, $\omega_i = -1$.

Fine propagator : The Monte Carlo algorithm

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2. **Sampling the flights**

   Probability of collision between $s > 0$ and $s + ds > 0$ is $p(s)ds = \Sigma_t e^{-\Sigma_t s} ds$. The path is obtained by the direct inversion of the cumulative $s = -\frac{1}{\Sigma_t} \ln(1 - \xi)$ with $\xi \sim \mathcal{U}([0,1])$

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3. **Collision**

   $\xi_1 \sim \mathcal{U}([0,1])$. If $\xi_1 \leq \frac{\Sigma_s}{\Sigma_t}$ scattering event $\Rightarrow$ sample a new direction and flight. If $\frac{\Sigma_s}{\Sigma_t} < \xi_1 \leq \frac{\Sigma_s}{\Sigma_t} + \frac{\Sigma_a}{\Sigma_t}$ absorption event $\rightarrow$ the neutron is dead.
   If $\xi_1 > \frac{\Sigma_s}{\Sigma_t} + \frac{\Sigma_a}{\Sigma_t}$ fission event. The mother neutron is dead and $\overline{\nu}$ child neutrons are emitted. New directions and flights have to be sampled for each child neutrons.

Fine propagator : The Monte Carlo algorithm

1. **Sampling the initial guess**

   $\rightarrow$ Position of particles (direct inversion of cumulative, table lookup, rejection...)

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   Probability of collision between $s > 0$ and $s + ds > 0$ is $p(s)ds = \Sigma_t e^{-\Sigma_t s} ds$. The path is obtained by the direct inversion of the cumulative $s = -\frac{1}{\Sigma_t} \ln(1 - \xi)$ with $\xi \sim \mathcal{U}([0,1])$

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   If $\xi_1 > \frac{\Sigma_s}{\Sigma_t} + \frac{\Sigma_a}{\Sigma_t}$ fission event. The mother neutron is dead and $\overline{\nu}$ child neutrons are emitted. New directions and flights have to be sampled for each child neutrons.

4. **Monte Carlo computation**

   Compute an approximation of $\int_\Omega (\psi_+ + \psi_-)(x,t)\, dx = \int_\Omega \Phi(x,t)\, dx$

Coarse propagator : A reaction-diffusion model

$$\frac{\partial \phi}{\partial t}(x,t) - \mathcal{D}\frac{\partial^2 \phi}{\partial x^2}(x,t) + \Sigma_a \phi(x,t) + (\nu - 1)\Sigma_f \phi(x,t) = 0 \quad \text{in} \quad \Omega \times [0,T]$$

$$\phi(x,0) = \phi^0(x) \quad \text{in} \quad \Omega$$

$$\phi(x,t) = 0 \quad \text{on} \quad \partial\Omega \times]0,T[$$

Cell-centered finite volume method: a single constant value per cell: $\forall 1 \leq n \leq N_t - 1$ we let

$$\mathbf{\Phi}^n := (\phi_K^n)_{K \in \mathcal{T}_h} \in \mathbb{R}^{N_e} \quad \phi_K^n := \frac{1}{|K|}\int_K \phi^n(x)\, dx$$

By integration over the element K and using the Green's formula we obtain

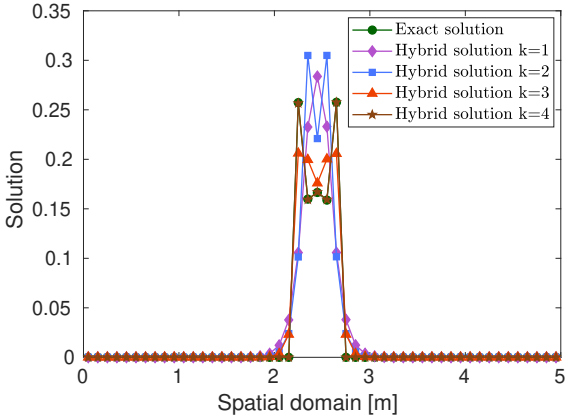
$$\frac{|K|}{\Delta t_n}\phi_K^n + \mathcal{D}\sum_{\sigma \in \mathcal{E}_K} \mathfrak{F}_{K,\sigma}^n - |\sigma|\frac{\phi_K^n}{d_{K\sigma}} + \Sigma_a \phi_K^n + (\nu - 1)\Sigma_f \phi_K^n = Q_K^{n-1} \quad \forall K \in \mathcal{T}_h.$$

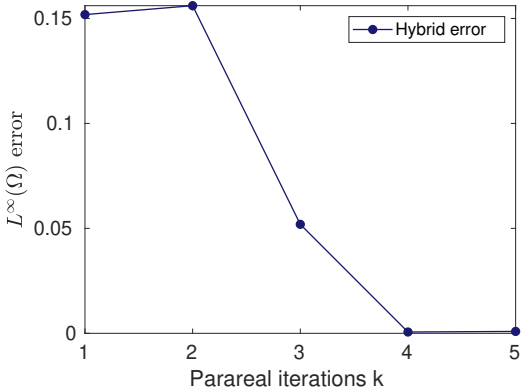
$\mathbf{\Phi}^n$ is solution to a linear system of equations

Numerical experiments

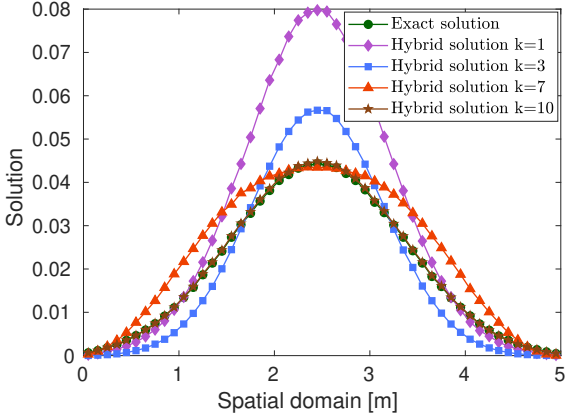
$\Sigma_a = \Sigma_f = 0$

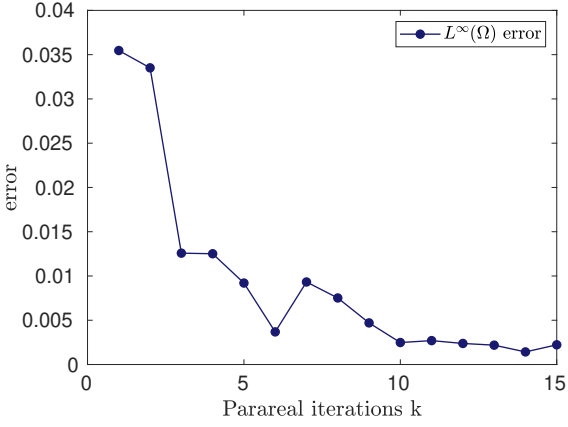
$n = 4$





$n = 80$





J. Dabaghi, Y. Maday, A. Zoia, *A hybrid parareal Monte-Carlo algorithm for the Boltzmann equation in neutronics.* In preparation (2021)

Outline

Conclusion

- We devised for the diffusion equation a hybrid parareal algorithm.
- Our approach reduces the CPU time of a Monte-Carlo simulation.

Ongoing work:

- Extension to the Boltzmann equation in neutronics with absorption and fission

Thank you for your attention!