A micro-macro parareal algorithm for singularly perturbed ODEs

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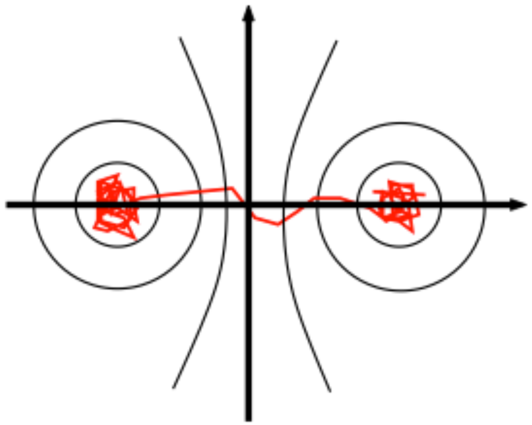
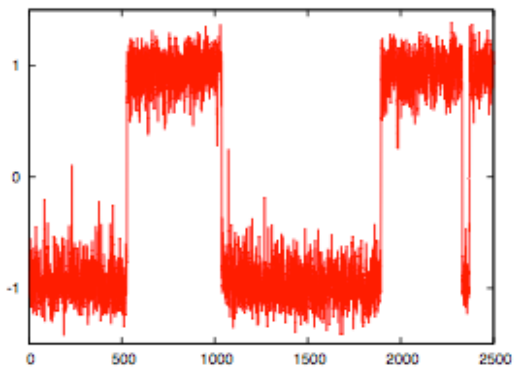
Motivation: effective dynamics of SDEs

- (Overdamped) Langevin equation for molecular dynamics

$$\frac{du}{dt} = -\nabla V(u) + \sqrt{2\beta^{-1}}\frac{dW}{dt}, \qquad u \in \mathbb{R}^N$$

- Metastability





- Effective dynamics for single reaction coordinate $\xi(u)$

- Under time-scale separation assumptions, we have

$$\xi(u(t)) \approx X(t) \quad \text{solution of} \quad \frac{dX}{dt} = -b(X) + \sigma(X)\frac{dB}{dt}$$

Legoll and Lelievre, Nonlinearity, 2010

Motivation: Fokker-Planck setting

- A single instance of the process follows the SDE

$$\frac{du}{dt} = -\nabla V(u) + \sqrt{2\beta^{-1}}\frac{dW}{dt}, \qquad u \in \mathbb{R}^N$$

- Probability density follows the Fokker-Planck equation

$$\partial_t p(u,t) - \nabla_u \cdot [\nabla V(u) p(u,t)] = \frac{1}{2\beta}\Delta_u p(u,t)$$

- For the effective dynamics, the Fokker-Planck equation is in 1D

- **Computational issues**:
  - High dimensionality of Fokker-Planck equations ➔ Monte Carlo
  - Time-scale separation leads to stiffness

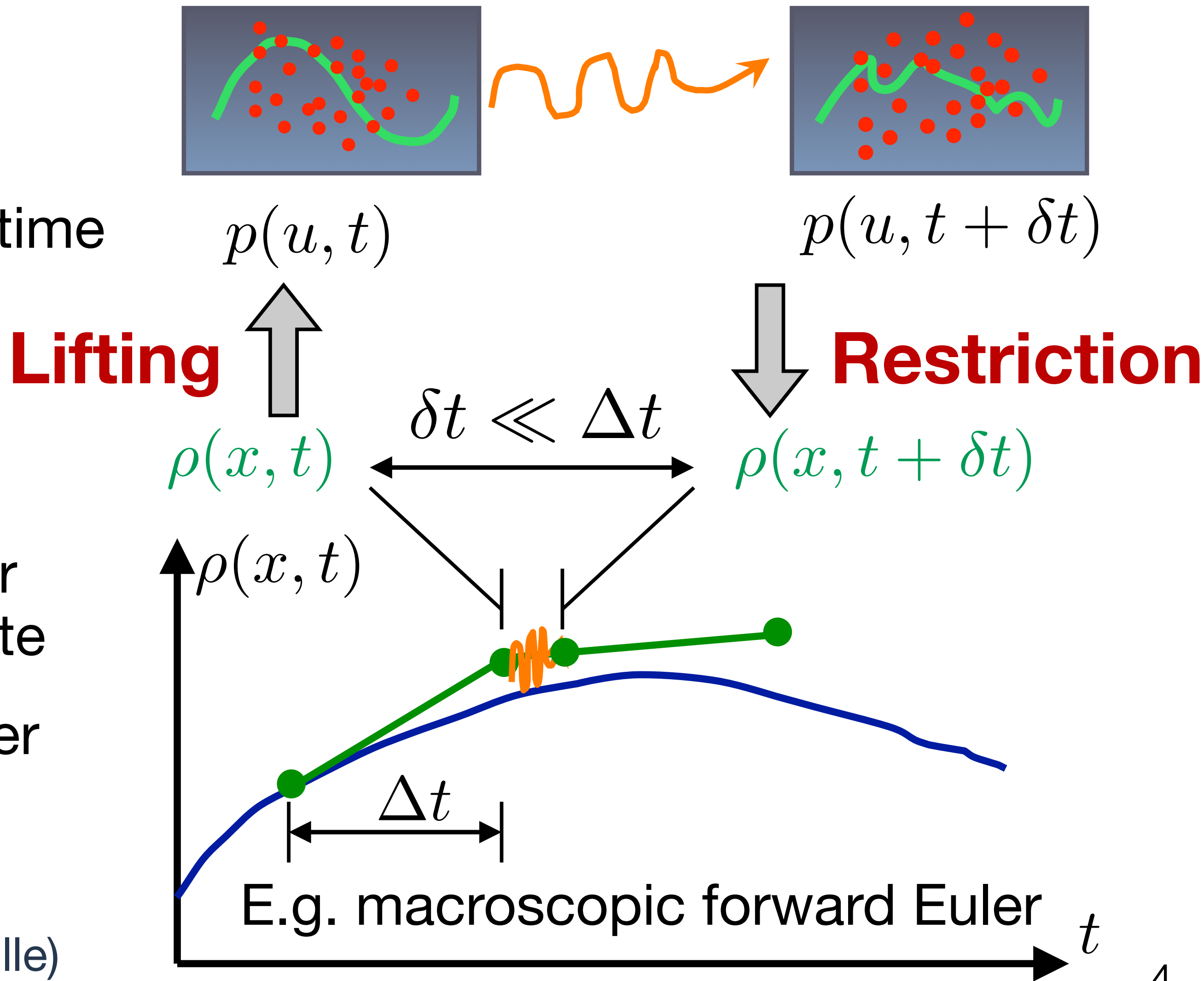
Computational multiscale framework
Based on *coarse projective integration*

Microscopic level

- model available
- simulate over short time interval

Macroscopic level

- model incomplete or insufficiently accurate
- want to simulate over long time interval



Kevrekidis et al, 2003 - …
E et al, 2003 - … (incl. Abdulle)

Goals of the present work

Observations

- Coarse projective integration does not directly exploit the available *approximate* macroscopic model
- Extrapolation in the presence of noise is problematic

Goal: increase efficiency and accuracy by

- Explicitly using the approximate macroscopic model
- Avoiding extrapolation in time

… using a parareal approach

The simplest possible setting
Singularly perturbed ODEs

- We have a multiscale ODE for $u = (x, y)$

$$\frac{dx}{dt} = f(x, y)$$
$$\frac{dy}{dt} = \frac{1}{\epsilon}\left(\eta(x) - Ay\right)$$

- Macroscopic model exists when $\epsilon \to 0$

$$\mathcal{R}u = x$$
$$\mathcal{L}X = (x, \eta(X))$$

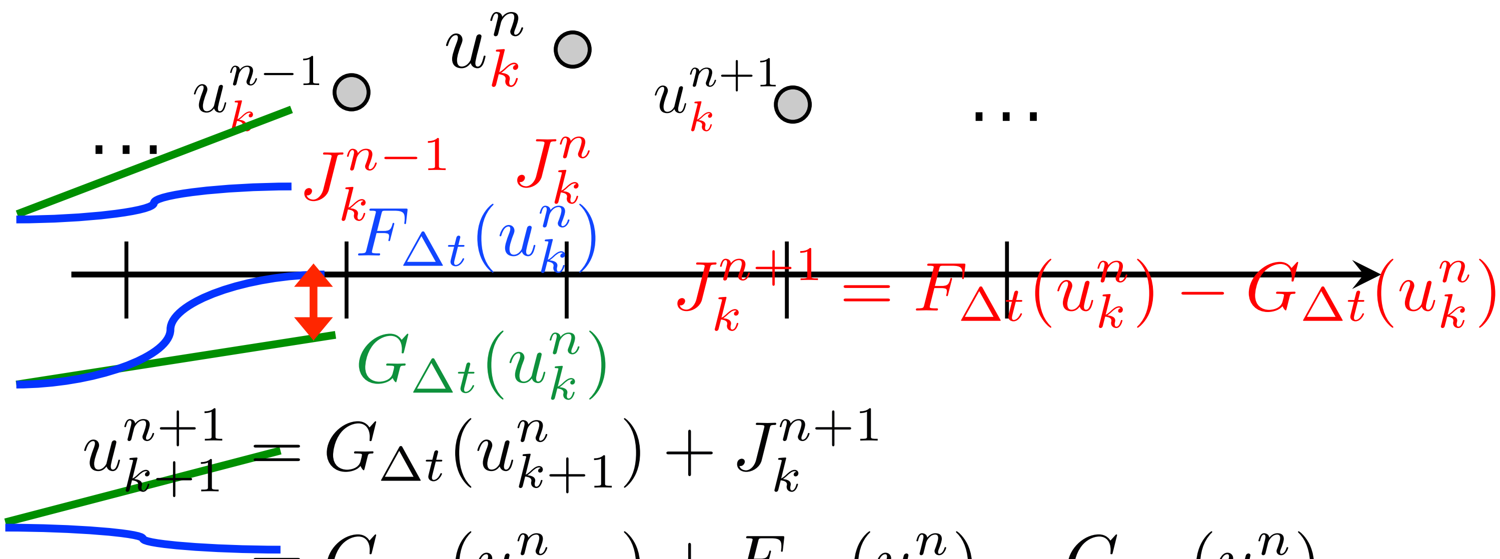
$$\frac{dX}{dt} = F_0(X) = f(X, \eta(X))$$

- We aim at showing that the parareal method has
  - Higher accuracy than the macroscopic limit
  - Lower computational cost than full microscopic simulation

Pavliotis and Stuart, Springer, 2008 / Givon, Kupferman, Stuart, Nonlinearity, 2004

Parareal algorithm for ODEs $\dot{u} = f(u)$

- Cheap, inaccurate solver $u^{n+1} = G_{\Delta t}(u^n)$
- Expensive, accurate solver $u^{n+1} = F_{\Delta t}(u^n)$
- Iteratively correct approximation parallel-in-time

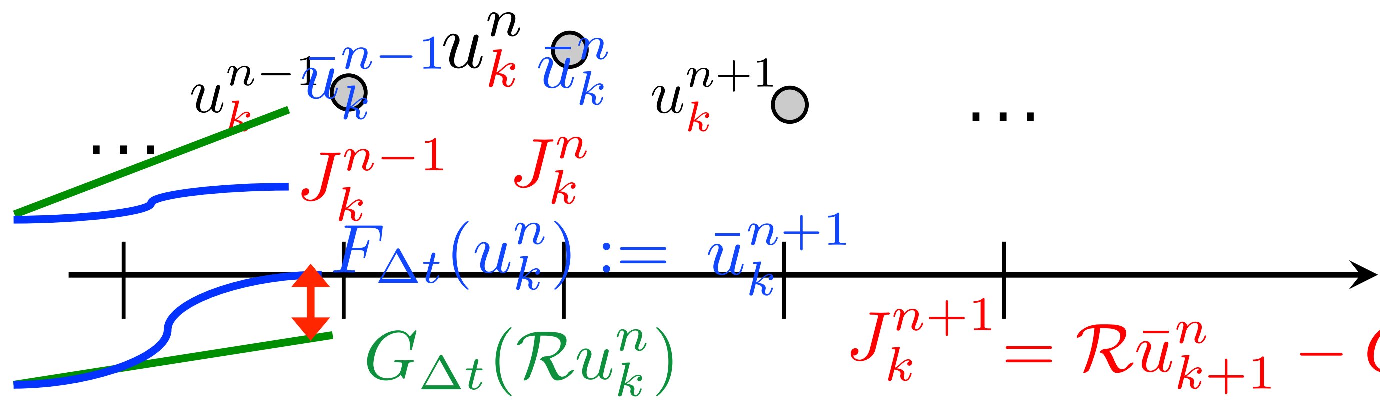


$$\begin{aligned} u_{k+1}^{n+1} &= G_{\Delta t}(u_{k+1}^n) + J_k^{n+1} \\ &= G_{\Delta t}(u_{k+1}^n) + F_{\Delta t}(u_k^n) - G_{\Delta t}(u_k^n) \end{aligned}$$

Lions, Maday and Turinici, CRAS, 2001

Micro-macro parareal algorithm

- Cheap, inaccurate solver $$X^{n+1} = G_{\Delta t}(X^n)$$
- Expensive, accurate solver $$u^{n+1} = F_{\Delta t}(u^n)$$



$$J_k^{n+1} = \mathcal{R}\bar{u}_{k+1}^n - G_{\Delta t}(\mathcal{R}u_k^n)$$

$$\begin{aligned} X_{k+1}^{n+1} &= G_{\Delta t}(X_{k+1}^n) + J_k^{n+1} \\ &= G_{\Delta t}(u_{k+1}^n) + \mathcal{R}\bar{u}_k^{n+1} - G_{\Delta t}(\mathcal{R}u_k^n) \end{aligned}$$

$$u_{k+1}^n = \mathcal{P}(X_{k+1}^n, \bar{u}_k^n)$$

Legoll, Lelievre, S, SISC, 2013

Elements in the convergence proof

$$\begin{aligned} X_{k+1}^{n+1} &= G_{\Delta t}(X_{k+1}^{n}) + J_k^{n+1} \\ &= G_{\Delta t}(u_{k+1}^{n}) + \mathcal{R}\bar{u}_{k+1}^{n} - G_{\Delta t}(\mathcal{R}u_k^n) \end{aligned}$$

$$u_{k+1}^{n} = \mathcal{P}(X_{k+1}^{n}, \bar{u}_k^n) \quad = (X_{k+1}^{n}, \bar{y}_k^n)$$

- Accuracy of the approximate macroscopic model

$$\|X(t) - \mathcal{R}(u(t))\| \leq C\epsilon \|x_0\|, \qquad \forall t > 0$$

- Time-scale separation between macroscopic and microscopic degrees of freedom

$$\left\|y(t) - A^{-1}\eta(x(t))\right\| \leq C\epsilon \|x_0\|, \qquad \forall t > t_{BL} = \mathcal{O}(\epsilon \log(1/\epsilon))$$

- Properties of the matching operator

$$\mathcal{P}(\mathcal{R}(u), u) = u$$

Convergence result

- Definition of macroscopic and microscopic errors

$$E_k^n = X_k^n - \mathcal{R}u(t_n) \qquad\qquad e_k^n = u_k^n - u(t_n)$$

- We then have the following error bound

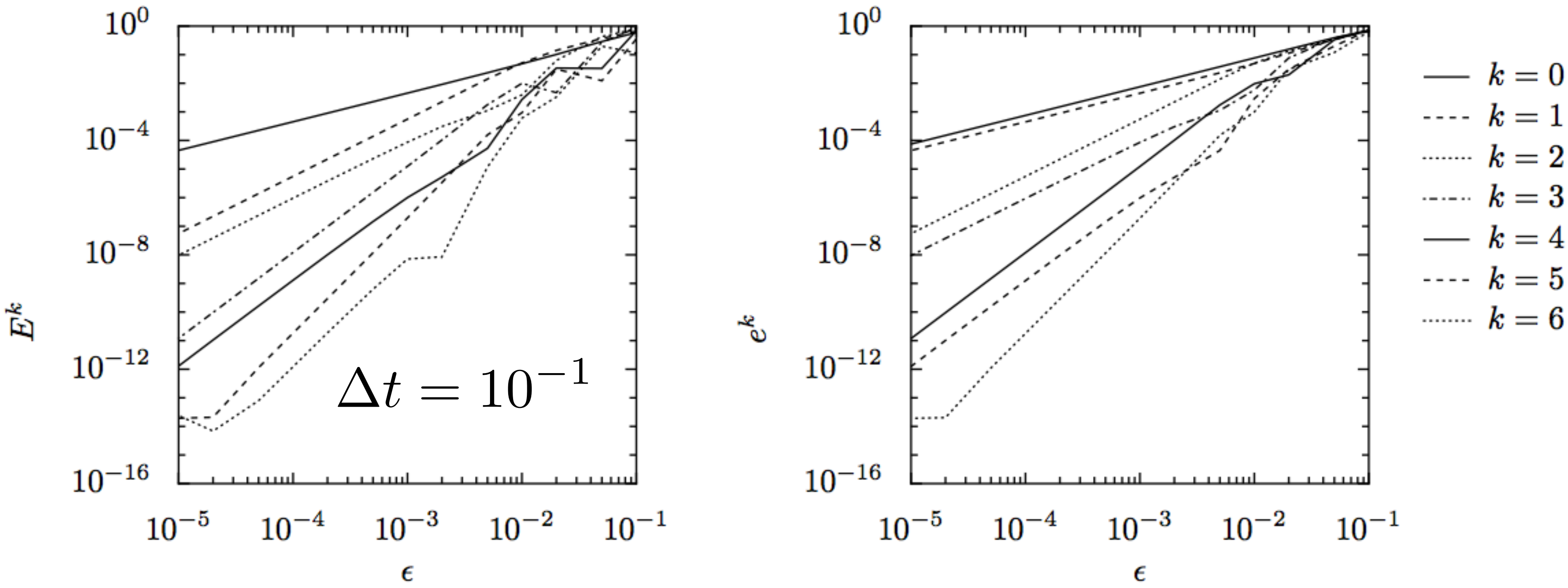
$$\forall\, k \geq 0, \qquad \sup_{0 \leq n \leq N} |E_k^n| \leq C_k \epsilon^{1+\lceil k/2 \rceil}$$

$$\forall\, k \geq 0, \qquad \sup_{0 \leq n \leq N} \|e_k^n\| \leq C_k \epsilon^{1+\lfloor k/2 \rfloor}$$

- Iterations alternatingly improve macroscopic and microscopic error

Legoll, Lelievre, S, to appear in SISC, 2013

Convergence properties in terms of ϵ

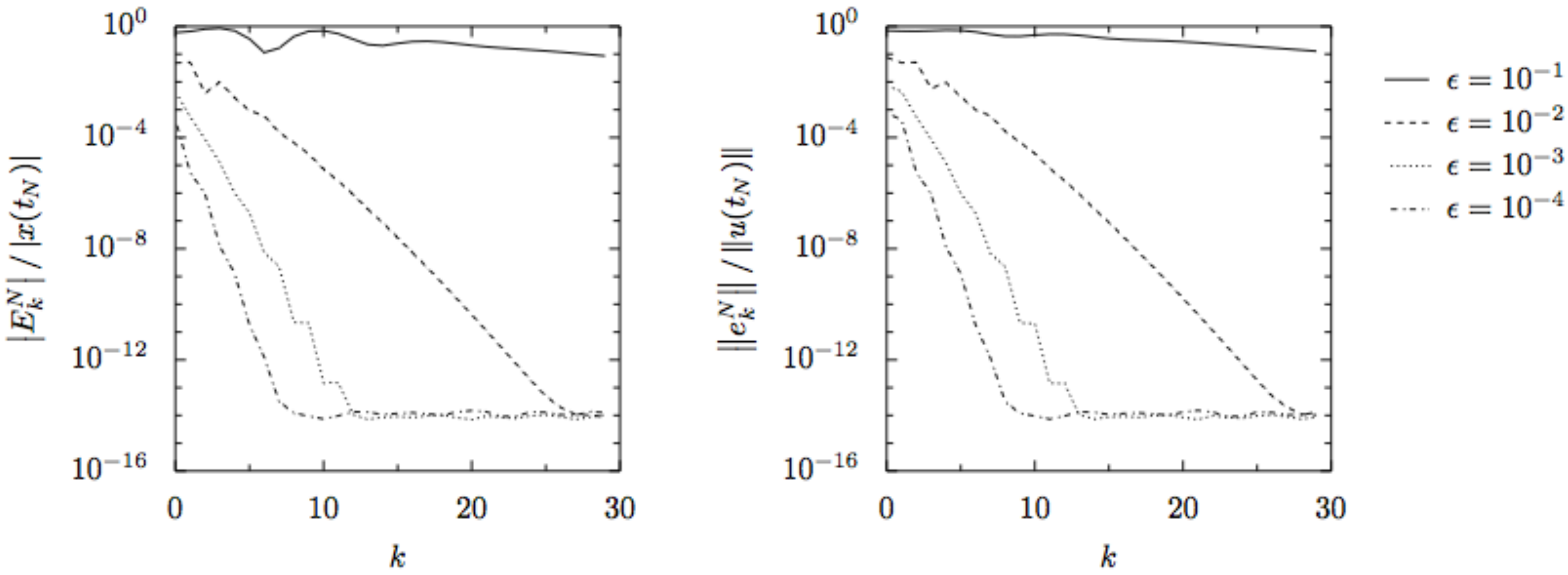


Left: macroscopic relative error **Right: microscopic relative error**

- Algorithm alternatingly improves macroscopic and microscopic errors
- Numerical results confirm sharpness of analytical result

Convergence in terms of iteration number

$\Delta t = 10^{-1}$



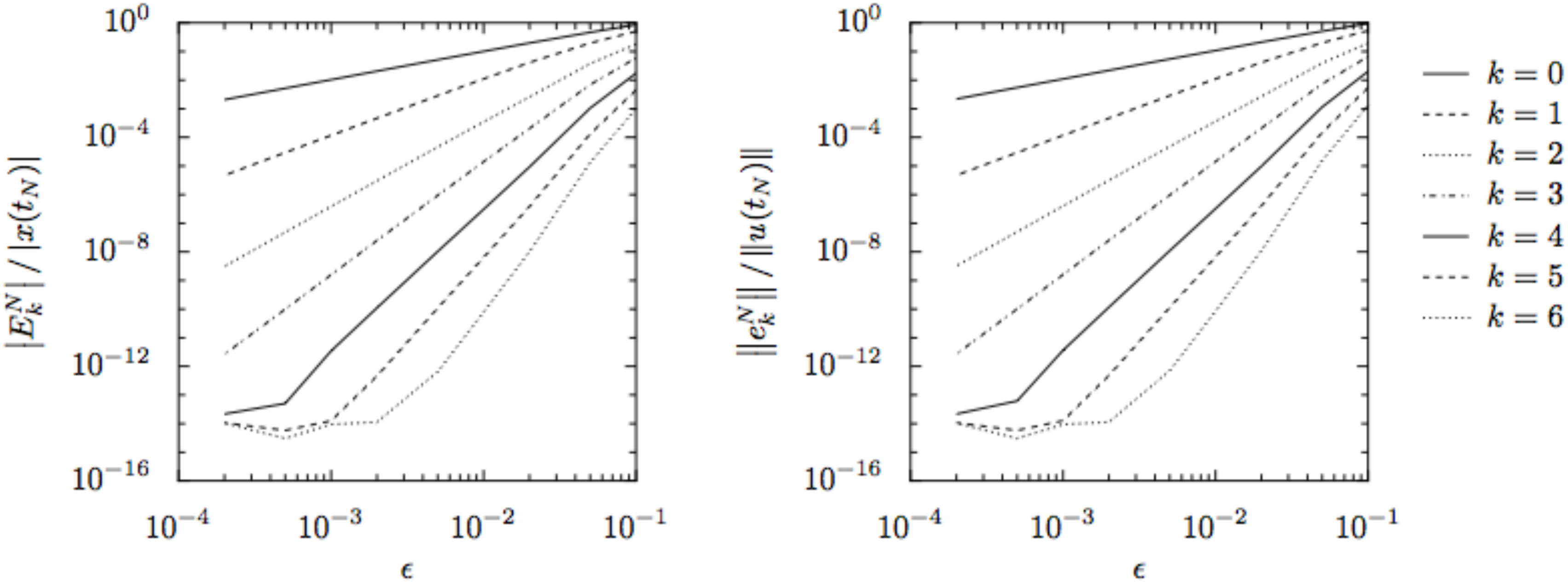
Convergence to exact solution in very few iterations

A nonlinear model

$$
\begin{aligned}
\dot{x}_1 &= A - (y+1)x_1 + x_1^2 x_2, \\
\dot{x}_2 &= y x_1 - x_1^2 x_2, \\
\dot{y} &= \frac{1}{\epsilon}(B_0 - y) - y x_1.
\end{aligned}
$$

No analysis in this case

Similar convergence behaviour



Conclusions and comments

- Parareal algorithm with macroscopic *model* as the coarse propagator

- Convergence to the exact microscopic dynamics proved in a simple case

- Application to more complex problems only relies on straightforward assumptions on time-scale separation and matching operator

- An alternative algorithm in the same spirit exists (Maday, 2007). Our analysis shows that that algorithm converges faster, but is less easily implemented.