Numerical issues in multiscale simulation and the role of approximate macroscopic models

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Based on joint work with

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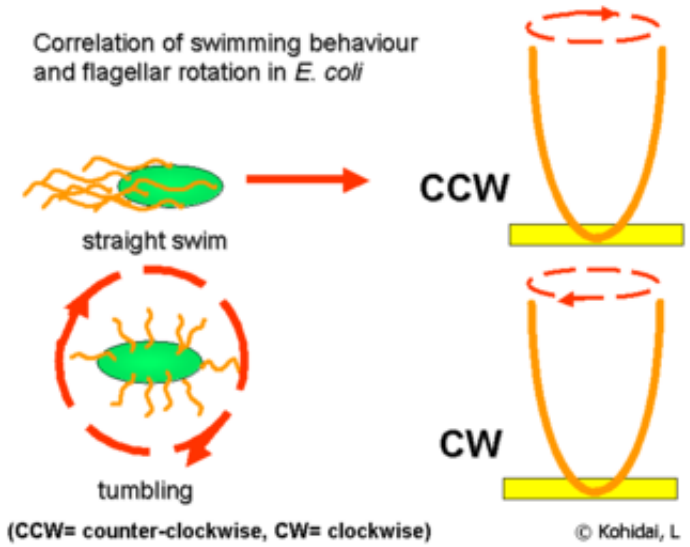
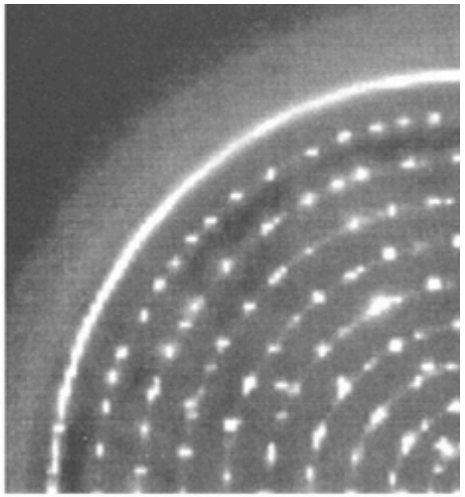
Our challenge in multiscale simulation

Problem statement: Discrepancy between

- macroscopic level of observation/simulation
- microscopic level of the available model



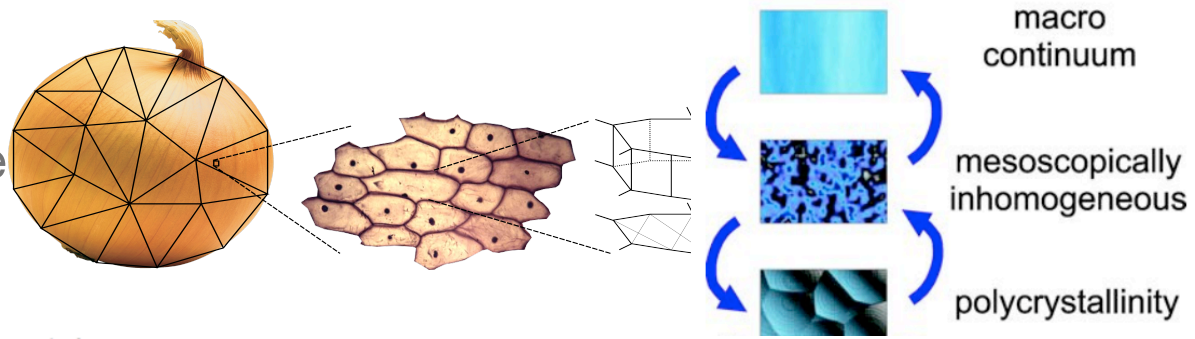


Example : bacterial chemotaxis

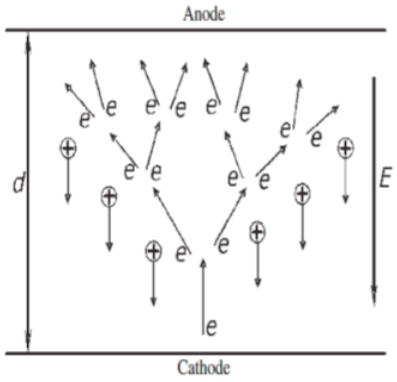
- Microscopic: detailed model for individual bacterium
- Macroscopic: advection-diffusion equation for population

Other example applications

- Deformation of complex (e.g., biological) materials
- Heterogeneous microstructure (polycrystalline, cellular)

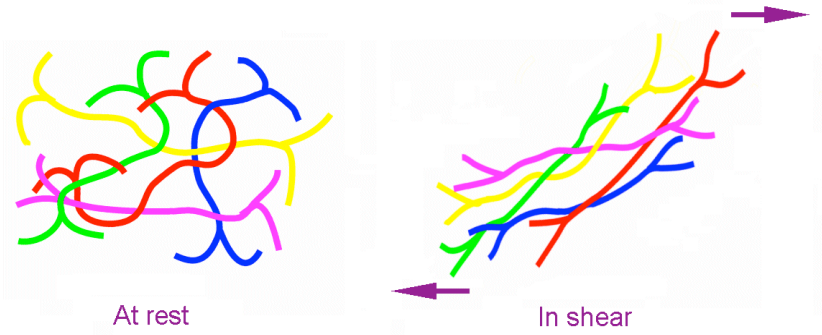


taken from V. Kouznetsova



- Ionization waves in gases
- Model for collisions between individual electrons

- Complex fluid flow: e.g., dilute solution of polymers
- Polymer distribution results in non-Newtonian stress tensor



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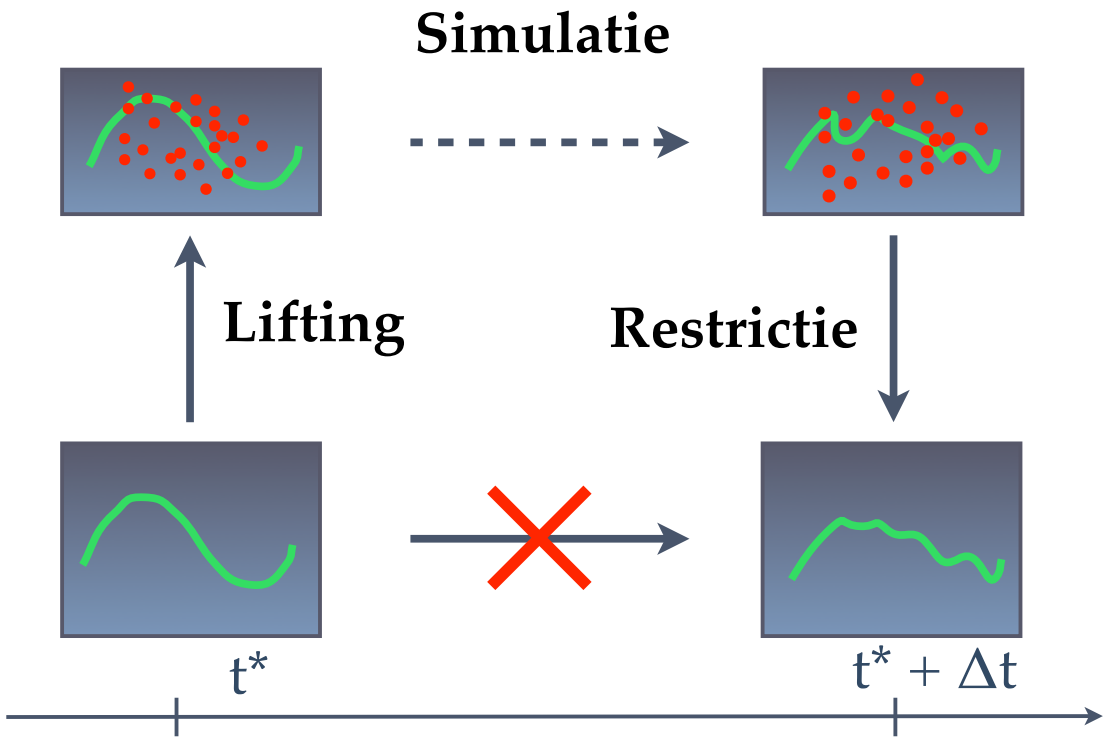
Connecting the levels of description

Microscopic level

- **known model**
- simulation code available

Macroscopic level

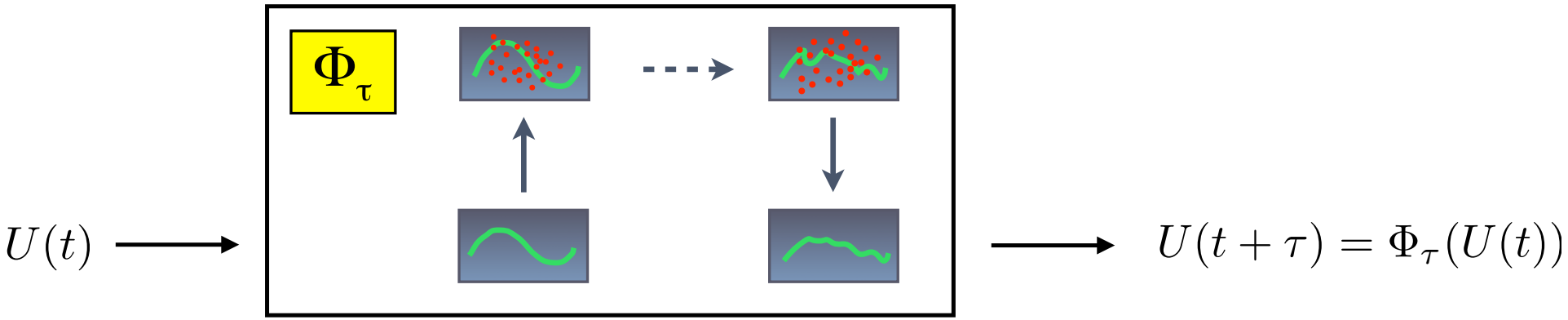
- only **state variables**
- unknown evolution equations



- **Coarse time-stepper** is a wrapper around a microscopic simulation
- Generic building block for computational multiscale algorithms

Kevrekidis et al., 2000 - ... / Kevrekidis & **S**, Annual Review on Physical Chemistry 60:321-344, 2009

Coarse based bifurcation analysis

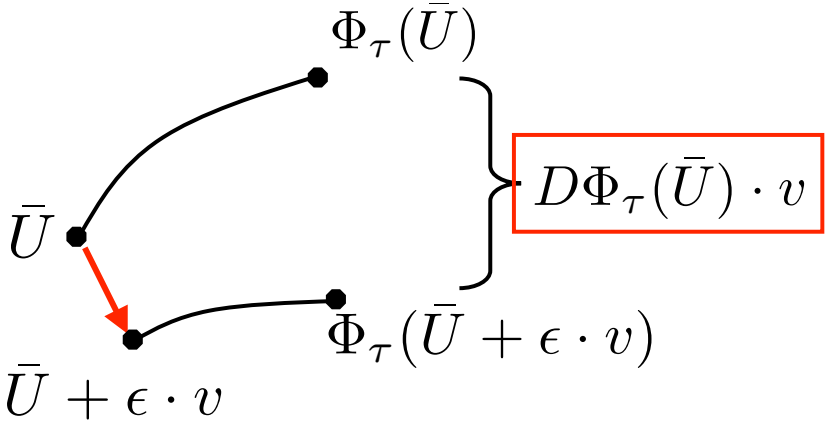


- Time-stepper is a **black box**
- Directly compute macroscopic steady states and their stability

$$U^* - \Phi_\tau(U^*) = 0$$

- Use (matrix-free) iterative methods (RPM, Newton-Krylov) -> **equation-free**

Matrix-vector products



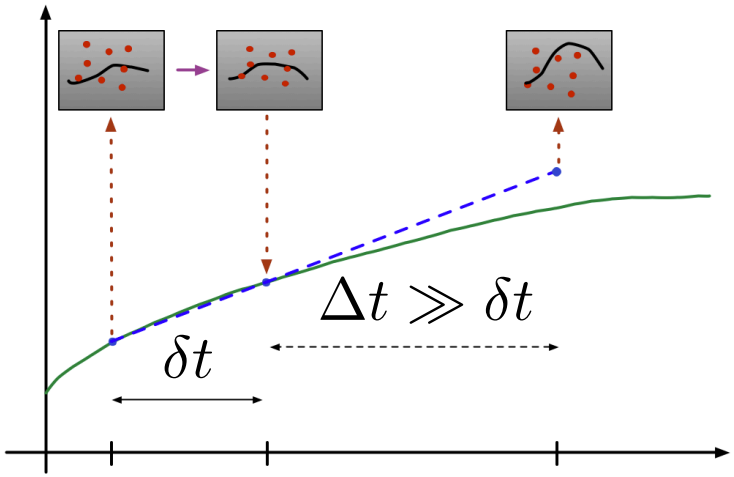
Kevrekidis et al., 2000 - ... / Kevrekidis & **S**, Annual Review on Physical Chemistry 60:321-344, 2009

Acceleration of macroscopic simulation

Exploit a separation in spatial and temporal scales

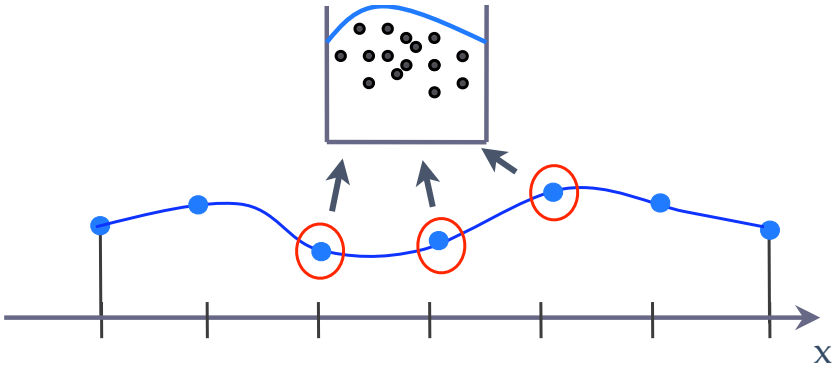
Coarse projective integration

Extrapolate macroscopic state forward in time



Patch dynamics

Interpolate between microscopic simulation in small subdomains



Gear, Kevrekidis, SISC. 24:1091-1106, 2004 / Lafitte, **S**, SISC, 2010, submitted.
S, Roose, Kevrekidis, SIAM MMS 4:278-306, 2005 / **S**, Kevrekidis, Roose, JCP 213(1):264-287, 2006.

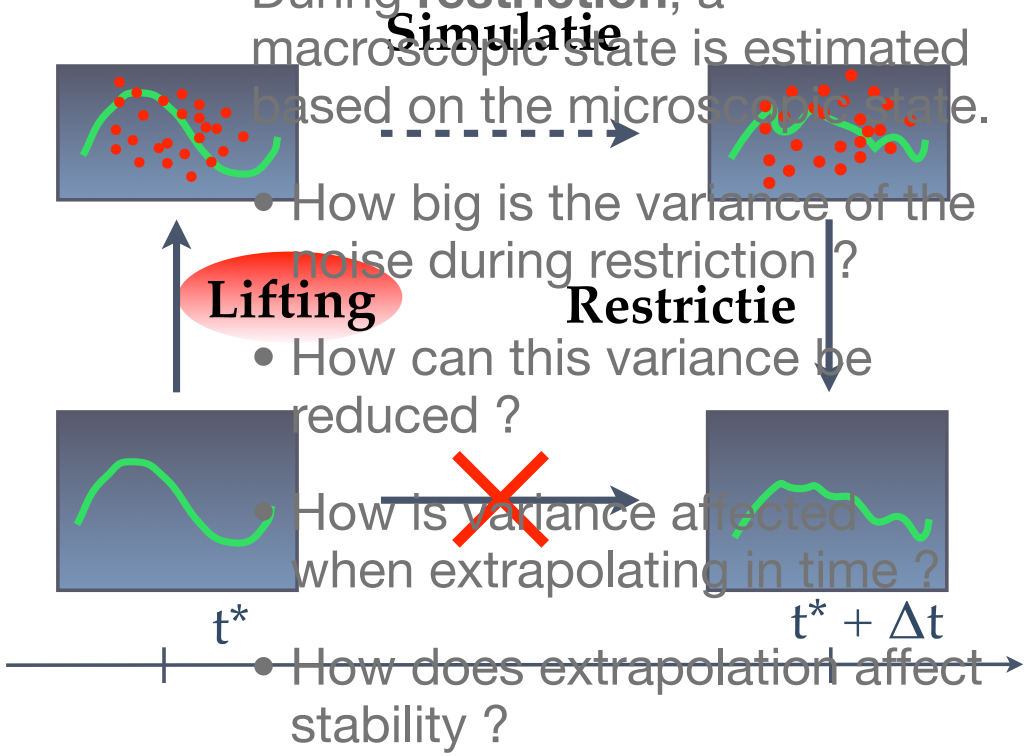
Questions from a numerical analysis viewpoint

During **lifting**, missing microsocpic information is filled in based on the macroscopic state.

- What are appropri macroscopic state variables ?
- How accurate is the reconstruction ?
- What is the influence of lifting errors on macroscopic evolution ?

During **restriction**, a macroscopic state is estimated based on the microscopic state.

- How big is the variance of the noise during restriction ?
- How can this variance be reduced ?
- How is variance affected when extrapolating in time ?
- How does extrapolation affect stability ?



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S, Lelievre, Legat, Computers and Fluids, 2010, in press.

The heterogeneous multiscale methods
An alternative formulation

- Postulate a general form for the unknown macroscopic equation
- Supplement this equation with an estimation of missing macroscopic quantities from a microscopic simulation
  - Initialization of the microscopic model from a given macroscopic state
  - Estimation of a macroscopic quantity from microscopic data
- This formulation has advantages from a numerical analysis viewpoint

E, Engquist, Vanden-Eijnden, et al., 2003 - ...

Plan of the presentation

- Introduction
- Projective and coarse projective integration for singularly perturbed ODEs
- Micro/macro accelerated Monte Carlo simulation of polymeric fluids
- Micro/macro parallel-in-time (parareal) simulation
- Concluding remarks

Multiscale ODEs with invariant manifold structure

- We have a multiscale ODE

$$\begin{aligned} \frac{dx}{dt} &= f(x,y) \\ \frac{dy}{dt} &= \frac{1}{\epsilon} g(x,y) \end{aligned} \qquad \lim_{t\to\infty} \varphi_\xi^t(y) = \eta(\xi) \qquad g(\xi,\eta(\xi)) = 0$$

- Explicit methods have time-step limitation $\delta t = O(\epsilon)$

- We know that a macroscopic model exists when $\epsilon \to 0$

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

- For this macroscopic model, we have $\Delta t = O(1)$

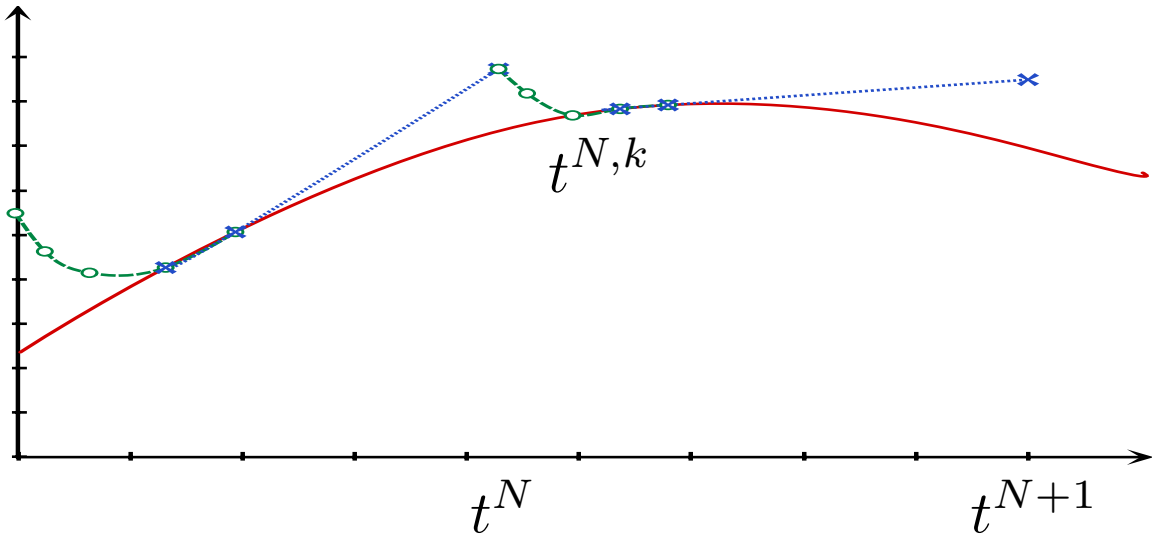
Projective (forward Euler) integration

- Perform $K+1$ explicit "inner" time steps of size $\delta t = O(\epsilon)$

$$u^{N,k+1} = S_{\delta t} u^{N,k}, \qquad t^{N,k} = N\Delta t + k\delta t$$

- Extrapolate forward in time on the large time scale : "outer" step size Δt

$$u^{N+1} = u^{N,K+1} + (\Delta t - (K+1)\delta t)\frac{u^{N,K+1} - u^{N,K}}{\delta t}$$



Gear, Kevrekidis, SISC. 24:1091-1106, 2004

Stability regions in the limit of infinite scale separation

- We know that, for the scale-separated problem, we want

$$\delta t = O(\epsilon), \qquad \Delta t = O(1)$$

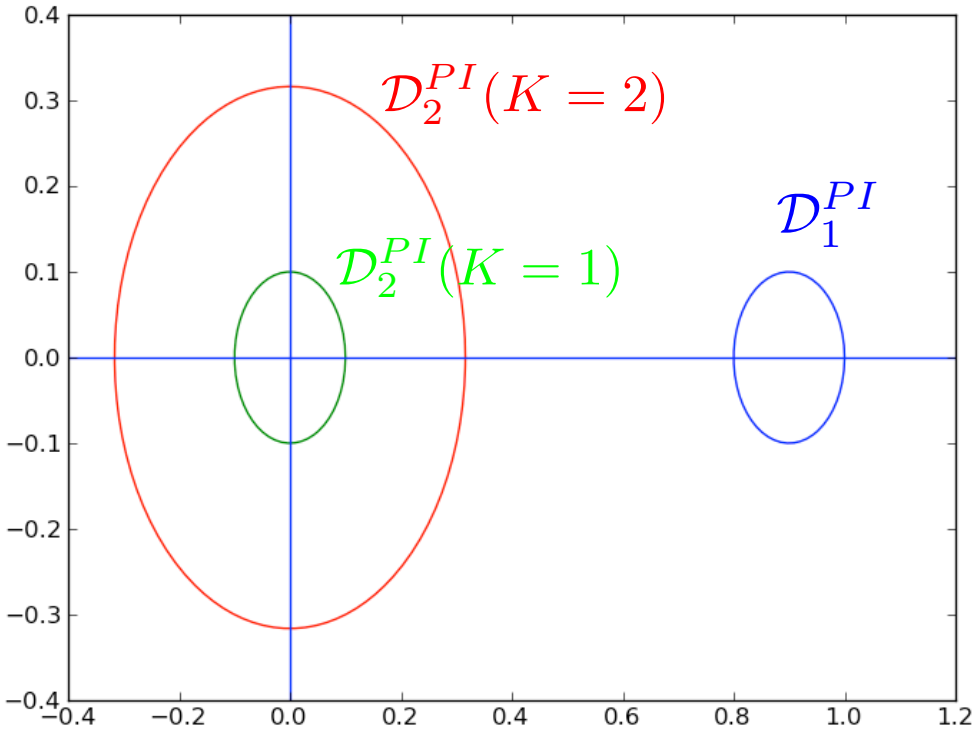
- We therefore look at the limit

$$\delta t / \Delta t \to 0$$

- Then, the projective integration is stable if the eigenvalues of are inside one of two discs

$$\mathcal{D}_1^{PI} = \mathcal{D}\left(1 - \frac{\delta t}{\Delta t}, \frac{\delta t}{\Delta t}\right)$$

$$\mathcal{D}_2^{PI} = \mathcal{D}\left(0, \left(\frac{\delta t}{\Delta t}\right)^{1/K}\right)$$



Gear, Kevrekidis, SISC. 24:1091-1106, 2004

Choice of method parameters : outer time step Δt

- We consider a linear system with multiple time scales, and its forward Euler time discretization

$$\frac{dx}{dt} = \lambda x \qquad x^{n+1} = x^n(1 + \lambda\delta t) = \rho_x x^n$$

$$\frac{dy}{dt} = -\frac{1}{\epsilon} y \qquad y^{n+1} = y^n(1 - \delta t/\epsilon) = \rho_y\, y^n$$

- Slow mode needs to be in a disc

$$\mathcal{D}_1^{PI} = \mathcal{D}\left(1 - \tfrac{\delta t}{\Delta t}, \tfrac{\delta t}{\Delta t}\right) \longrightarrow \boxed{|\lambda \Delta t| < 2}$$

The condition on Δt is independent of δt !!

- Fast mode needs to be in a disc

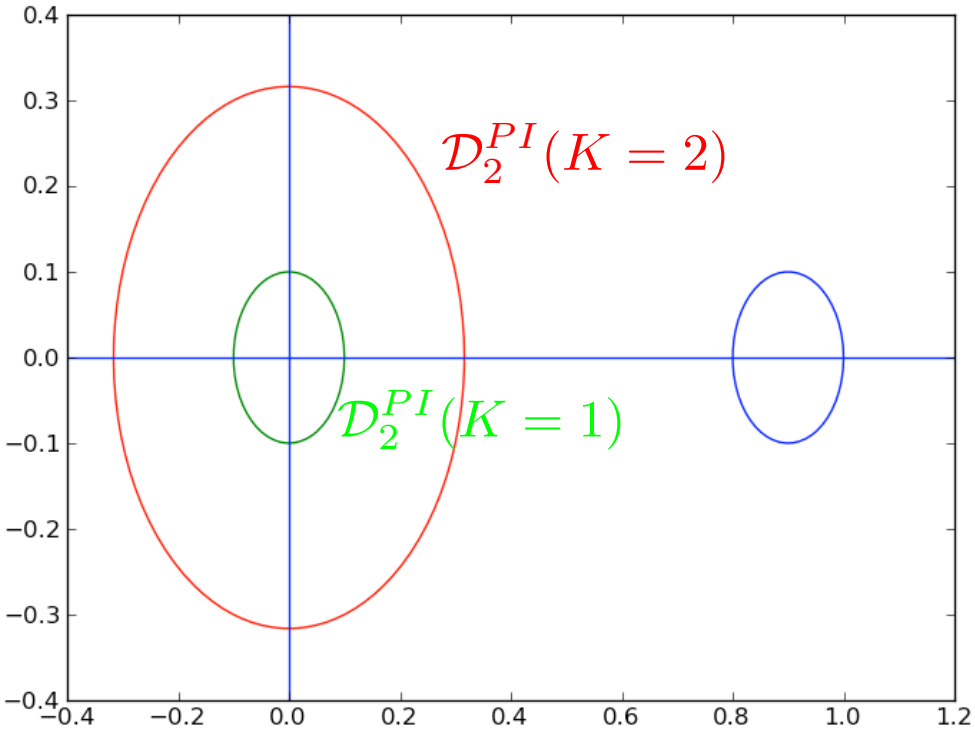
$$\mathcal{D}_2^{PI} = \mathcal{D}\left(0, \left(\tfrac{\delta t}{\Delta t}\right)^{1/K}\right) \longrightarrow \delta t = \alpha\epsilon$$

$$\rho_y = 1 - \alpha$$

Choice of method parameters: number of inner steps K

- Choose K such that the fast eigenvalues are all inside the disc

$$\mathcal{D}_2^{PI} = \mathcal{D}\left(0, \left(\frac{\alpha\epsilon}{\Delta t}\right)^{1/K}\right)$$



- With some algebra, this leads to

$$K = C\log(\epsilon^{-1})$$

Consistency of projective forward Euler
Extrapolation of fast modes

- Consider inner forward Euler/projective forward Euler for the fast equation

$$\frac{dy}{dt} = -\frac{1}{\epsilon}y \qquad\qquad y^{n+1} = y^n(1-\alpha)$$

- Projective integration for the fast modes reads

$$y^{N+1} = y^{N,K+1} + (\Delta t - (K+1)\delta t)\,\frac{y^{N,K+1} - y^{N,K}}{\delta t}$$

- We have

$$\frac{y^{N,K+1} - x^{N,K}}{\delta t} = \frac{((1-\alpha)-1)(1-\alpha)^K y^N}{\alpha\epsilon} = \frac{-(1-\alpha)^K y^N}{\epsilon}$$

- Unlike for the slow modes, this is not a good approximation to the time derivative (only damping is achieved !) -> we make an $O(1/\epsilon)$ during extrapolation, which needs to be damped -> $K = O(\log(1/\epsilon))$

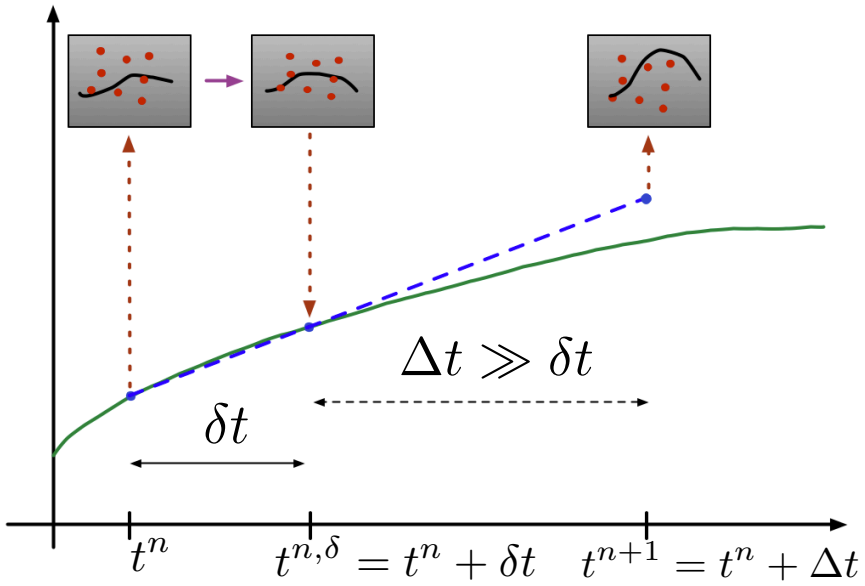
Coarse projective integration

- Start from a macroscopic state

$$X = X^n$$

- **Lift** to the corresponding microscopic state

$$\mathcal{L} : X = X^n \mapsto (x^n = X^n, y^n \approx \eta(X^n))$$



- Evolve over a microscopic time step

$$s : t^n \to t^n + \delta t :: (x^n, y^n) \mapsto \left(x^{n,\delta}, y^{n,\delta}\right)$$

- **Restrict** to macroscopic state

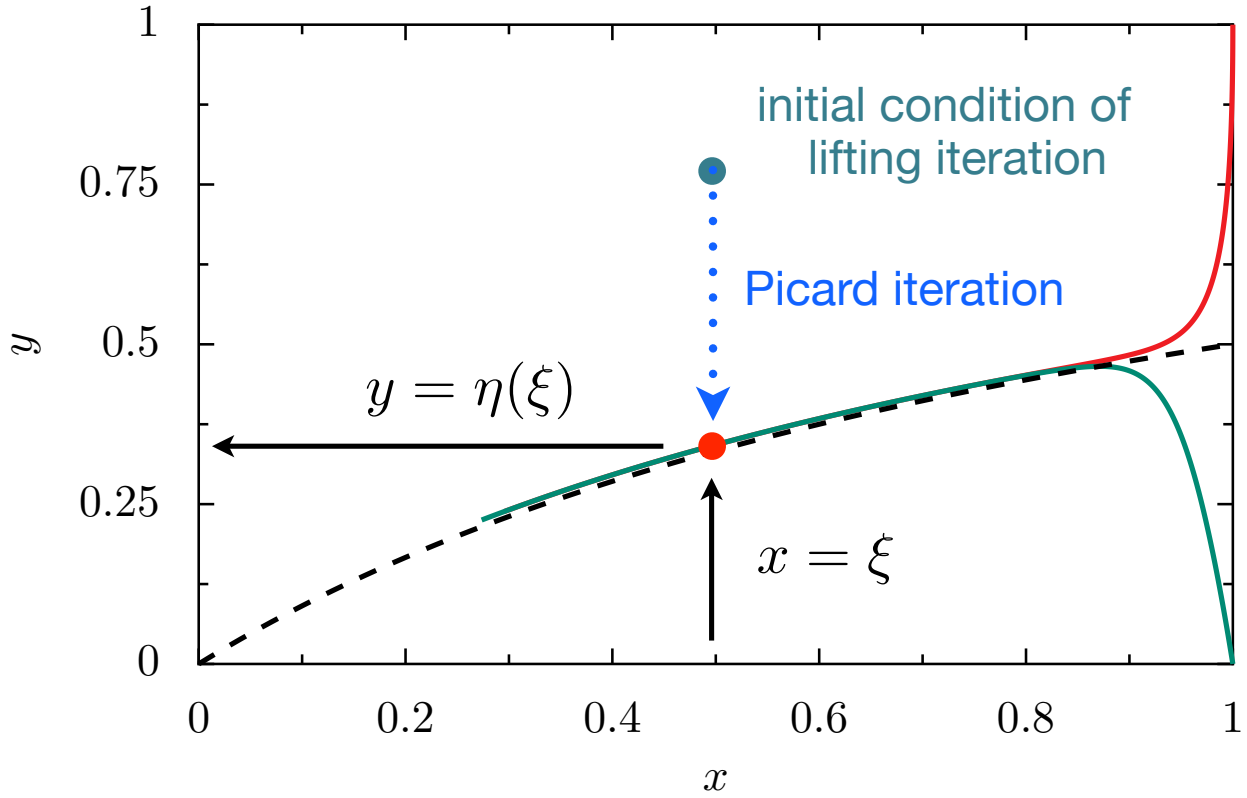
$$X^{n,\delta} = x^{n,\delta}$$

- Extrapolate macroscopic state

$$X^{n+1} = X^{n,\delta} + (\Delta t - \delta t)\frac{X^{n,\delta} - X^n}{\delta t}$$

One strategy for lifting : Picard iteration

$$y^{n,m+1} = y^{n,m} + \delta t \; g(x^n, y^{n,m}), \qquad m = 0, \ldots, M$$



When we just keep $y^{n,0} = y^{n-1,K}$, then $K = O(1)$

Challenge for multiscale SDEs

- We have a multiscale SDE

$$\begin{aligned} dx &= f(x,y)dt \\ dy &= \frac{1}{\epsilon}g(x,y)dt + \frac{1}{\sqrt{\epsilon}}\beta(x,y)dW \end{aligned}$$

$$\lim_{t\to\infty} \rho_\xi(y,t) = \rho_\xi^\infty(y)$$

- Implicit methods don't work; explicit methods have a time-step restriction

$$\delta t = O(\epsilon)$$

- We know that a macroscopic model exists when $\epsilon \to 0$

$$\frac{dX}{dt} = F(X) = \int f(X,y)d\mu_X(y) = \int f(X,y)\rho_X^\infty(y)dy$$

- For this macroscopic model, we have $\Delta t = O(1)$

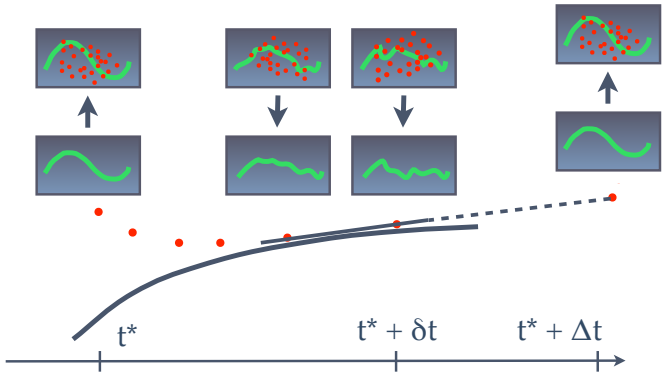
Coarse projective integration for problems that require averaging

- Start from a macroscopic state

$$X = X^n$$

- Lift to the corresponding microscopic state

$$\mathcal{L} : X = X^n \mapsto \{(x_i^n = X^n, y_i^n)\}_{i=1}^I, \quad y_i^n \sim \mu_{X^n}(y)$$



- Evolve each of the realizations over a microscopic time

$$s : t^n \to t^n + \delta t :: \{(x_i^n, y_i^n)\}_{i=1}^I \mapsto \left\{\left(x_i^{n,\delta}, y_i^{n,\delta}\right)\right\}_{i=1}^I$$

- Restrict to macroscopic state

$$X^{n,\delta} = \frac{1}{I}\sum_{i=1}^{I} x_i^{n,\delta}$$

- Extrapolate macroscopic state

$$X^{n+1} = X^{n,\delta} + (\Delta t - \delta t)\frac{X^{n,\delta} - X^n}{\delta t}$$

Heterogeneous multiscale method for problems that require averaging

- Historically, for problems that require averaging, a slightly different algorithm was proposed first in the context of the heterogeneous multiscale method
- Propose a numerical method for the unknown macroscopic equation

$$X^{n+1} = X^n + \Delta t \; F(X^n)$$

- Supplement with an estimator for the unknown function F
  - Lifting for macroscopic state to microscopic state

$$\mathcal{L} : X = X^n \mapsto \{(x_i^n = X^n, y_i^n)\}_{i=1}^I \,, \quad y_i^n \sim \mu_{X^n}(y)$$

  - Replace restriction by the required estimation

$$F(X^n) = \frac{1}{I} \sum_{i=1}^{I} f(X^n, y_i^n)$$

Constrained simulation to sample invariant measure

- We want the invariant distribution of

$$dy = \frac{1}{\epsilon} g(\xi, y)dt + \frac{1}{\sqrt{\epsilon}} \beta(\xi, y)dW$$

- **Use ergodicity :**
  - if a time average is equivalent to an ensemble average, we can simulate

$$y^{m+1} = y^n + g(\xi, y^m)\Delta t + \beta(\xi, y^m)\Delta W$$

  - and compute the restriction as

$$\hat{F}(X^n) = \frac{1}{M} \sum_{m=1}^{M} f(X^n, y^m) \approx \int f(X^n, y) d\mu_{X^n}(y)$$

Plan of the presentation

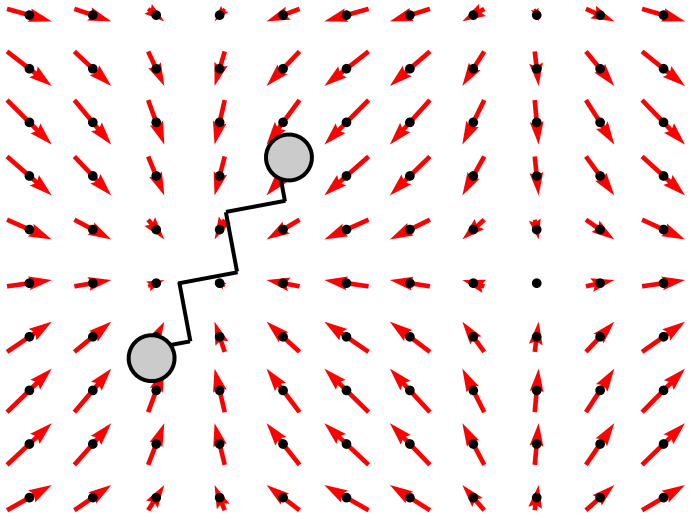
- Introduction
- Projective and coarse projective integration for singularly perturbed ODEs
- **Micro/macro accelerated Monte Carlo simulation of polymeric fluids**
- Micro/macro parallel-in-time (parareal) simulation
- Concluding remarks

Micro-macro simulation of dilute polymer solutions

Macroscopic part : Navier-Stokes equations for solvent

$$\mathrm{Re}\left(\frac{\partial u}{\partial t} + u \cdot \nabla u\right) = (1-\epsilon)\Delta u - \nabla p + \mathrm{div}(\tau_p)$$

$$\mathrm{div}(u) = 0$$



Coupling : non-Newtonian stress tensor (Kramers' formula)

$$\tau_p = \frac{\epsilon}{\mathrm{We}}\langle X \otimes F(X)\rangle - \mathrm{Id}$$

Microscopic part : Stochastic differential equation (SDE) for the configuration of an individual polymer

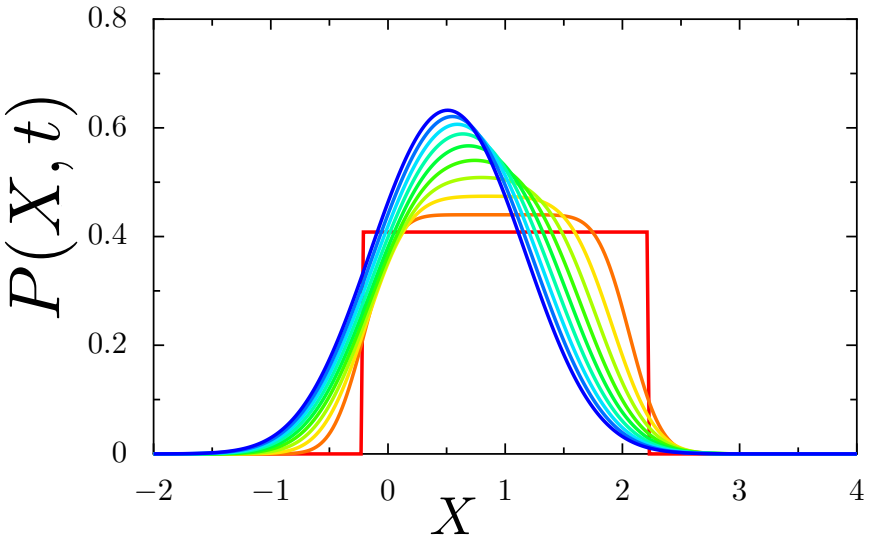
$$dX = \left[\kappa(t)\, X - \frac{1}{2\mathrm{We}} F(X)\right] dt + \frac{1}{\sqrt{\mathrm{We}}} dW_t,$$

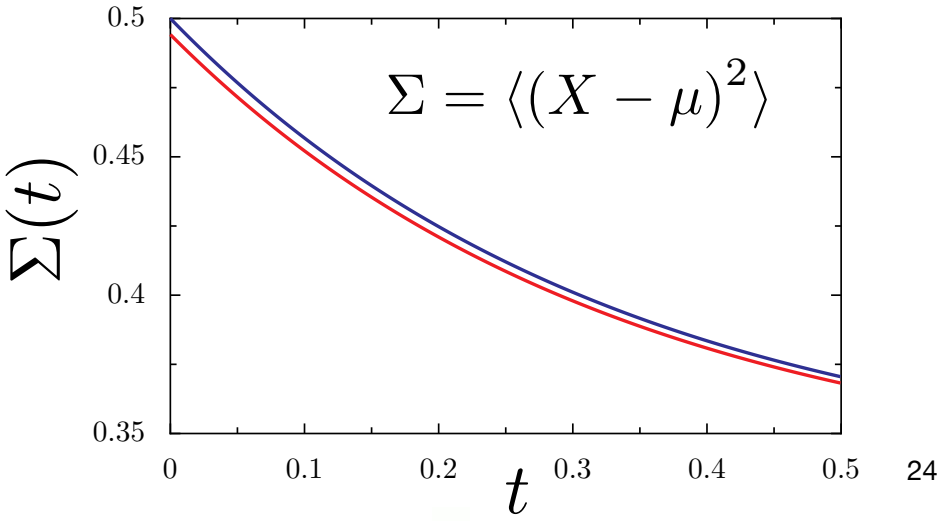
Laso, Öttinger, J. Non-Newtonian Fluid Mech. 47 (1993) 1-20.

Example 1 : Linear springs

$$dX = \left[\kappa(t)\, X - \frac{1}{2\mathrm{We}} F(X)\right] dt + \frac{1}{\sqrt{\mathrm{We}}} dW_t, \qquad F(X) = X$$

- Stress tensor $\tau_p \sim \langle X F(X) \rangle \propto \langle X^2 \rangle$
- Sign of X is irrelevant (length of spring), so $\mu = \langle X \rangle \to 0$
- Distribution of X evolves towards a Gaussian
- Closed model for evolution of the variance $\dfrac{d\Sigma}{dt} = -2\left(\kappa(t) - \dfrac{1}{2\mathrm{We}}\right)\Sigma + \dfrac{2}{\mathrm{We}}$





Example 2 : FENE springs

- Finitely extensible nonlinearly elastic (FENE)

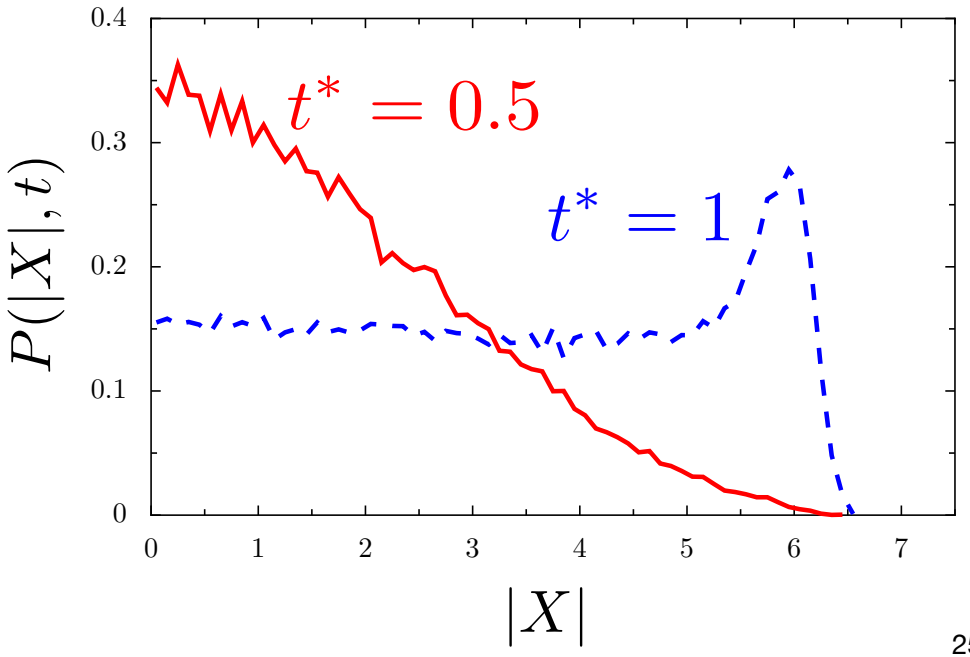
$$dX = \left[\kappa(t)\, X - \frac{1}{2\mathrm{We}} F(X)\right] dt + \frac{1}{\sqrt{\mathrm{We}}} dW_t, \qquad F(X) = \frac{X}{1 - X^2/b}$$

- Distribution becomes non-Gaussian (with sharp peak)

- Impossible to represent exactly with a finite number of moments

$$\mathbf{U}^{[L]} = (U_l)_{l=1}^{L}$$
$$U_l = \left\langle X^{2l} \right\rangle$$

- Monte Carlo simulation required (especially in higher dimensions !)

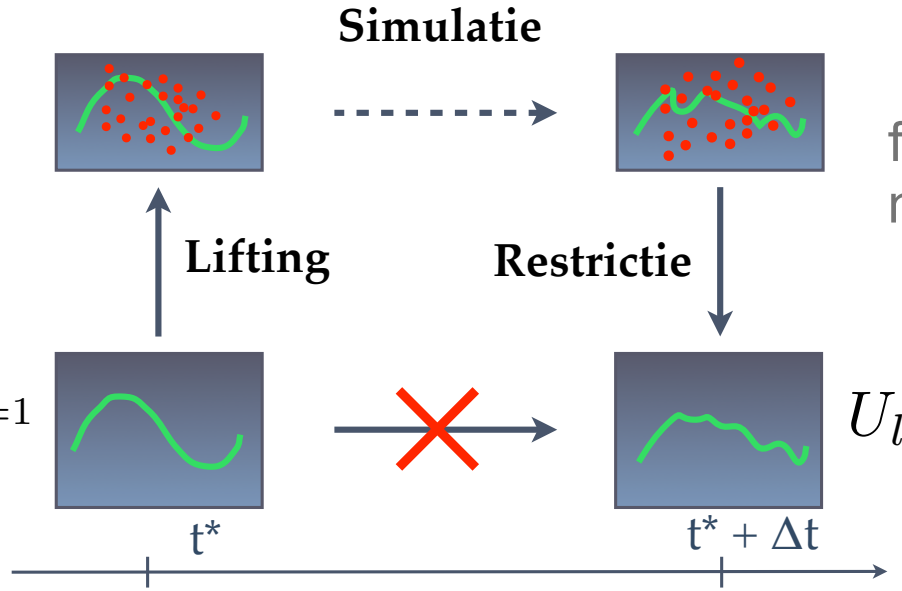


Coarse time-stepper for Monte Carlo simulation

Microscopic level

$$d\mathcal{X} = \left[\kappa(t)\,\mathcal{X} - \frac{1}{2\mathrm{We}}F(\mathcal{X})\right]dt + \frac{1}{\sqrt{\mathrm{We}}}d\mathcal{W}_t$$

$$\mathcal{X}^{k+1} = s_X(\mathcal{X}^k, \kappa(t), \delta t)$$



from moments to an ensemble

$\mathcal{L} : \mathbf{U} \mapsto \mathcal{X} = \{X_j\}_{j=1}^{J}$

from an ensemble to moments

$\mathcal{R} : \mathcal{X} \mapsto \mathbf{U}$

$U_l = \frac{1}{J}\sum_{j=1}^{J} f_l(X_j)$

Macroscopic level

$$\mathbf{U}^{[L]} = (U_l)_{l=1}^{L}$$

$$U_l = \left\langle X^{2l} \right\rangle$$

$$\frac{d\mathbf{U}}{dt} = \mathcal{H}(\mathbf{U}, \kappa(t))$$

$$\tau_p = T(\mathbf{U})$$

Lifting operator : constrained simulation

- Simulate with constrained macroscopic state until conditional equilibrium

$$\mathcal{X}^{*,m+1} = s_X(\mathcal{X}^{*,m}, \kappa^*, \delta t) + \Lambda \nabla_{\mathcal{X}} \mathcal{R}(\mathcal{X}^{*,m+1}),$$
$$\text{met } \Lambda \in \mathbb{R}^L \text{ zodanig dat } \mathcal{R}(\mathcal{X}^{*,m+1}) = \mathbf{U}^*$$

  - Time integration, followed by projection onto manifold defined by imposed macroscopic state

$$\mathcal{X}^{*,m+1} = \arg\min \left\| \mathcal{X}^{*,m+1} - s_X(\mathcal{X}^{*,m}, \kappa^*, \delta t) \right\|$$
$$\text{with constraint } \mathcal{R}(\mathcal{X}^{*,m+1}) = \mathbf{U}^*$$

- The result of the lifting is then given as (for M sufficiently large)

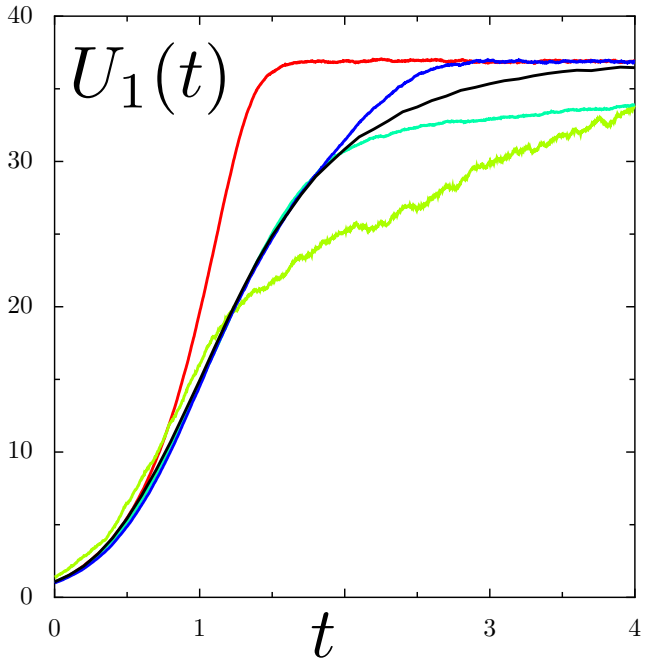
$$\mathcal{X}^* = \mathcal{L}(\mathbf{U}^*) := \mathcal{X}^{*,M}$$

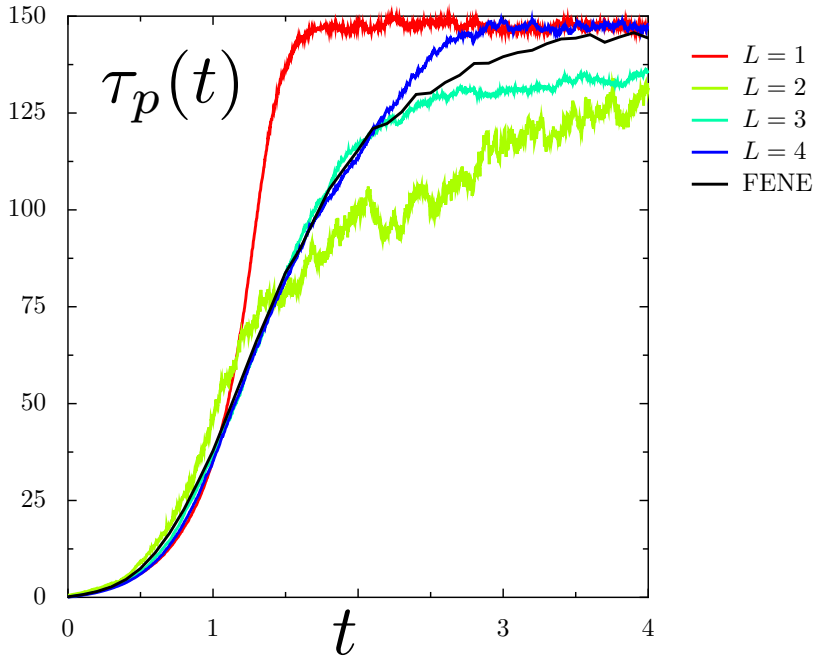
- Consistent initial condition also by projection of a nearby ensemble

S, Lelievre, Legat, Computers and Fluids, 2010, in press.

Lifting induces a closure approximation

- Experiment
  - Coarse time-stepper with very small time step
  - Macroscopic state variables : $\mathbf{U}^{[L]} = (U_l)_{l=1}^{L}, \qquad U_l = \langle X^{2l} \rangle$
  - (Much more expensive than full microscopic simulation)
- Lifting introduces **modeling error** that decreases for an increasing number of moments





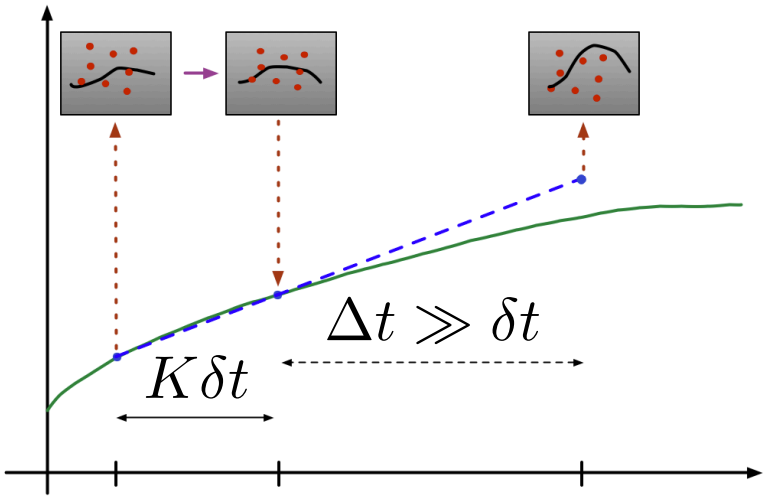
Extrapolation via coarse projective integration

- Start with a given macroscopic state

$$\mathbf{U} = \mathbf{U}^N$$

- **Lift** to the corresponding microscopic state

$$\mathcal{L} : \mathbf{U} = \mathbf{U}^N \mapsto \mathcal{X}^N = \mathcal{X}^{N,M}$$



- **Simulate** the ensemble over K microscopic steps

$$\mathcal{X}^{N,k+1} = s_X(\mathcal{X}^{N,k}, \kappa(t^{N,k}), \delta t), \quad k = 0, \ldots K-1$$

- **Restrict** to macroscopic state

$$\mathbf{U}^{N,K} = \mathcal{R}(\mathcal{X}^{N,K})$$

- **Extrapolate** macroscopic state

$$\mathbf{U}^{N+1} = \mathbf{U}^{N,K} + (\Delta t - K\delta t)\frac{\mathbf{U}^{N,K} - \mathbf{U}^N}{K\delta t}$$

Efficiency and accuracy of coarse projective integration

- Coarse projective integration is efficient if

$$\Delta t \gg (M + K)\delta t$$

Number of constrained steps during lifting

Number of steps to estimate time derivative

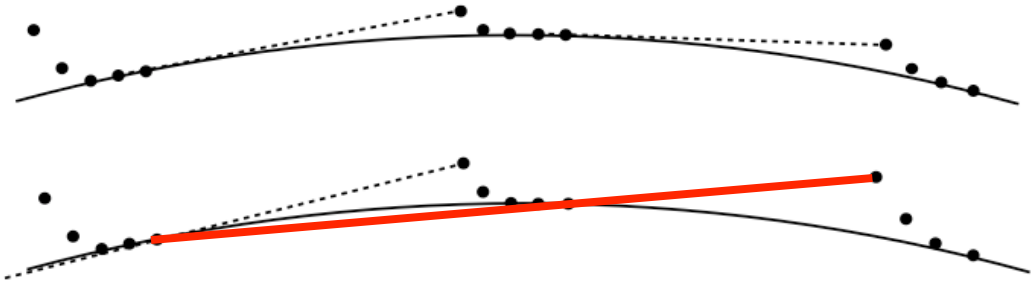
  - The bigger the time scale separation ($\mathrm{We} \to 0$), the smaller M can be
  - But: in the limit when $\mathrm{We} \to 0$, the macroscopic model is known !
  - *Real* acceleration is only possible for an intermediary regime

- During extrapolation, estimation noise is amplified with a factor $\Delta t / K \delta t$
  - A similar statistical error is obtained using less particles and no extrapolation
  - For equal statistical error, coarse projective integration requires as much computations as a full microscopic simulation (assuming M=0 !)

An alternative extrapolation strategy
Multistep state extrapolation

- Projective integration

$$\mathbf{U}^{N+1} = \mathbf{U}^{N,K} + (\Delta t - K\delta t)\frac{\mathbf{U}^{N,K} - \mathbf{U}^{N}}{K\delta t}$$



- Multistep state extrapolation
  - Extrapolate using the last point of each *sequence* of microscopic simulation

$$\mathbf{U}^{N+1} = \mathbf{U}^{N,K} + (\Delta t - K\delta t)\frac{\mathbf{U}^{N,K} - \mathbf{U}^{N-1,K}}{\Delta t}$$

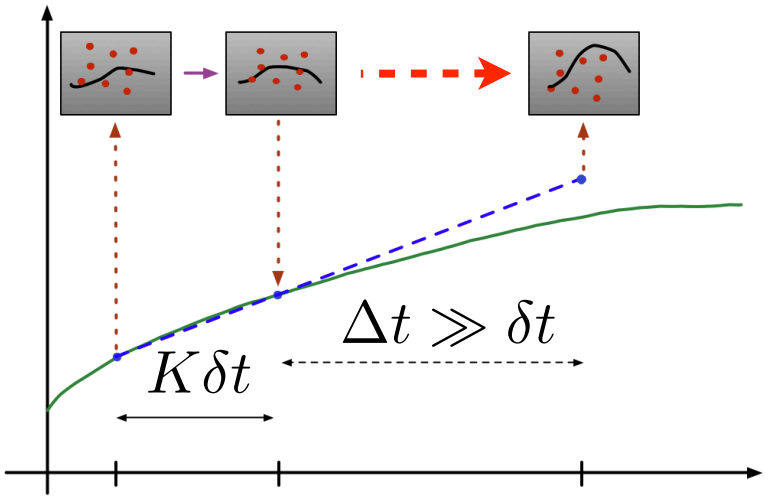
  - *Statistical* error is unaffected
  - *Systematic* error does get amplified with a factor $\Delta t / K\delta t$
  - But we want to extrapolate ***just because*** we can tolerate a larger systematic error !

Sommeijer, Comput. Math. Appl. 19 (6) (1990) 37–49.

Projection: an alternative for lifting

- "Classical" lifting :
  - project an ensemble on $t = t^{N,K}$ onto an extrapolated macroscopic state on $t = t^{N+1}$
  - simulate with macroscopic constraint until conditional equilibrium (M steps)
- Alternative : perform projection **without** constrained simulation
  - The time gained during extrapolation is not lost during constrained simulation
  - The projected ensemble now also depends on the ensemble at the previous time step !

$$\mathcal{X}^{N+1,N+1} = \mathcal{P}(\mathbf{U}^{N+1,N+1}; \mathcal{X}^{N,K})$$

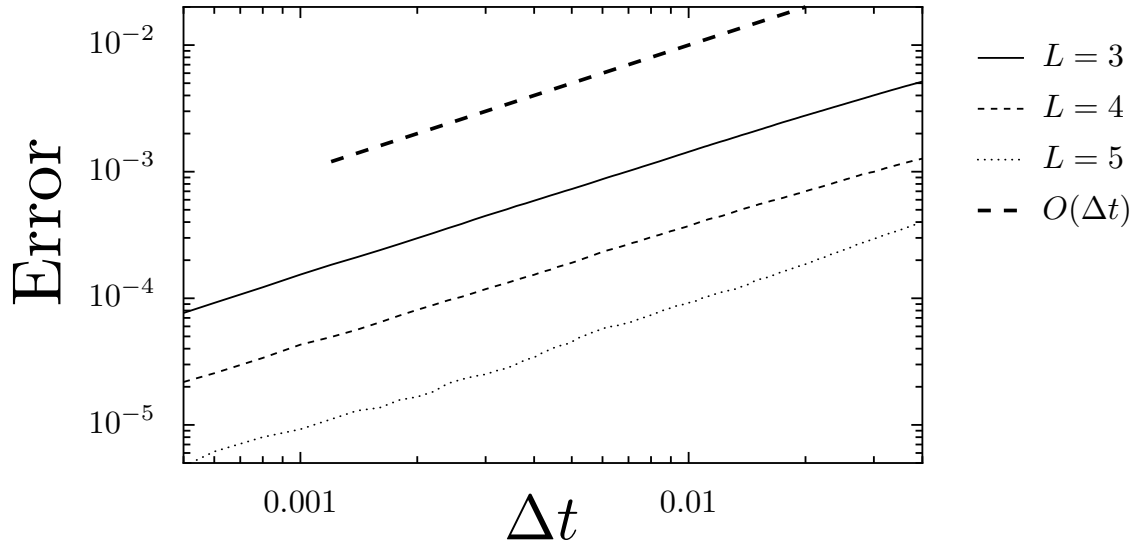


Debrabant, **S**, SIAM MMS, 2010, submitted.

Accuracy of projection operator

- Experiment
  - Macroscopic state variables : $\mathbf{U}^{[L]} = (U_l)_{l=1}^{L}, \qquad U_l = \langle X^{2l} \rangle$
  - Simulate until time t*
  - Project $\mathcal{X}(t^* - \Delta t)$ onto manifold defined by $\mathbf{U}^{[L]}(t^*)$ and compare with $\mathcal{X}(t^*)$
- Projection introduces a modeling error that decreases with
  - increasing number of moments
  - decreasing extrapolation time step

$$\text{Error} \sim C_L \Delta t$$

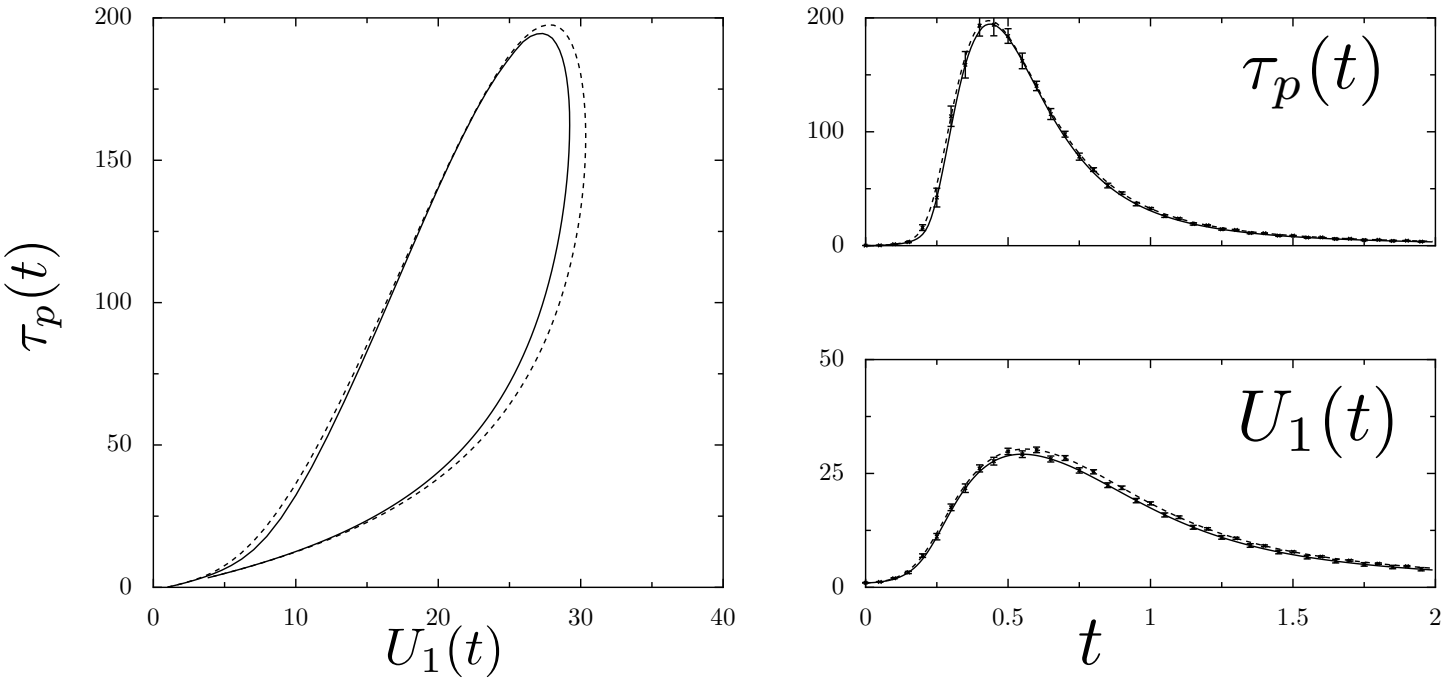


2-sample K-S test

L	p-value
3	0
4	7,00E-06
5	0,28
6	0,25
7	0,84

Numerical illustration

- Experiment
  - macroscopic state variables $U_1 = \langle X^2 \rangle,\ U_2 = \langle X F(X) \rangle$
  - strongly time dependent velocity gradient $\kappa(t) = 100\ t\ (1-t)\ \exp(-4t)$
  - adaptive macroscopic time step
- Average gain of factor 4 in regime without strong scale separation



Plan of the presentation

- Introduction
- Projective and coarse projective integration for singularly perturbed ODEs
- Micro/macro accelerated Monte Carlo simulation of polymeric fluids
- **Micro/macro parallel-in-time (parareal) simulation**
- Concluding remarks

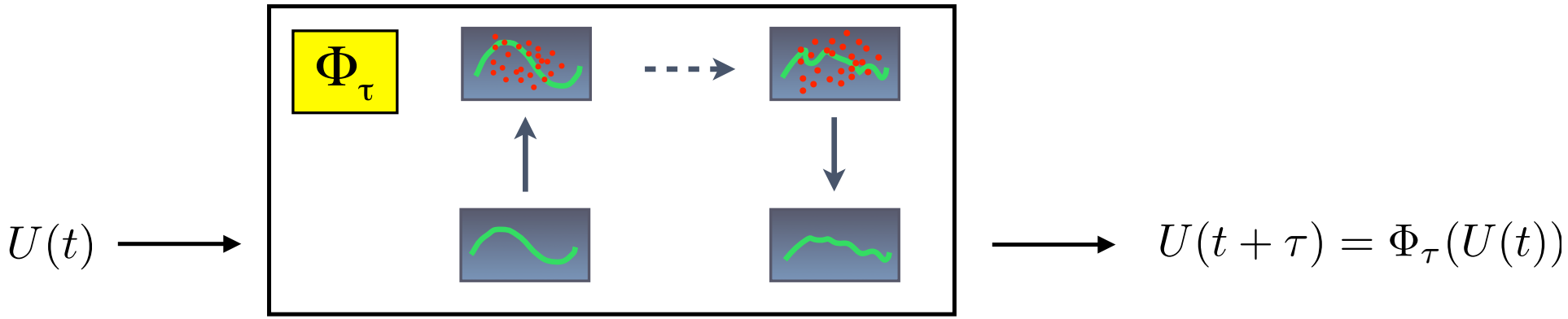
Conclusions

- Coarse projective integration is a technique to accelerate simulation **by inducing a numerical closure approximation**
- The numerical closure is imposed by the lifting and prohibits convergence to the macroscopic image of the microscopic dynamics
- Replacing the lifting by a projection of the microscopic state on the manifold defined by a certain macroscopic state allows for full convergence

What I did not talk about

- Approximate macroscopic models can be used in a multilevel hierarchy, similar to multigrid
- Approximate macroscopic models can be useful to precondition Krylov methods in coarse bifurcation analysis
- One can build variance reduction techniques based on a limiting macroscopic equation
- Multiscale algorithms of this type can have significant advantages in several applications: polycrystalline materials, biological tissue, electromagnetism, ...

Equation-free time-stepper based bifurcation analysis

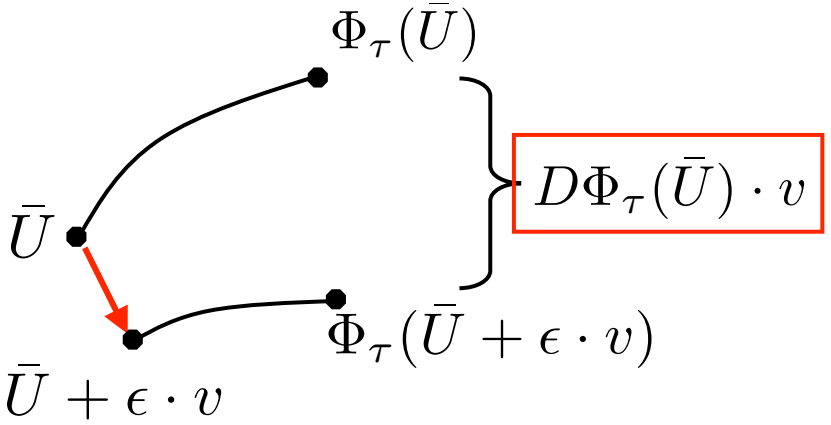


- Time-stepper is a **black box**
- Directly compute macroscopic steady states and their stability

$$U^* - \Phi_\tau(U^*) = 0$$

- Use (matrix-free) iterative methods (RPM, Newton-Krylov)

Matrix-vector products



Kevrekidis et al., 2000 - ... / Kevrekidis & **S**, Annual Review on Physical Chemistry 60:321-344, 2009