Colloquium du CERMICS

École des Ponts
ParisTech

Multiscale dynamical systems and parareal algorithms

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7 juin 2018

Multiscale dynamical systems and parareal algorithms

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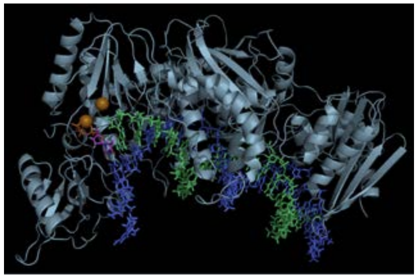
CERMICS Colloquium, École Nationale des Ponts et Chaussées, June 7, 2018

Outline

1. The challenge of multiscale dynamical systems
2. Information theory and averaging
3. Heterogeneous multiscale methods for ODEs
4. Parareal: parallel integration in time
5. Milestoning
6. Phase plane map based parareal integration
7. Conclusions

1. The challenge of multiscale dynamical systems



Quantum mechanics "Schrödinger"	Molecular Dynamics "Newton"	Protein folding	Time (s)
10^{-15}	10^{-9}	1	

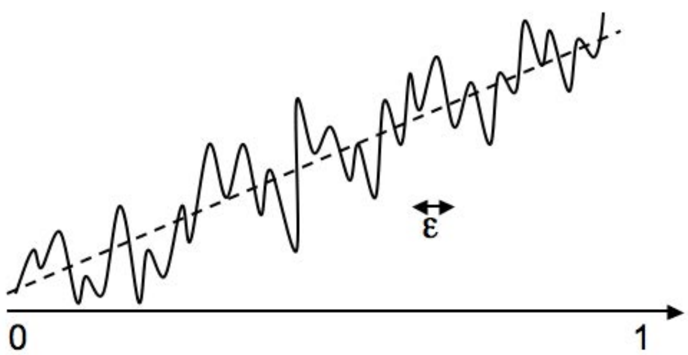
Comet passing	Planetary motion	Galaxy dynamics	Time (s)
10^{2}	10^{7}	10^{15}	

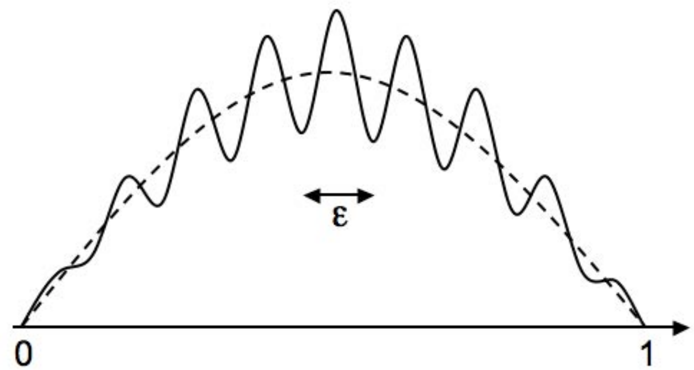
….the ultimate targets

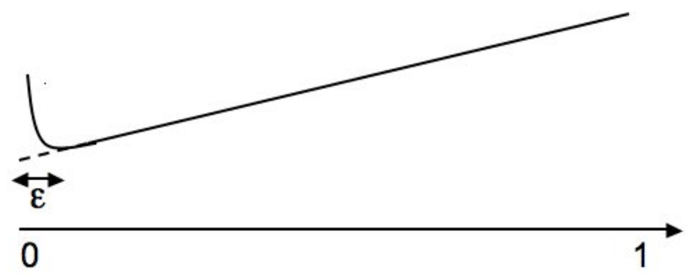
Multiscale functions

Examples of multiscale

Functions $u_\varepsilon(x)$







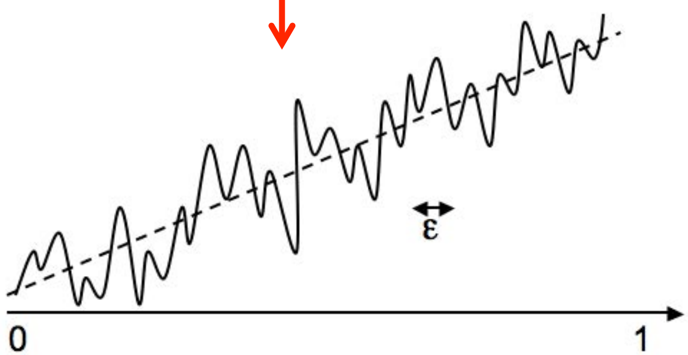
Random, periodic and

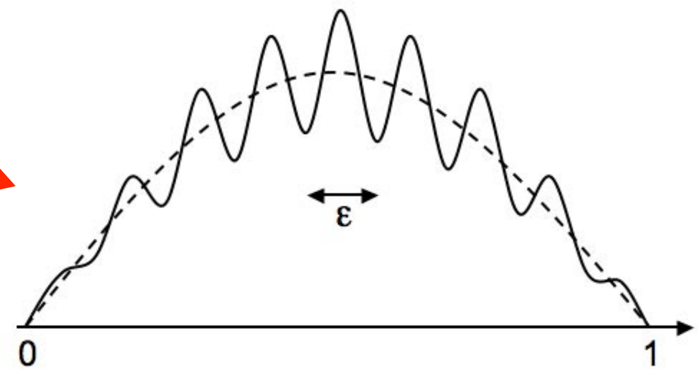
Localized multiscales

Multiscale functions

Microscales globally

focus for us now

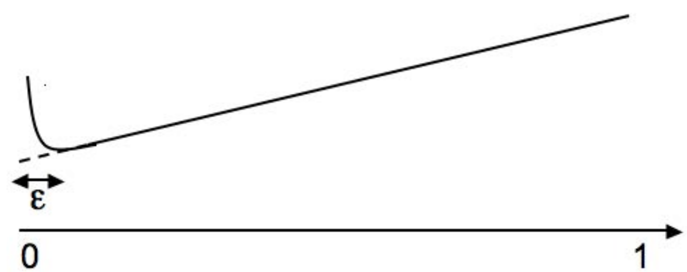




Localized microscales

typically resolved by adaptive

meshing and stiff solvers



Multiscale functions

1. In our analysis we will define the scales more explicitly, for example, by a scaling law. The function $u_\varepsilon(x) = u(x,x/\varepsilon)$ for local and oscillatory

$$u(x,y) \to U(x),\ \ y \to \infty, \quad u(x,y)\ periodic\ in\ y$$

2. The scales are also naturally described by a scale-based transform of a function as, for example, Fourier series

$$u_\varepsilon(x) = a_0 + \sum_{j=1}^{J} b_j \sin(2\pi jx) + a_j \cos(2\pi jx)$$

- For clarity in the presentation we will often consider "two-scale" problems: a macro-scale in the range of O(1) and a micro-scale with wave-lengths O(ε)

Computational challenges

- Large amount of data (variables, unknowns, degrees of freedom, samples, …) are needed to describe a multiscale object of function.
  - Nyquist – Shannnon sampling theorem: at least 2 data points per wavelength in each dimention (will return to this)
- Computing with a large number of variable requre a large number of computer operations, flops

$$\#\, samples > (2/\varepsilon)^d$$

$$\#\, flop = O((N(\delta,\varepsilon)/\varepsilon)^{dr})$$

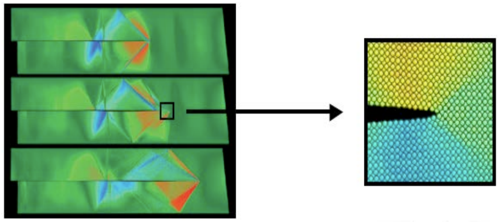
ε: smallest wavelength, domain O(1)
N: unknowns / wavelength for given accuracy δ,
r : exponent for number of flops/unknown

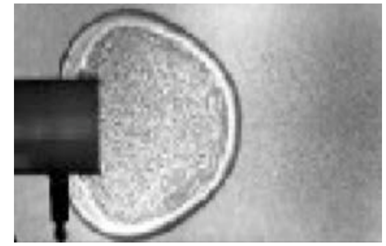
The Heterogeneous Multiscale Method (HMM)

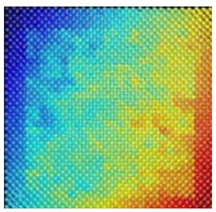
- We will follow the framework of Heterogeneous Multiscale Methods (HMM) for designing numerical methods coupling models with different scales, [E, E. 2003]
  - Design macro-scale scheme for the desired variables. The scheme efficient but may not be accurate enough
  - Use micro-scale numerical simulations locally in time or space to supply missing accurate data in macro-scale model

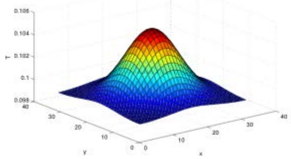
$$
\begin{aligned}
&Macro: \quad F_H(U_H, D(u_h)) = 0 \\
&Micro: \quad f_h(u_h, d(U_H)) = 0 \\
&\rightarrow \quad F_H(U_{HMM}, D_{HMM}(U_{HMM})) = 0
\end{aligned}
$$

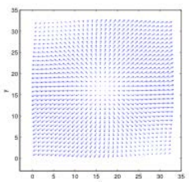
Applications

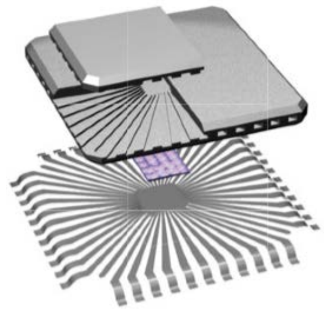


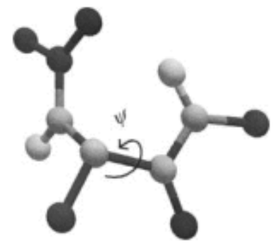


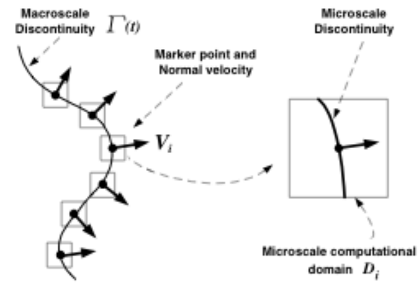


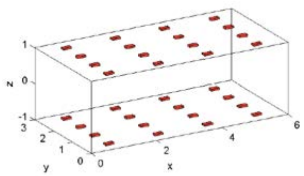


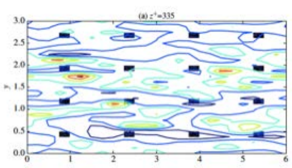


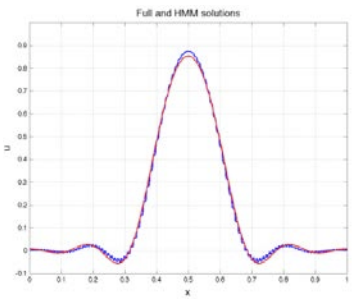


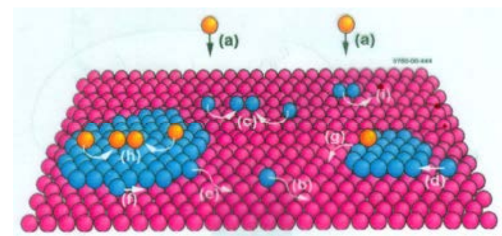


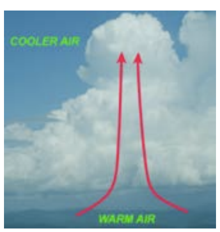


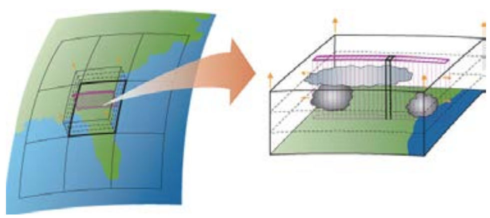


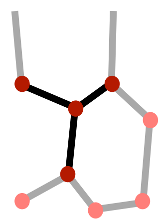


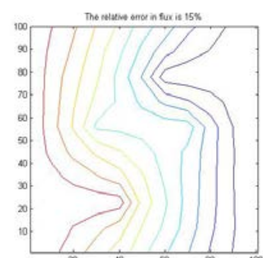


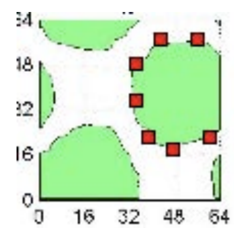


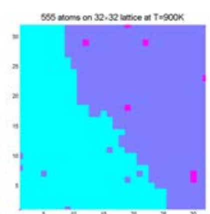












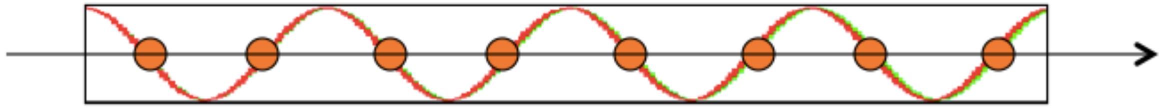
[Ariel, Caflisch, E, Eqt, Holst, Li, Ren, Runborg, Sharp, Sun, Tsai].

Mathematical foundation for computational multiscale ODE methods

1. Information theory applied to multiscale functions
   – Added information modifies sampling theorem
2. Analytical multiscale analysis
   – Averaging, (homogenization)

2. Information theory and averaging

- Nyquist-Shannon sampling theorem [Shannon 1948] from information theory
- A band limited signal can be stably reconstructed by equidistant samples if and only if the sampling rate is more than 2 points per shortest wavelength (frequency less than B)



$$f(t) = \sum_{n=-\infty}^{\infty} f(t_n) \frac{\sin(2Bt - n)}{\pi(2Bt - n)}$$

Multiscale functions

- If more is known of the function or signal: can sampling rate be reduced? – [E., Frederick, 2014], [Frederick 2016] [E., Frederick 2018]

$$f_{\varepsilon}(x) = f(x, x/\varepsilon) = f(x, y)$$

- f (x,y), band limited in x and y, 1 – periodic in y

Multiscale functions

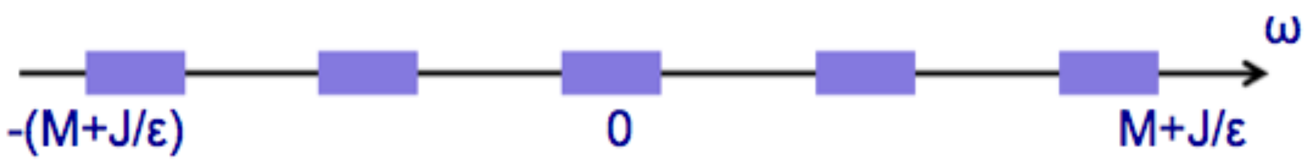
- If more is known of the function or signal: less sampling

$$f(x, x/\varepsilon)?$$

$$f(x,y) \ \ \textit{periodic in } y \rightarrow \textit{Fourier series representation}$$

$$f = \sum_{j--J}^{J} c_j(x)\exp(2\pi jx/\varepsilon), \quad \hat{c}_j \ \textit{supported in} \ (-M, M)$$

$$\hat{f}(\omega) = 0, \ \ \omega \notin \bigcup_{j\in J}\left([-M, M] + j/\varepsilon\right)$$



Multiscale functions

- Nyquist rate $f_N = 2(M+J/\varepsilon)$, sufficient for stable reconstruction
  - Necessary with uniform sampling
- Landau rate $f_L = 2JM$, necessary for reconstruction – any sampling, [Landau 1967]
- [Nitzan et. al. 2016], stable reconstruction (frame) if spectrum supported on set of finite measure

- So far only Nyquist-Shannon with explicit sampling strategy

Explicit multiscale sampling

Theorem [E. Frederick, 2014]: A band limited $f(x,x/\varepsilon)$ ($f(x,y)$, 1-periodic in y) can be uniquely and stably reconstructed by samples $f(z)$:

$$f(z),\ z\in X, \quad X=\{n\,\Delta x+k\,\delta x,\ n\in Z,\ k\in Z\cap[1,\ 2M\,]\}$$

$$N^{-1}\le\Delta x\le 1, \quad 0<\delta x<(2M+1)^{-1}N^{-1}$$

$$A\|f\|^2_{L^2(R)}\le\Delta x\sum_{z\in X}|f(z)|^2\le B\|f\|^2_{L^2(R)}$$

$$(2M+1)^{-1}\left(\prod_{m=1}^{2M}\sin(m\pi\delta x)\right)^2\le A\le B$$

Explicit multiscale sampling

Theorem [E. Frederick, 2014]: A band limited $f(x,x/\varepsilon)$ ($f(x,y)$, 1-periodic in y) can be uniquely and stably reconstructed by samples $f(z)$:

Remarks on proof

- Fourier series

$$f(x, x/\varepsilon) = f(x, y) = \sum_j c_j(x) e^{2\pi i j y} = \sum_m c_m(x) e^{2\pi i j N x},$$

$$supp(\hat{c}_j) \subset [-0.5, 0.5]$$

- Shannon type sampling for uniform sets $X_k = \Delta x (k\,\delta x + Z)$

Remarks on proof

- Fourier series

$$f(x, x/\varepsilon) = f(x, y) = \sum_j c_j(x) e^{2\pi i j y} = \sum_m c_m(x) e^{2\pi i j N x},$$

$$supp(\hat{c}_j) \subset [-0.5, 0.5]$$

- Shannon type sampling for uniform sets $X_k = \Delta x(k\,\delta x + Z)$
- Poisson summation and restricted Fourier transform

$$f_k(x) = \sum_{m=-M}^{M} c_m(x) e^{2\pi i m k \delta x}$$

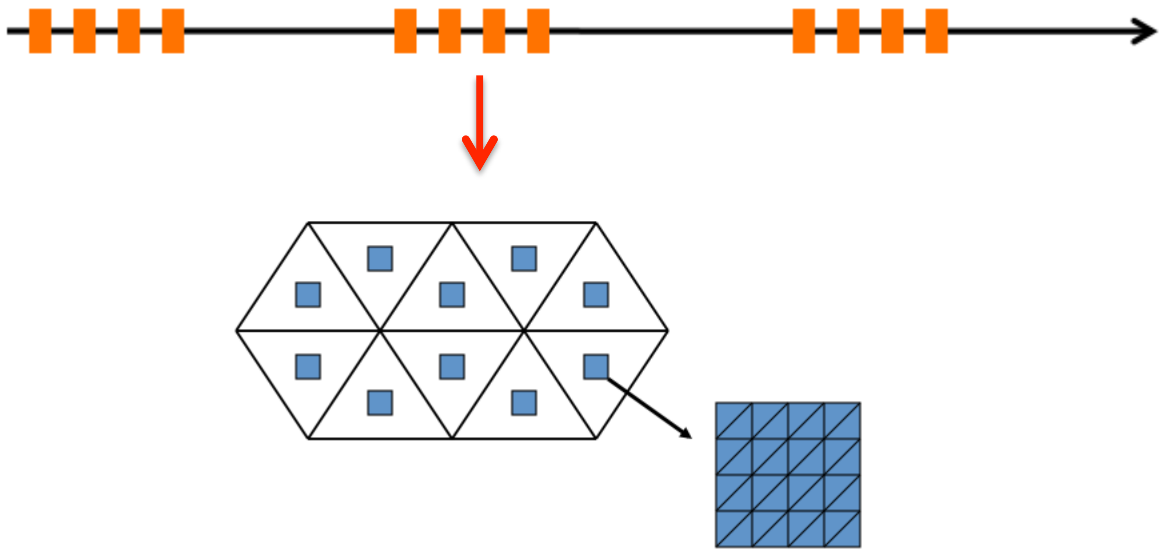
- Full matching $\longrightarrow$ Vandermonde system, [Gauchi 1990] estimate basis for explicit stability inequality

Remarks on extensions

- For dynamical systems: attraction to inertia manifold from:

$$u(x, x/\varepsilon) = u(x, y) \to U(x), \quad y \to \infty$$

- Theorem extends to clustering in higher dimensions



Background in averaging theory

- Mathematical model reduction: find effective equation as limit of equations with wider range of scales

$$F_\varepsilon(u_\varepsilon) = 0 \qquad \lim_{\varepsilon \to 0} u_\varepsilon = \bar{u}, \quad \bar{F}(\bar{u}) = 0$$

- Example of classical applied mathematics methods
  - Averaging of dynamical systems (“eliminate” oscillations)
  - Homogenization of elliptic operators (“eliminate” microstructure)
  - WKB, Geometrical optics, singular perturbation analysis,..

Averaging of oscillatory dynamical systems

- Typical applications: molecular dynamics, astrophysics
- Effective equation from averaging of ergodic process
- Find equation for averaged unknown *u* without the ε scale

$$x_\varepsilon' = f_\varepsilon(x_\varepsilon) \to \begin{cases} u_\varepsilon' = f(u_\varepsilon, v_\varepsilon) \\ v_\varepsilon' = \varepsilon^{-1} g(u_\varepsilon, v_\varepsilon) \end{cases} \qquad \varepsilon \to 0, \qquad \begin{matrix} u_\varepsilon \to \bar{u} \\ \bar{u}' = \int_v f(\bar{u}, v)\, d\mu \end{matrix}$$

- Integration with respect to invariant measure *μ*: "averaging over fast motion". *v* – dynamics ergodic
- Rich theory – we will consider cases when above averring is true, in particular when *v*-equation has ε-periodic solutions:

$$v_\varepsilon' = \varepsilon^{-1} g(U, v_\varepsilon)$$

$$x_\varepsilon(t) = x(t, t/\varepsilon)$$

v

Example we will come back to

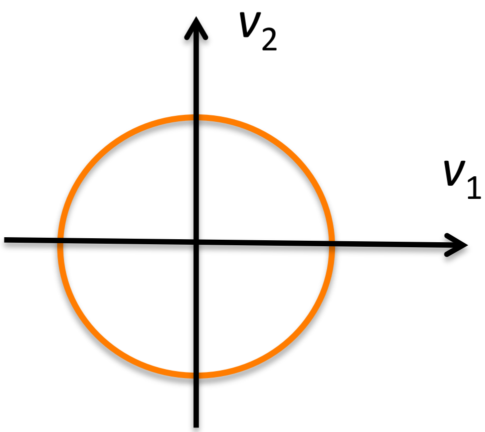
$$\frac{du}{dt} = v_1^2, \quad \frac{dv_1}{dt} = \varepsilon^{-1} v_2, \quad \frac{dv_2}{dt} = -\varepsilon^{-1} v_1$$

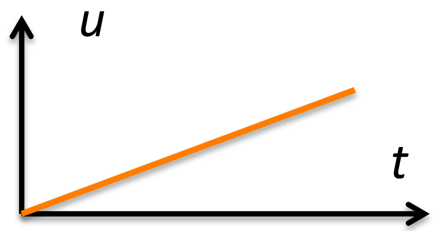
$$u(0) = 0,\ v_1(0) = 0,\ v_2(0) = 1$$

$$v_1(t) = \sin(t/\varepsilon),\ v_2(t) = \cos(t/\varepsilon)$$

$$\rightarrow \frac{du}{dt} = \left(\sin(t/\varepsilon)\right)^2 \rightarrow \int_0^1 \left(1 - \cos(2\pi s)/2\right) ds = 1/2$$

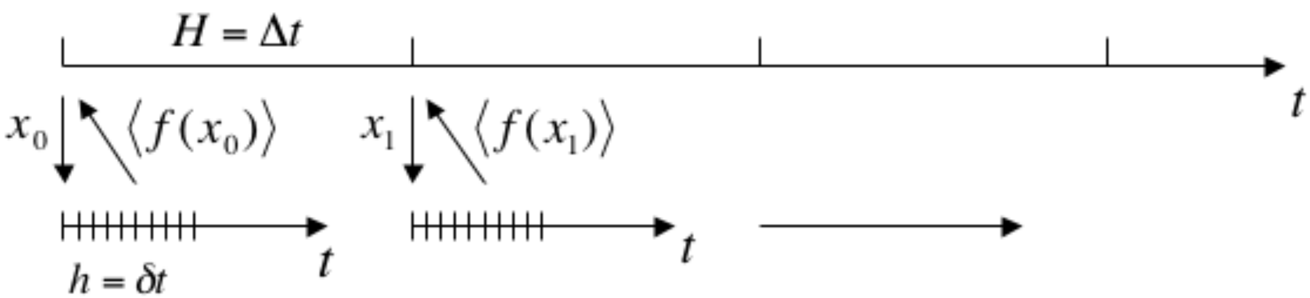
$$\Rightarrow \bar{u}(t) = t/2, \quad \left(u = \bar{u} + O(\varepsilon)\right)$$





3. Heterogeneous Multiscale Methods for ODEs

$$\dot{x}_\varepsilon = f_\varepsilon(x_\varepsilon, t)$$



- Effective $\langle f \rangle$ value for macro-scale solver from average of micro-scale data, mimicking the analytic process, [E, E., 2003], [E,Tsai, 2005]

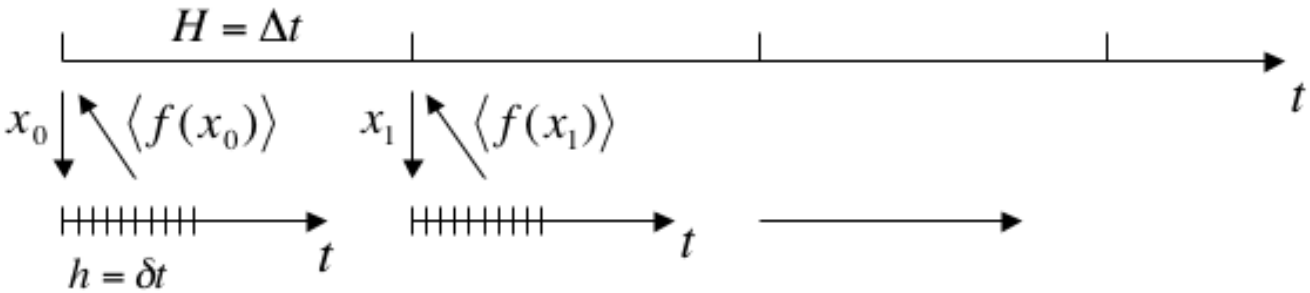
$$\langle f \rangle_j \approx \sum_k K_k f_{j+k}, \quad \frac{d\bar{u}}{dt} = \int f(\bar{u}, v)\, d\mu_{\bar{u}}(v)$$

$$f(t, t/\varepsilon), \quad f(t, \tau) \ \ periodic\ in\ \tau$$

- The computational grid is also based on analysis

Heterogeneous Multiscale Methods for ODEs

$$\dot{x}_\varepsilon = f_\varepsilon(x_\varepsilon, t)$$



- Three processes, course (upper line) and fine solver (lower line) and the coupling (average force)

$$x_{N+1} = F_H(x_N), \quad x_N = x_0 + NH, \quad x_{n+1} = F_h(x_n), \quad x_n = x_0 + nh$$

$$\langle f \rangle_j \approx \sum_k K_k f_{j+k}$$

Convergence analysis contains the same three processes

Averaging example: HMM – theory

- The HMM framework applies directly (harmonic oscillator + slow)

$$\frac{du}{dt} = v_1^2, \quad \frac{dv_1}{dt} = \varepsilon^{-1} v_2, \quad \frac{dv_2}{dt} = -\varepsilon^{-1} v_1,$$

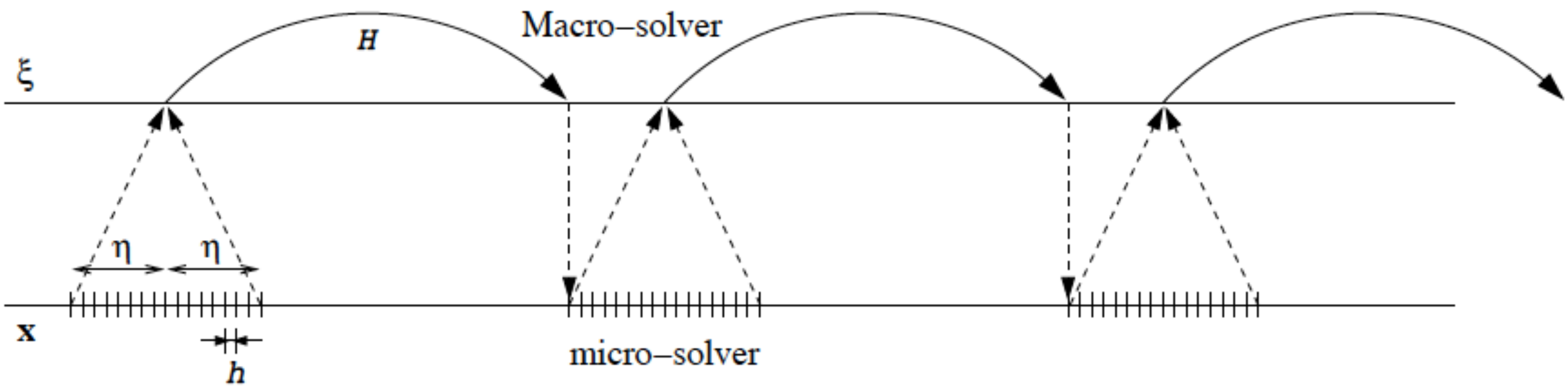
- The basic HMM method works well and can be proved to converge. Generalization to other equation possible

$$\left\langle f(x_\varepsilon(t)) \right\rangle = \sum_k K_k f_{j+k}, \ \ K \in C^s, \quad \int_{t-\delta/2}^{t+\delta/2} K(t,\tau)\tau^l \, d\tau = \begin{cases} 1, & l = 0 \\ 0, & 0 < l \le q-1 \end{cases}$$

$$\left\| \bar{x}_\varepsilon - x_{HMM} \right\| = O\left(H^{p_M} + \left(\frac{h}{\varepsilon}\right)^{p_m} \frac{\delta}{H} + \left(\frac{\varepsilon}{\delta}\right)^s + \delta^q\right)$$

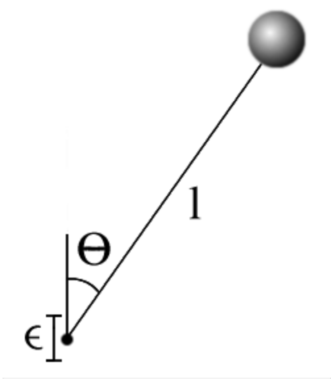
Heterogeneous Multiscale Methods for ODEs

- There are different variants, for example, symmetric integration for time reversible processes
- Convergence in case of inertia manifold attractors is possible



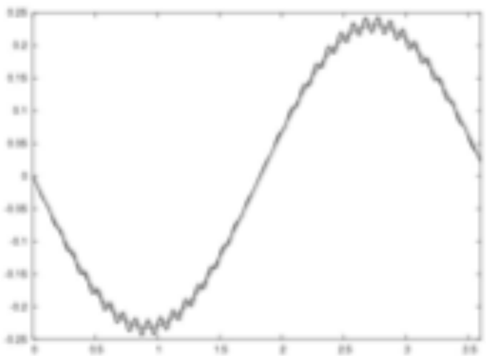
$$\langle f \rangle_j \approx \sum_k K_k f_{j+k}, \quad K \text{ symmetric}$$

Kapitza pendulum



$$l\frac{d^2\theta}{dt^2} = (g + \varepsilon^{-1}\sin(2\pi\varepsilon^{-1}t))\sin(\theta)$$

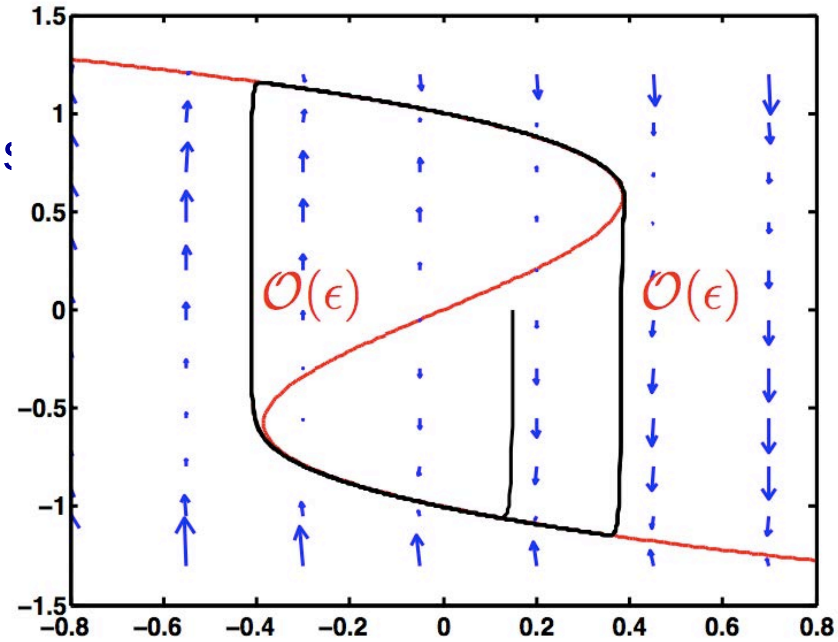
If the pivot is forced to oscillate rapidly, slow stable oscillations around θ =0 are possible.



HMM example

- This relaxation oscillator is a suitable example for numerical resolution of fast process [Dahlquist et al, 1981]
- Two-scale fast process
- Numerical multiscale methods only possibility challenging for exp. methods

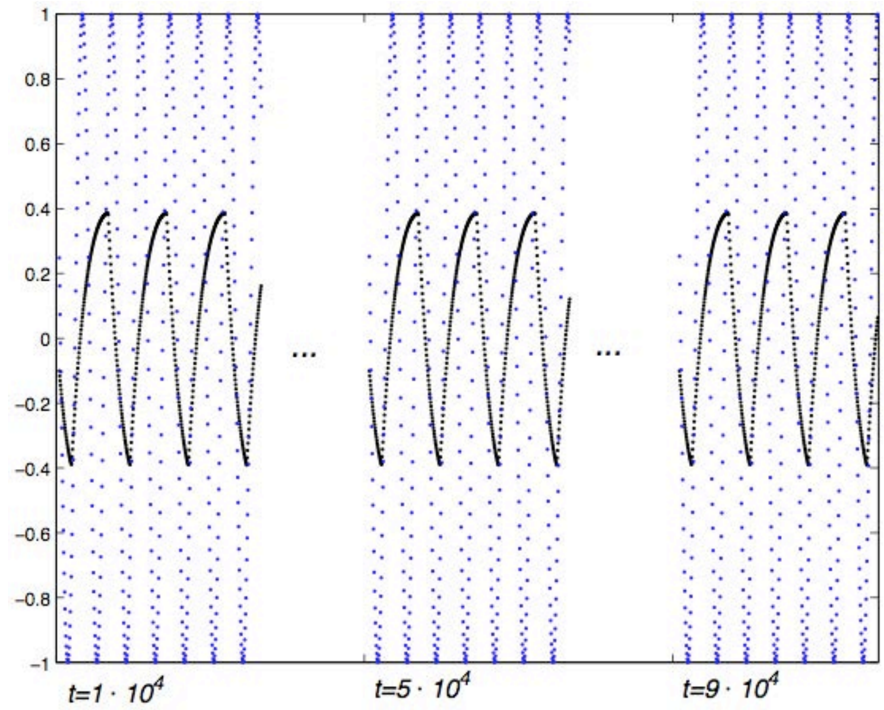
$$\begin{cases} \dot{x}_1 = -1 - x_1 + 8x_2^3 \\ \dot{x}_2 = \frac{1}{\varepsilon}\left(-x_1 + x_2 - x_2^3\right) \end{cases}$$



HMM phase locking

- 3 scales $O(\varepsilon)$, $O(1)$, $O(\varepsilon^{-1})$

$$\begin{cases} \dot{x}_1 = -1 - x_1 + 8x_2^3 + \varepsilon\lambda x_3 \\ \dot{x}_2 = \dfrac{1}{\varepsilon}\left(-x_1 + x_2 - x_2^3\right) \\ \dot{x}_3 = \omega x_4 \\ \dot{x}_4 = -\omega x_3 \end{cases}$$



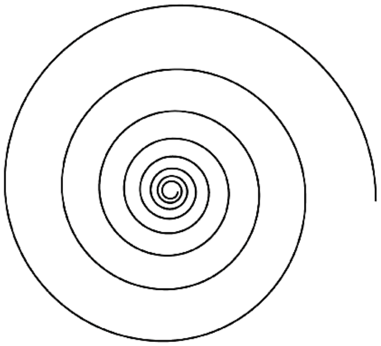
Challenge: initial values for microscale

- Convergence lost if the "fast" equations not ergodic. (resonance)
- Error from re-initialization

$$\frac{du}{dt} = v_1^2, \quad \frac{dv_1}{dt} = \varepsilon^{-1} v_2 + v_1, \quad \frac{dv_2}{dt} = -\varepsilon^{-1} v_1 + v_2,$$

$$u(0) = 0,\ v_1(0) = 0,\ v_2(0) = 1$$

$$\Rightarrow u = (e^t - 1)/2,\ v_1 = e^t \sin(t/\varepsilon),\ v_2 = e^t \cos(t/\varepsilon)$$



- The basic HMM method will not converge, $\langle f_2 \rangle = \langle f_3 \rangle = 0$.
- The initialization of the micro-scale is not correct.
- The *v*-system is not ergodic. There is a "hidden" slow variable: *r*

$$\left(\dot{r} = \sqrt{v_1^2 + v_2^2} = r\right)$$

Controlling “slow variables” for consistent re-initialization

- Related to the closure problem for effective equations. Problem for molecular dynamics

(a) Follow “slow variable” in established cases

(b) Find numerically (or analytically) explicit approximations of a complete set of the “slow variables”

(c) Compute averages of relevant moments and use as constraints. Implicit type of technique (Compare, thermostats)

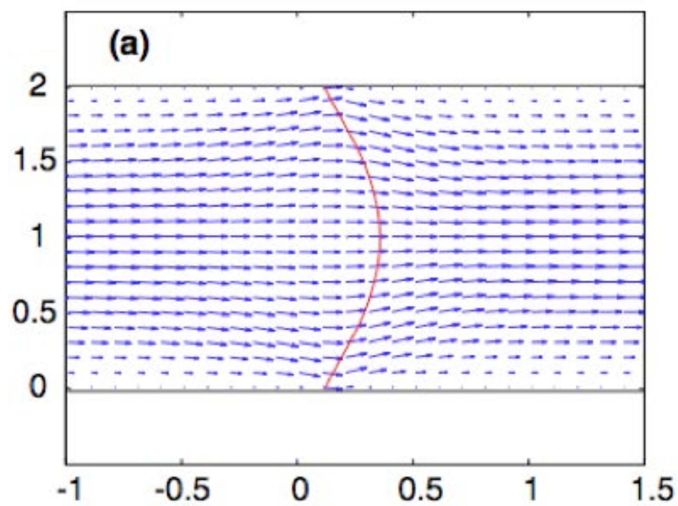
Example use variables u, r, θ in our model problem

(d) If possible separate f_ε in fast (ergodic) and slow remaining part (all slow variables does not need to be identified)

(e) Compute phase plane maps for parareal simulations (✔)

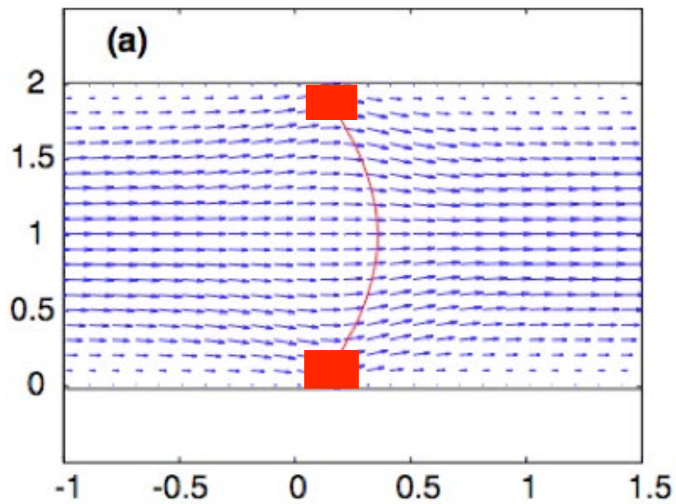
(a) “Established case”
fluid – MD coupling, slip line

- No slip boundary condition for Naver-Stokes fails at slip line



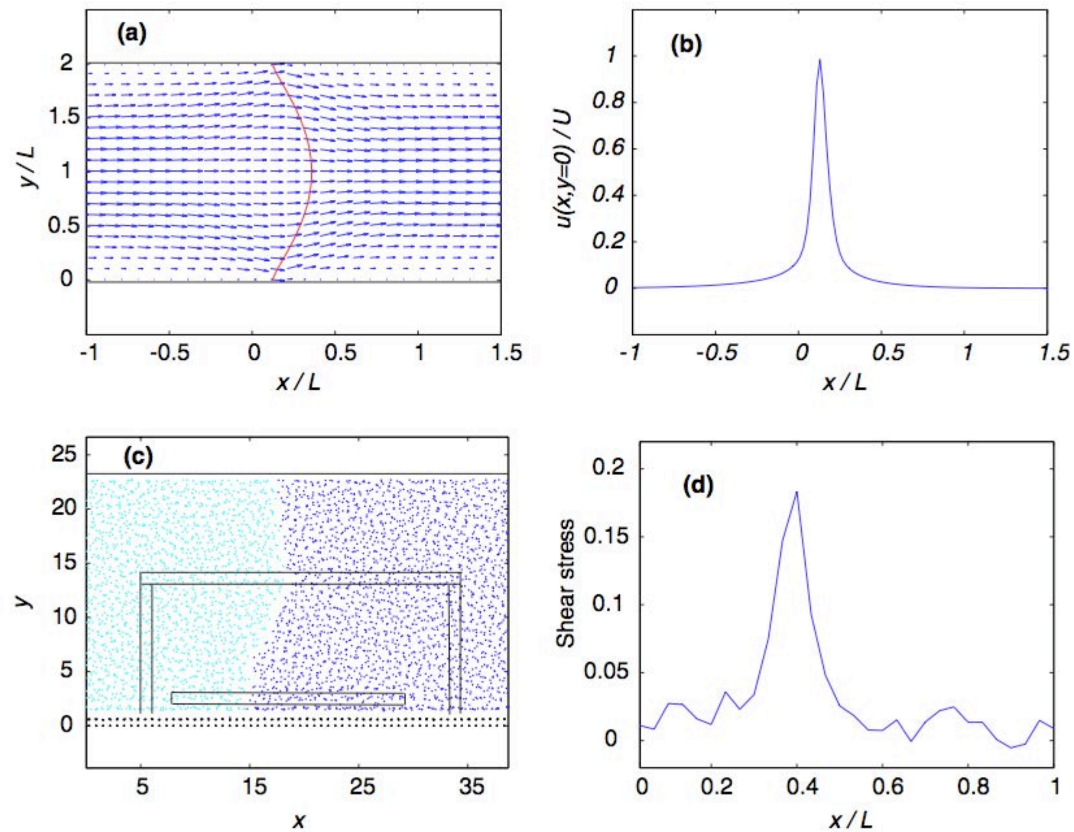
Slip line example

- No slip boundary condition for Naver-Stokes fails at slip line



Slip line example

- Coupling: fluid and line velocity and shear stress
- Heat bath for MD
- Velocity, pressure slow outside of slip line – compare closure problem



(b) Determine complete set of slow variables

- Goal is to find maximal set of slow observables or variables

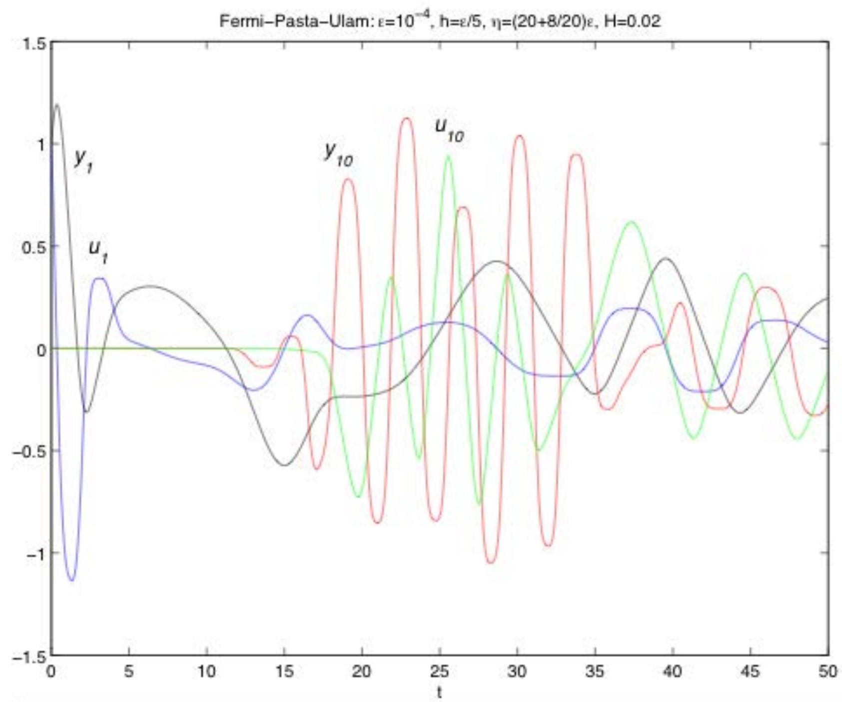
$$\left\{\xi_j(x)\right\}_{j=1}^{r}, \quad \left|\frac{d\xi_j(x(t))}{dt}\right| \leq C, \quad j = 1,..r$$

- Using the micro solver, determine coefficient in an algebraic form of diffeomorphism $\Phi(x)=(\xi(x),..)$ orthogonal to trajectory, simple HMM then applies
- Typical ξ-variables
  - Null space of principle (ε^{-1}) part of system Jacobian
  - Amplitude of local oscillator
  - Phase difference between oscillators
  - u, $(v_1^2 + v_2^2)$ in our model example

Fermi-Pasta-Ulam problem, finding all “slow variables”

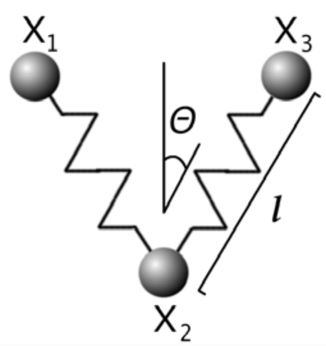
- 1-D system with alternating stiff linear and soft nonlinear springs

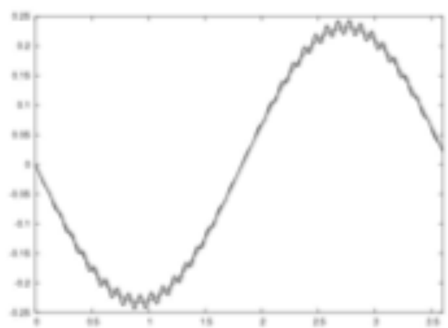
- Numerical example with 10 springs
- Only one “fast variable”
- Recall radius in expanding spiral example

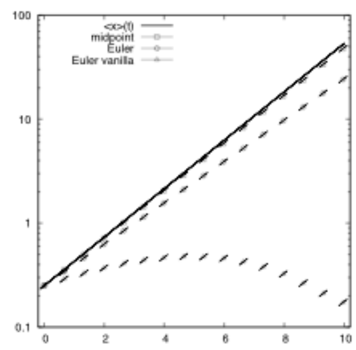


(c) Compute averages of relevant moments and use as constraints

- By also tracking $\langle (v_1)^2 \rangle$ in example above and reinitialize such that the moment average is consistent, convergence can be achieved. Re-initialization implicitly defined
- Example: three body harmonic springs





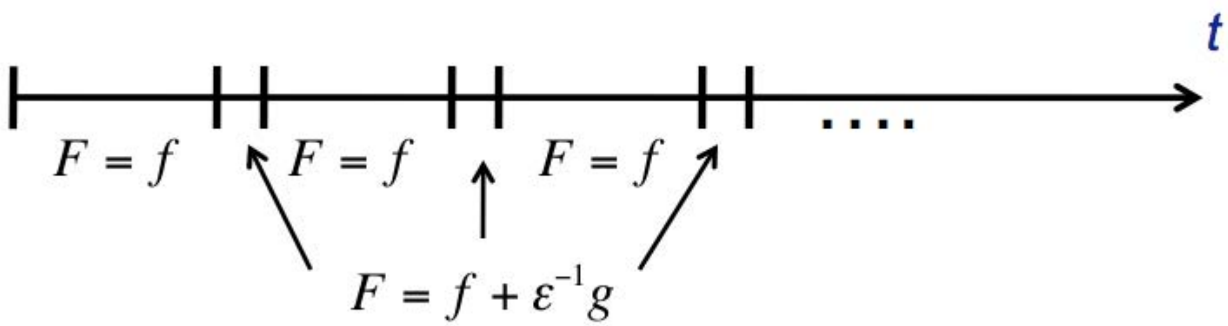


(d) Seamless HMM and FLAVORS

- FLow AVeraging integratORS (FLAVORS) [Tao, Owhadi, Marsden 2010], compare, seamless HMM [E, Vanden-Eijnden 2009]
- We used later [E. Lee 2014] variable step sizes to avoid "just rescaling ε

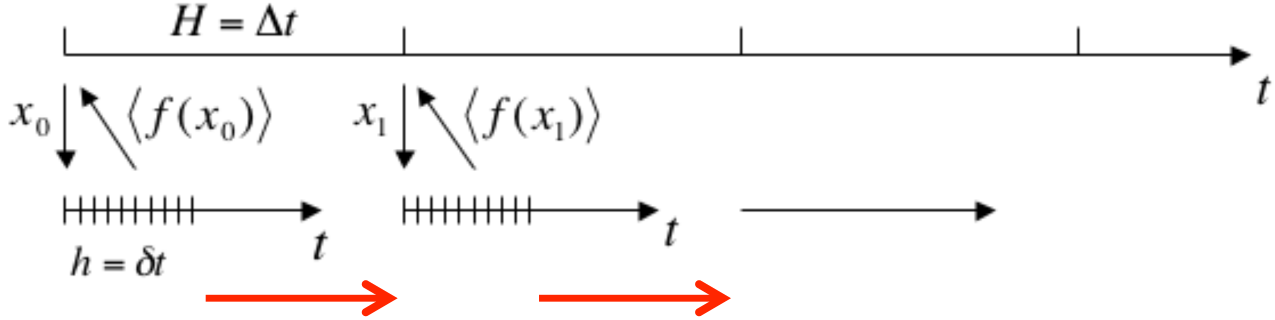
$$\frac{dx}{dt} = f_\varepsilon(x) = f(x) + \varepsilon^{-1} g(x)$$

- FLAVORS: Staggered or fractional step evolution



(e) Local micro-simulations $\longrightarrow$ parareal

- Ultimate "solution" to re-initialization challenge: full domain fine solver
- For HMM: ideally extend microscale integration domain – efficiency from distributed computing
- Re-initialization challenge is replaced by course scale solver challenge



4. Parareal: parallel integration in time

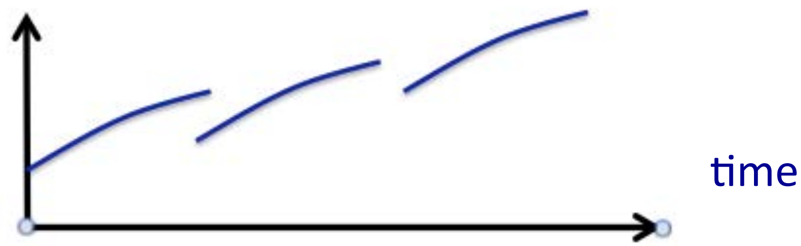
- Motivation: higher computer performance now essentially only from increases in distributed processing

Moore's law

Processor speed → parallelization

Parallel computing

- Parareal: technique for parallel in time computations of dynamical systems. Parallel in space common
  - Challenge in time: causality compare space
  - Predictor corrector method for domain decomposition in time
  - Initial application: dissipative systems, Early paper [Lions, Maday, Turinici 2001]

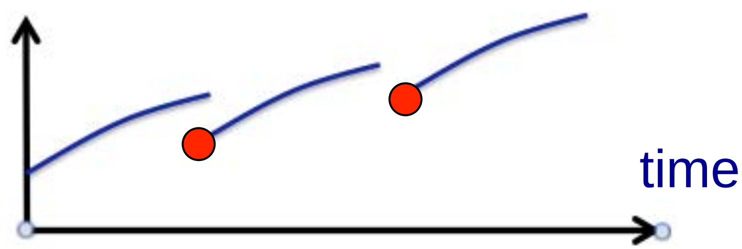


Parareal

- Recall parareal: technique for parallel in time computations of dynamical systems.
  - Challenge in time: causality
  - Predictor corrector algorithm, compare parallel shooting
  - Based on coarse solver ( ) and high resolution solver ( )

Coarse solver

$$x_0^0 = x_0, \quad x_n^0 = C_H x_{n-1}^0$$

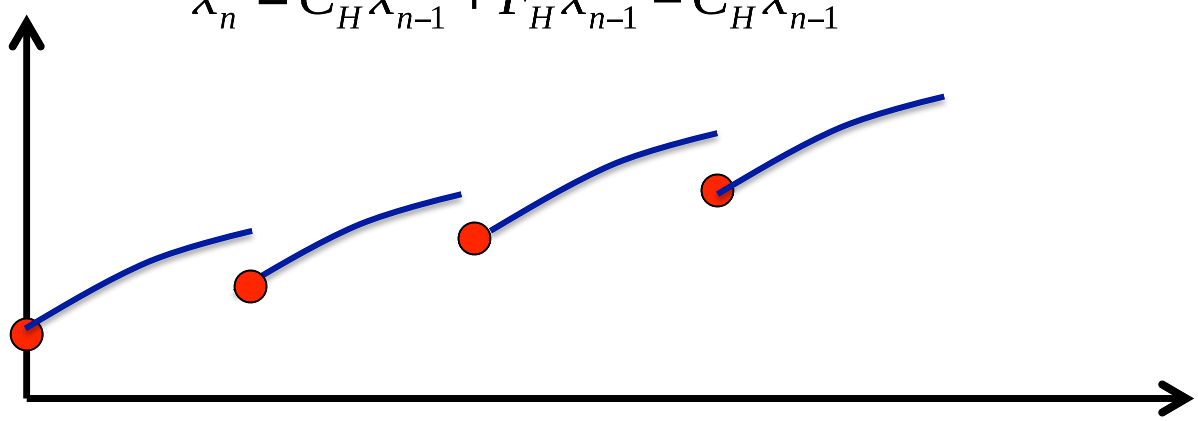


Parareal correction

- A framework for parallel in time algorithms
  - Local simulations covering fully the sub-intervals
  - Macroscale: *C*, microscale: *F*

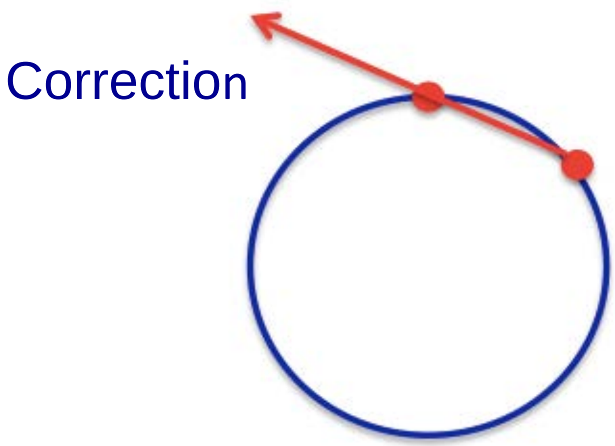
$$For\ k = 1,..,K$$

$$x_n^k = C_H x_{n-1}^k + F_H x_{n-1}^{k-1} - C_H x_{n-1}^{k-1}$$



Convergence

- Convergence based on:
  - Dissipative process (short memory), [Lions, Maday, Turinici, 2001]
  - Accurate coarse global solver for all initial values and suitable initial value update procedures, [Gander, Hairer, 2007,2014]
- Hamiltonian systems require highly accurate global course integrator [Gander, Petcu, 2007]



- Coarse numerical approximation: solver with larger step size or larger ε – too many iterations – even blowup possible

Challenge: parareal for oscillatory systems

- Coarse solver needs to be quite accurate even for the “highest frequency”
- [Gander, Hairer, 2007]: accuracy requirement for “parareal convergence”

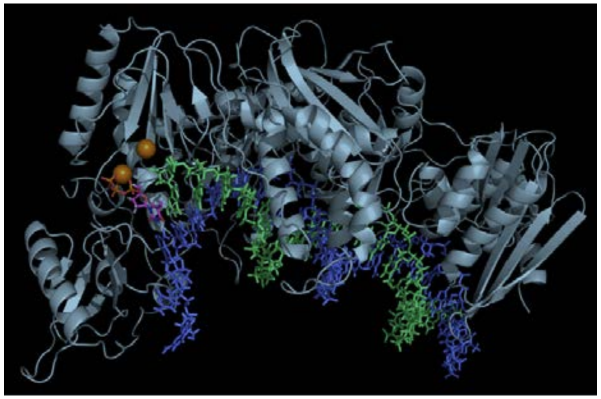
$$F_H x - C_H x = c(x) H^{p+1}, \quad \| C_H x - C_H y \| \le (1 + cH) \| x - y \|$$

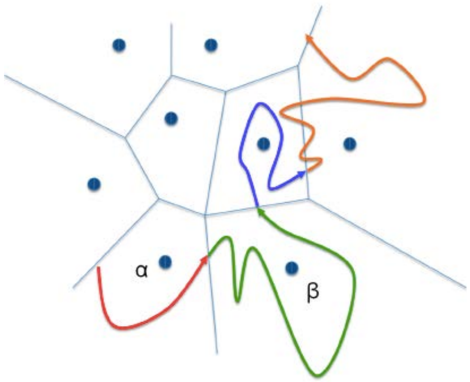
$$\rightarrow \quad \| x(t_n) - x_n^k \| \le \frac{c t_n^{k+1}}{(k+1)!} H^{p(k+1)}$$

- Problem for natural coarse integrators: changing *ε* of *h*
- In MD already F_H has low accuracy
- Motivation to consider phase plane map as coarse solver
- Compare “milestoning”

5. Milestoning

- Milestoning: a domain decomposition technique for multiscale Molecular Dynamics (MD) simulations
  - Challenge: extend molecular dynamics simulations to much larger time than what is possible in direct simulations (example protein folding)
  - Early paper [Elber, Faradjian, 2004]

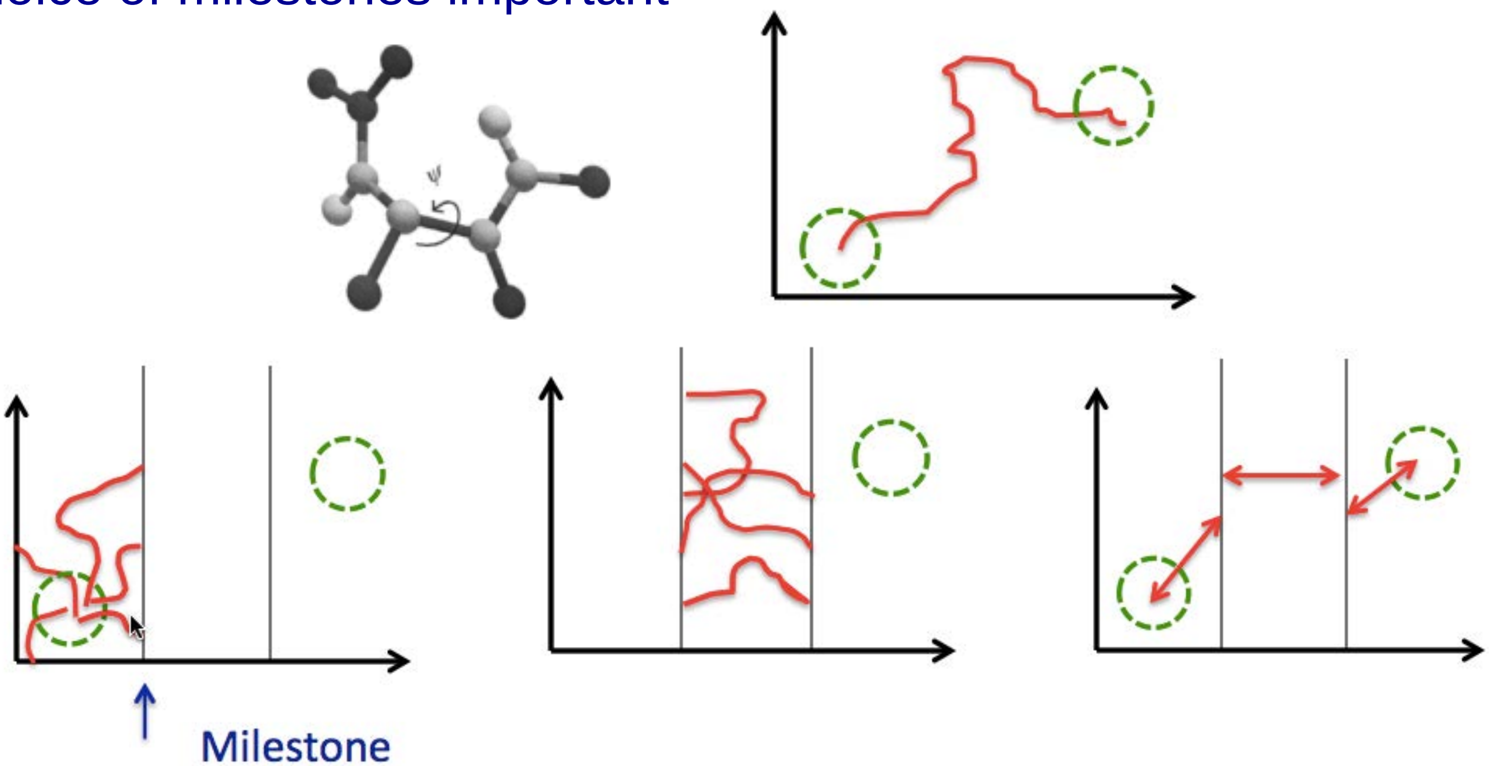




Projected phase plane

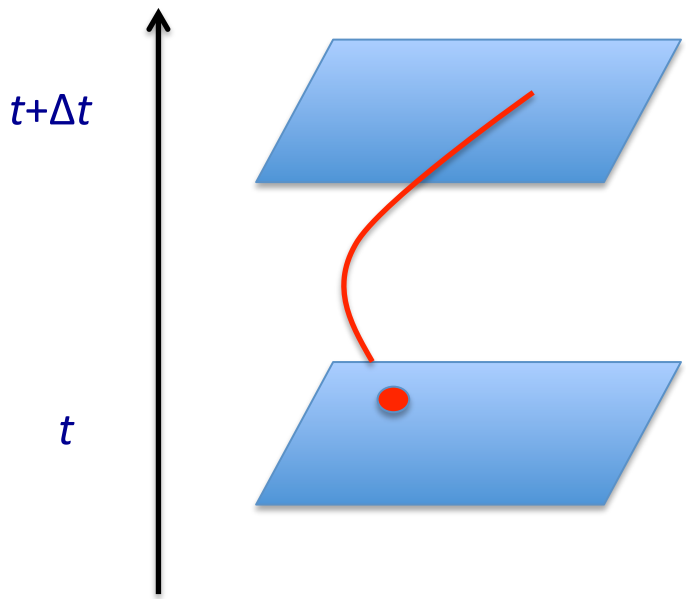
Milestoning: domain decomposition

- The phase space of a Hamiltonian system or a stochastic differential equation is decomposed into domains separated by milestones
- Phase space high dimensional – milestones low dimensional (1 to 3)
- Choice of milestones important



6. Phase plane map based parareal integration

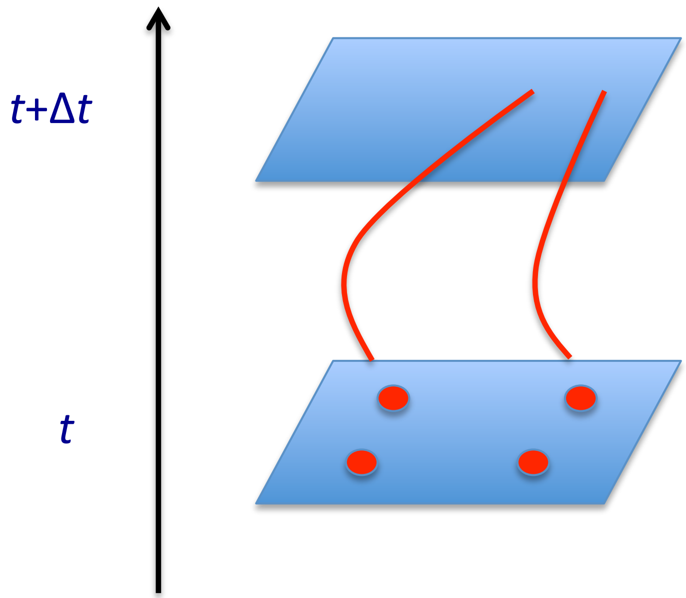
- Coarse global integrator for autonomous systems
- Determine map $x(t)$ to $x(t+\Delta t)$ for number of x – values in parallel



$$\begin{cases} \dfrac{dx_\varepsilon}{dt} = f_\varepsilon(x_\varepsilon), \quad t < t < t + \Delta t, \\ x_\varepsilon(t) = x^0 \end{cases} \qquad \left(x : R^+ \to R^d\right)$$

Phase plane map

- Coarse global integrator for autonomous systems
- Determine map $x(t)$ to $x(t+\Delta t)$ for number of x – values in parallel
- Use these x – values with interpolation as course global integrator

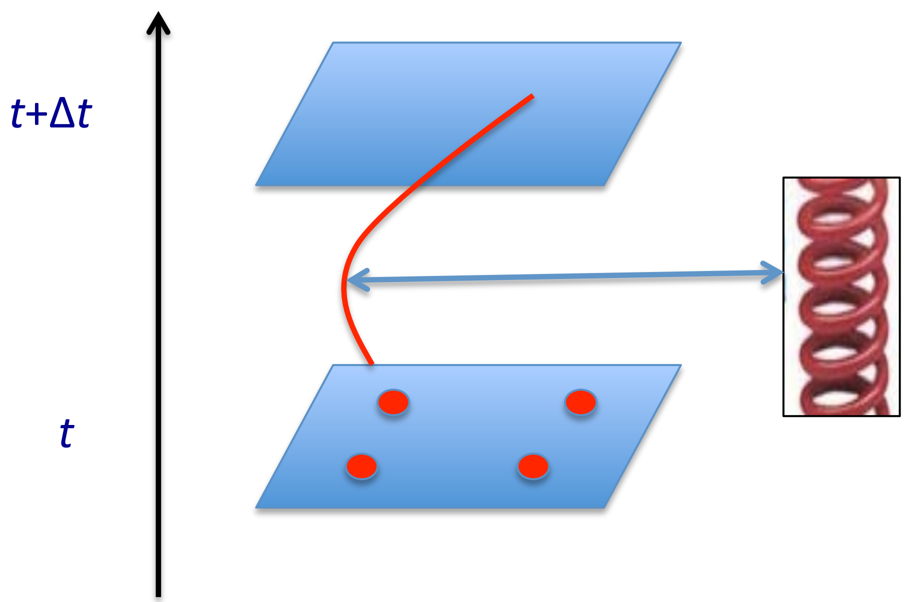


Goal: reduce phase error

Compute in parallel several snapshots defining the map

Phase plane map

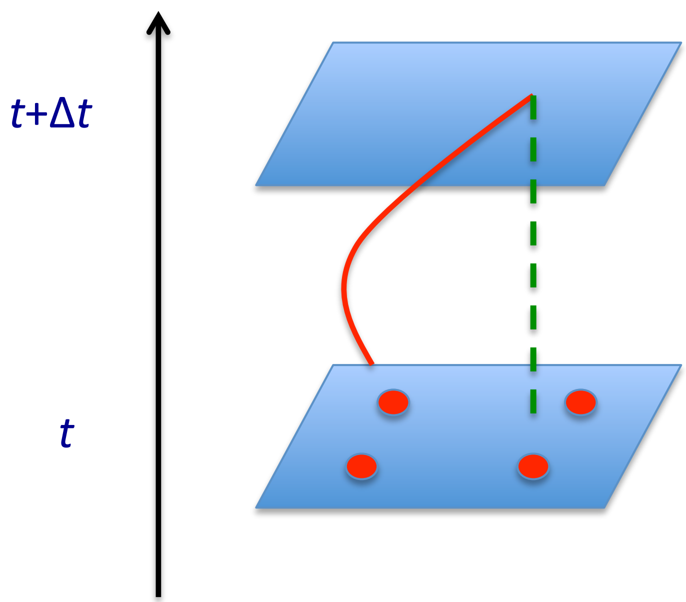
- Coarse global integrator for autonomous systems
- Determine map $x(t)$ to $x(t+\Delta t)$ for number of x – values in parallel
- Use these x – values with interpolation as course global integrator



Highly oscillatory solutions
do not reduce regularity of map
(no ε dependence)

Phase plane map

- Coarse global integrator for autonomous systems
- Determine map $x(t)$ to $x(t+\Delta t)$ for number of x – values in parallel
- Use these x – values with interpolation as course global integrator



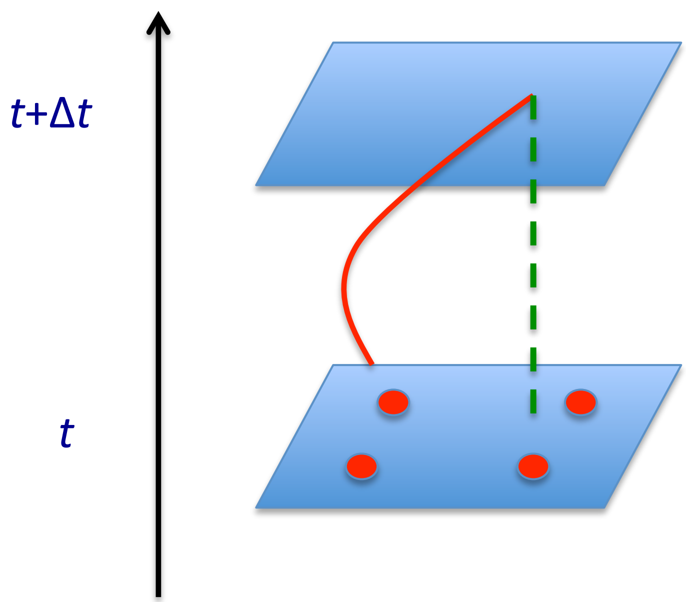
Coarse global integrator:
very good phase accuracy

$$\frac{dx_\varepsilon}{dt} = (i\varepsilon^{-1})\,x_\varepsilon, \quad t < t < t + \Delta t, \quad x_\varepsilon(t) = x^0$$

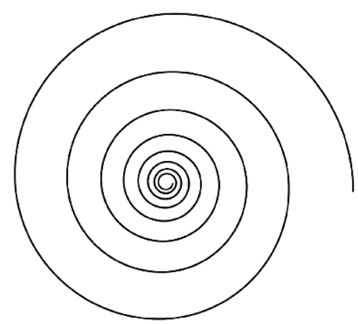
$$\left|\frac{dx_\varepsilon}{dt}\right| = O(\varepsilon^{-1}), \quad \left|\frac{\partial x_\varepsilon(t+\Delta t)}{\partial x^0}\right| = \left|e^{i/\varepsilon}\right| = O(1)$$

Phase plane map

- Coarse global integrator for autonomous systems
- Determine map $x(t)$ to $x(t+\Delta t)$ for number of x – values in parallel
- Use these x – values with interpolation as course global integrator

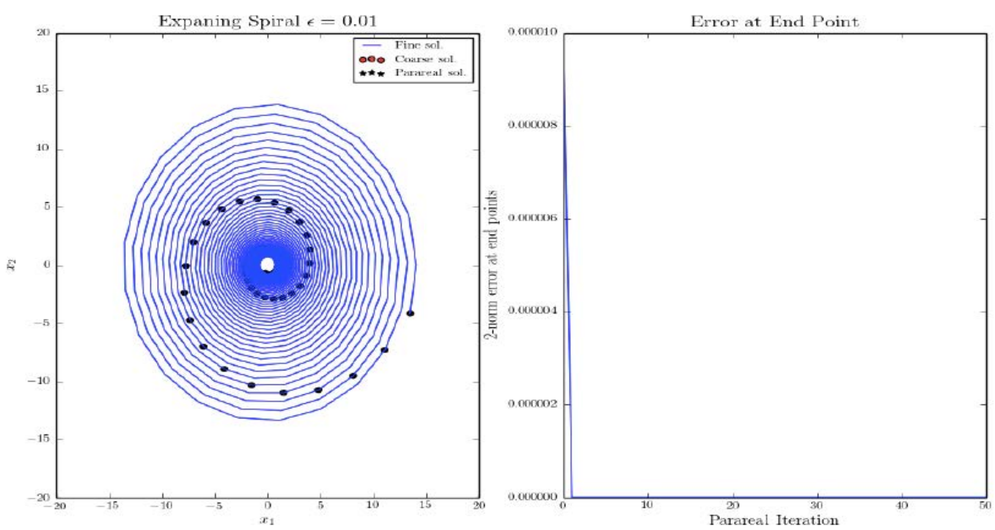


Works very well in parareal setting
for our spiral problem
Linear problem: # int. pts. = d+1



Expanding spiral

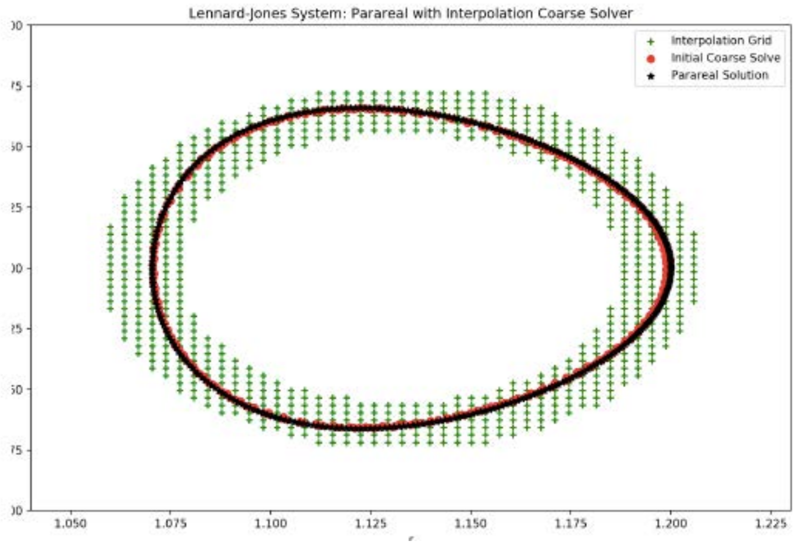
- 2 DOF only 3 parallel fine scale simulation defines this linear phase plane map “exactly”. Linear system with d DOF requires d+1 simulations
- For very high dimensions, neural networks are alternatives

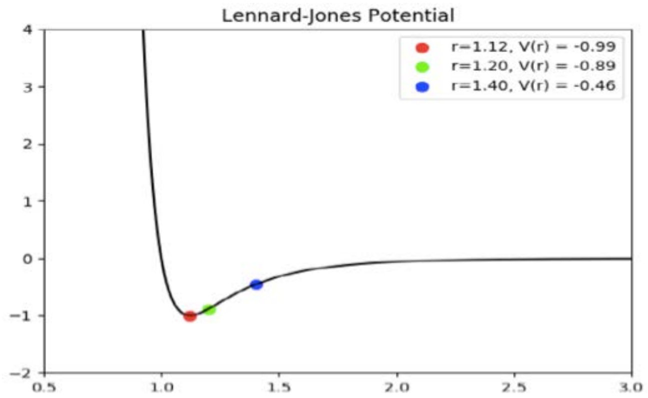


MD: Lennard-Jones potential

- 2 DOF, 2 atoms
- Piecewise linear interpolation near orbit

$$V = c_1 r^{-12} - c_2 r^{-6}$$

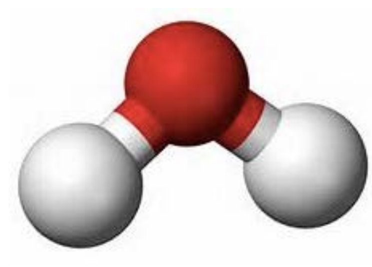




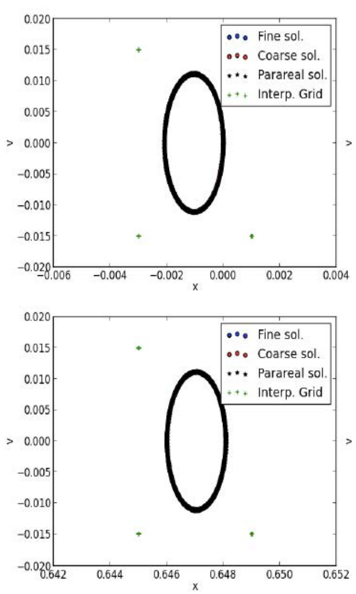
Grid Points (m)	Iterations
10	19
50	10
100	8
500	4
1000	3

MD: Lennard-Jones potential

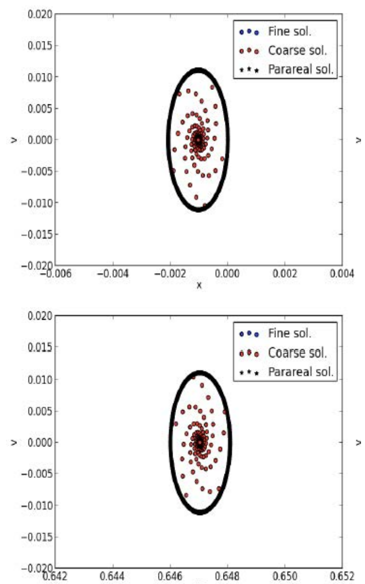
- 12 DOF, target molecule with 3 atoms
- Initial condition closer to minimal potential
- Piecewise linear interpolation near orbit
- 400 *H*-intervals



PP-map



RK4

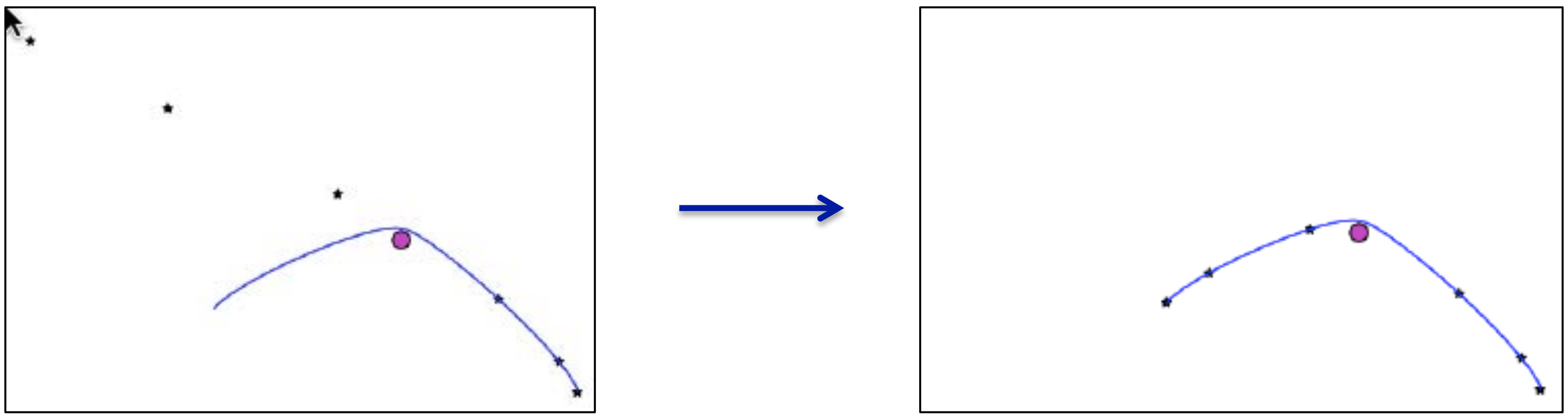


4 parareal iterations vs 34 for 10^{-3} accuracy

Localized multiscales

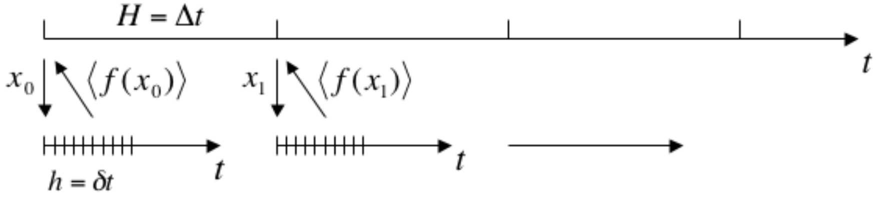
- Gravitational N-body problem of “near miss”
- Convergence in one parareal iteration

$$m_i \ddot{x}_i = \sum_{j=1}^{N} \frac{g m_i M_j}{\left|x_j - x_i\right|^2} \frac{(x_j - x_i)}{\left|x_j - x_i\right|}$$



7. Conclusions

- HMM – ODE based on information theory and averaging
- Simulations require decomposition into slow and fast (ergodic) variables



- Oscillatory and transient cases
- Paraeal parallel-in-time simulation using phase plane maps for coarse solver is a promising alternative
- For more realistic degrees of freedom: sparse grids, higher order interpolation, symplectic integrators …