Introduction to Multiscale Modeling

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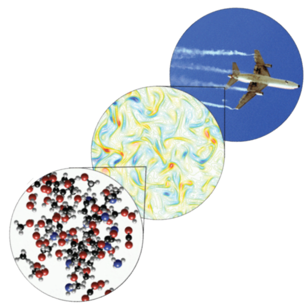
Outline

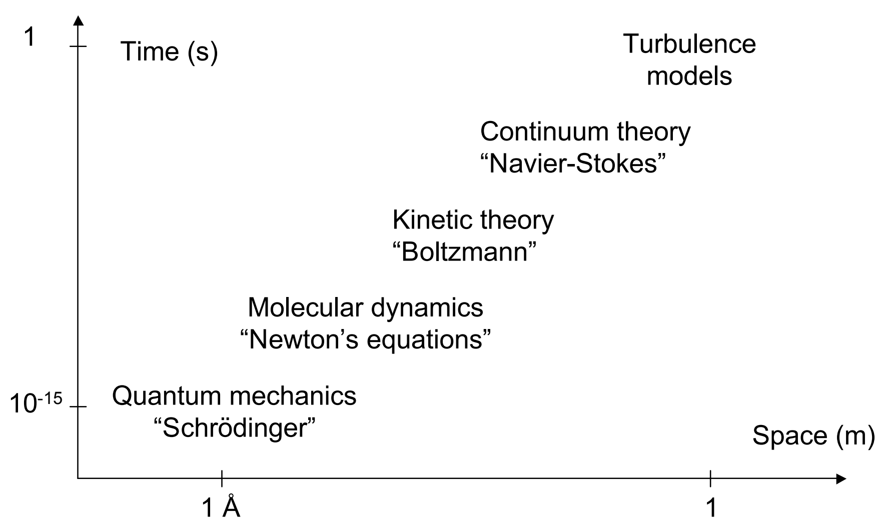
I Overview of Multi-scale Modeling
1. The challenge of multi-scale problems
2. Modeling strategies
3. Classical analytical techniques
4. Numerical methods

II Heterogeneous Multi-scale Methods (HMM)
1. Structure of HMM
2. Analysis
3. Applications
4. Computational issues

1. The challenge of multi-scale problems

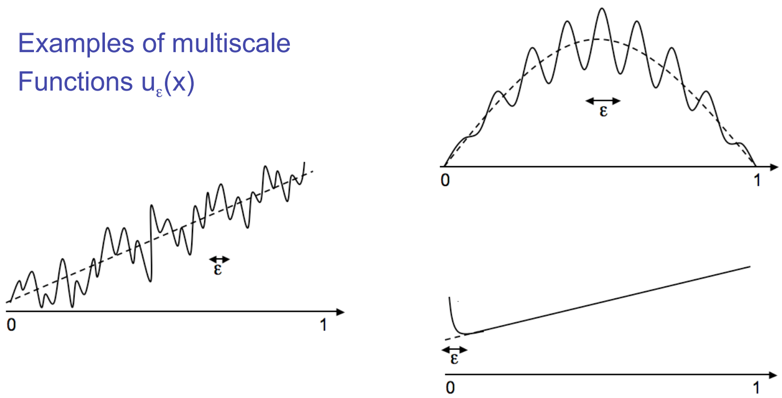


The space and time sales in this picture vary strongly from atomistic to full airplane processes. Different models are typically derived independently for the different scales. We will focus on problems where more than one scale and model is needed and where the micro-scale model is too computationally costly.



Multiscale functions

Examples of multiscale Functions $u_\varepsilon(x)$



Multiscale functions

- In our analysis we will define the scales more explicitly, for example, by a scaling law.The function $u_\varepsilon(x) = u(x,x/\varepsilon)$, where $u(x,y)$ is 1-periodic in y, or where $u(x,y) \to U(x)$ as $y \to \infty$, are said to contain the scales 1 and ε.
- The scales are also naturally described by a scale-based transform of a function as, for example, Fourier or wavelet transforms.

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

- For clarity in the presentation we will mainly consider "two-scale" problems: a macro-scale in the range of O(1) and a micro-scale with wave-lengths $O(\varepsilon)$ rather than full multi-scale problems or sometimes a range of scales between $O(\varepsilon)$ and O(1)

Multiscale problems

Let us formally write the original multi-scale differential or integral equation as,

$$F_\varepsilon(u_\varepsilon) = 0$$

where F_ε represents the differential equations with initial and boundary conditions. Analytically we are interested in the following limit process

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

The type of convergence could be different for different cases.

Computational complexity

- A major reason for deriving effective equations with a narrow range of scales is the high computational cost of directly solving highly oscillatory problems.
- With the size of the computational domain = L in each direction and the smallest wavelength = ε the typical number of operations in the solution of a multi-scale differential equation in d dimensions for a fixed prescribed accuracy is,

$$flop = O((N(L/\varepsilon)(L/\varepsilon)^{-1})^{dr}) = O((L/\varepsilon)^{\alpha}), \quad \alpha \geq d$$

$$\#\ unknowns \geq O((L/\varepsilon)^{d}) \quad [Shannon]$$

With L=1 we have,

$$flop = O((N(\varepsilon,\delta)\varepsilon^{-1})^{dr})$$

N(ε): number of unknowns per wavelength to achieve a given accuracy ($N(\varepsilon) \geq 2$ from Shannon sampling theorem,

$N(\varepsilon) \approx O(\varepsilon^{-1/2})$ for standard second order finite difference methods). N typically scales as $O(\delta^{-s})$, s>0, where δ is the prescribed accuracy

ε: the shortest wavelength to be approximated

δ: prescribed accuracy

d: number of dimensions

r: exponent for number of flops per unknown in the numerical method (r=1 for explicit methods and r=3 for Gaussian elimination of dense matrices)

Even with the best numerical methods:, r = 1, N(ε) bounded,

$$flop = O(\varepsilon^{-d})$$

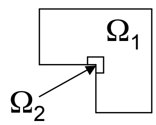
and this prohibits numerical simulation based on direct atomistic models over sizes in the millimeter range or more.

The upper limit for a teraflop computer is thus practically $\varepsilon = 10^{-3}$ with 10000 degrees of freedom in each dimension, R^{3+1}.

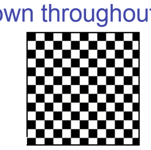
New approximate effective equations must be derived or the computation must be reduced to a small sample of the original domain if ε is very small.

Two basic types of problems for which the macro-scale model fails

- Type A: Macro-scale model is accurate enough in most of computational domain Ω_1. Micro-scale model used in the complement Ω_2. Compare mesh refinement and heterogeneous domain decomposition.



- Type B: A Macro-scale model is not fully known throughout computational domain. Sampling the micro-scale



2. Modeling strategies

- Modeling: analytical and numerical models
- Analytical models
  - Purpose: find equations for appropriate range of scales for analysis and numerical computations
  - Use science, mathematics and experiments

    (Here mainly as background for understanding the numerical methods.)
- Numerical models
  - Purpose: increase computational efficiency and accuracy
  - Efficient algorithms and coupling of different models

General mathematical modeling

1. Models derived from physical laws and engineering practice
2. Models derived from other usually more complex models via mathematical derivations (model reduction)
3. Models derived from a predetermined form by adjusting coefficients to match data (ex. linear models, neural nets)

The models are typically differential or integral equations but could also be algebraic equations. There could be composite models that couple simpler models.

Computational strategies

Let the equation below represent a multi-scale problem with range of scales O(ε) to O(1)

$$F_\varepsilon(u^\varepsilon) = 0$$

In the ideal case we can find an analytic model reduction which produces a model (effective or homogenized equation) with a narrow range of scales

$$F_\varepsilon(u^\varepsilon) = 0$$

$$\swarrow$$

$$\overline{F}(\overline{u}) = 0$$

This model can then be efficiently numerically approximated

$$F_\varepsilon(u^\varepsilon) = 0$$

$$\swarrow$$

$$\overline{F}(\overline{u}) = 0$$

$$\downarrow$$

$$\overline{F}_h(\overline{u}_h) = 0$$

If appropriate effective equations are not available special numerical techniques are needed. With ε very small direct numerical simulation is too costly and a numerical model reduction is required

$$\begin{tikzcd}[column sep=small]
 & F_\varepsilon(u^\varepsilon)=0 \arrow[dl] \arrow[dr] & \\
\overline{F}(\overline{u})=0 \arrow[d] & & F_{\varepsilon,h}(u_{\varepsilon,h})=0 \\
\overline{F}_h(\overline{u}_h)=0 & &
\end{tikzcd}$$

Computational strategies

Left: discretize homogenized or effective equation for average or expected values
Right: discretize directly in some way

$$\begin{tikzcd}[column sep=small]
 & F_\varepsilon(u^\varepsilon)=0 \arrow[dl] \arrow[dr] & \\
\overline{F}(\overline{u})=0 \arrow[d] \arrow[drr, dashed] & & F_{\varepsilon,h}(u_{\varepsilon,h})=0 \arrow[d] \\
\overline{F}_h(\overline{u}_h)=0 & & \tilde{F}_{\varepsilon,h}(\tilde{u}_{\varepsilon,h})=0
\end{tikzcd}$$

Analytical model reduction

- These techniques are often found in the physics, mechanics or in the classical applied mathematics literature.
- They are commonly seen as part of the applied science rather than "just" a mathematical technique.
- They have been very useful for understanding multi-scale problems and for deriving effective equations but many have no rigorous mathematical justification.
- Many times the different models for different ranges of scales are derived independently and the connection between the models developed later.
- The purpose of the reduction may be for computational purposes or for easier analysis.
- We will only focus on methods developed in applied mathematics

3. Classical analytical techniques

Applied mathematics and mechanics related techniques

- Singular perturbations
- Stiff dynamical systems
- Homogenization methods
- Geometrical optics and geometrical theory of diffraction
- Boundary layer theory

Examples from theoretical physics

- Renormalization group methods
- Semi classical representation, path integral techniques, Wigner distributions
- Density function theory

Applied mathematics techniques

We will consider four classical techniques in somewhat more detail and they are chosen to give representative examples of a variety of analytic techniques.

- Singular perturbations of differential equations
- Stiff ordinary differential equations
- Homogenization of elliptic differential equations
- Geometrical optics

Singular perturbations

We will consider examples where the the micro scales are localized. The purpose is the derivation of the limiting effective equations and the study of the limiting process.

$$-\varepsilon \frac{d^2 u_\varepsilon}{dx^2} + a \frac{du_\varepsilon}{dx} + bu_\varepsilon = f(x) \quad 0 < x < 1, \quad a > 0,$$
$$u_\varepsilon(0) = u_L, \quad u_\varepsilon(1) = u_R$$
$$0 < \varepsilon << 1, \; a, b > 0$$

The formal limit of this differential equation is of first order and only requires one boundary condition. In this case we can solve the original problem to see which boundary condition should be kept

$$u_\varepsilon = u_{IH} + u_H$$

$$u_{IH}(x) = \int_0^x \exp(-(b/a)(x-\xi))f(\xi)d\xi + O(\varepsilon)$$

$$u_H(x) = A_1 \exp(z_1 x) + A_2 \exp(z_2 x)$$

The inhomogeneous part of the solution u_{IH} is smooth as $\varepsilon \to 0$. The homogenous part u_h matches the boundary conditions resulting from subtracting u_{IH} with z_1 and z_2 the roots of the characteristic equation,

$$-\varepsilon z^2 + az + b = 0$$

$$z_1 = a/(2\varepsilon) + \sqrt{(a/2\varepsilon)^2 + b}, \quad z_2 = a/(2\varepsilon) - \sqrt{(a/2\varepsilon)^2 + b},$$

Recall the form of the homogeneous part,

$$u_H(x) = A_1 \exp(z_1 x) + A_2 \exp(z_2 x)$$

$$z_1 = a/\varepsilon + O(\varepsilon), \quad z_2 = O(\varepsilon)$$

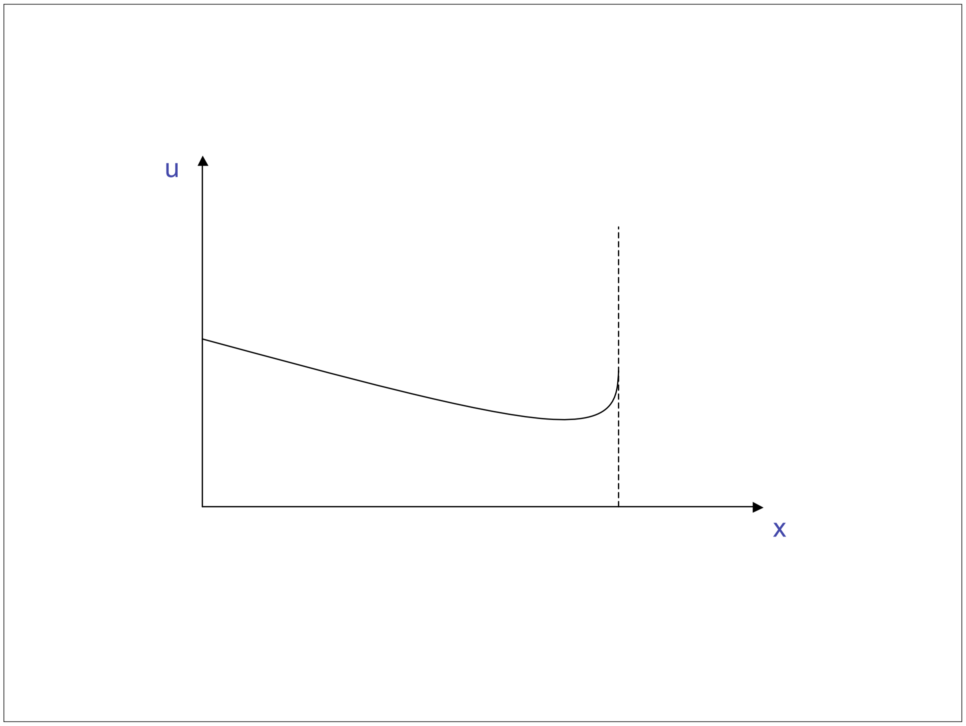
The coefficients A_1 and A_2 are determined to match the boundary conditions

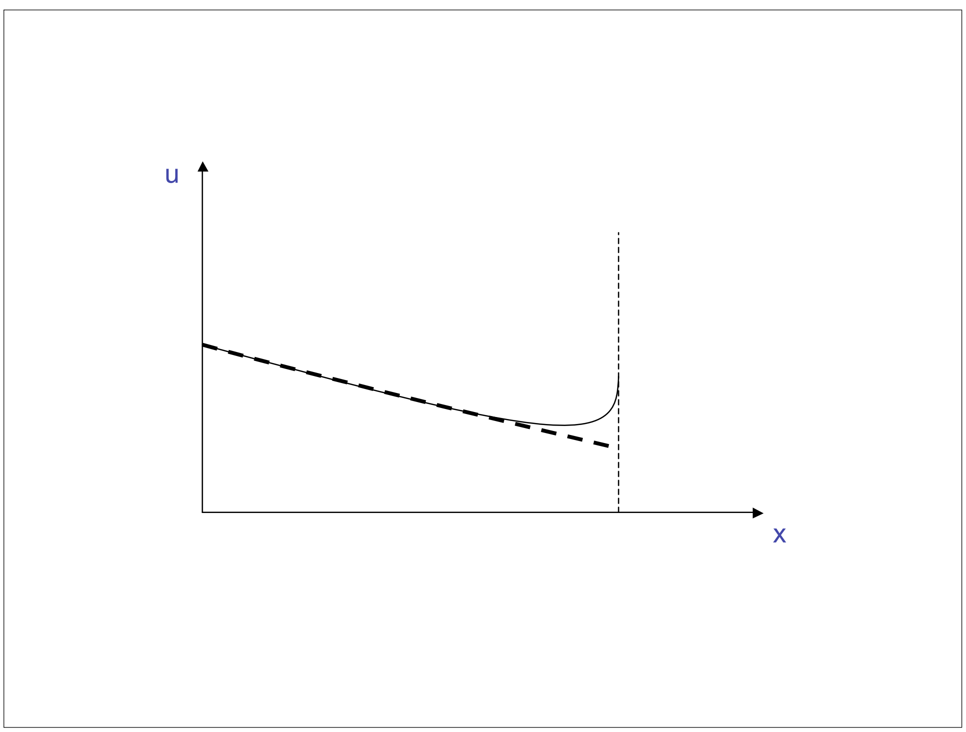
$$A_1 + A_2 = u_L - u_{IH}(0)$$

$$A_1 \exp(z_1) + A_2 \exp(z_2) = u_R - u_{IH}(1)$$

$$A_1 \approx 0, \quad A_2 \approx u_L - u_{IH}(0)$$

Thus u_H is close to a constant away from a boundary near x=1.


u
x


u
x

The effective equation is

$$a\frac{du}{dx} + bu = f(x), \quad 0 < x < 1$$
$$u(0) = u_L$$

and u^ε converges to u point wise in any domain $0 \le x \le r < 1$, with the error $O(\varepsilon)$.

The inner solution and the boundary layer solution can be matched together to form an approximation for the full interval. This type of approximation goes under the name of matched asymptotics.

$$a\frac{du_1}{dx} + bu_1 = f(x), \ u_1(0) = u_L, \quad 0 < x \le 1 - C(\varepsilon)\varepsilon$$
$$\begin{cases} -\varepsilon\frac{d^2u_2}{dx^2} + a\frac{du_2}{dx} + bu_2 = 0, & 1 - C(\varepsilon)\varepsilon < x < 1 \\ u_2(1 - C(\varepsilon)\varepsilon) = u_1(1 - C(\varepsilon)\varepsilon), & u_2(1) = u_R, \end{cases}$$

Prandtl boundary layer equations

One classical example of an effective boundary layer equation is the Prandtl equation as a limit of high Reynolds number Navier-Stokes equations,

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial p}{\partial x} = \frac{1}{R}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$
$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial p}{\partial y} = \frac{1}{R}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right)$$
$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \quad y > 0, -\infty < x < \infty, t > 0,$$
$$u(x,y,0), v(x,y,0) \ \textit{given initial values},$$
$$u = v = 0, \quad y = 0, \quad -\infty < x < \infty,$$

The Prandtl assumption is that the inertia terms are balanced by the viscous terms in the a boundary layer of thickness δ ($0<y<\delta$). Rescaling the independent variables $y/\delta \to \eta$ and using the divergence free condition,

$$\frac{\partial}{\partial y} \to \delta^{-1}\frac{\partial}{\partial \eta}, \quad \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

implies the scaling $u=O(1)$, $v=O(\delta)$. Following the tradition we will use y for the new variable η and study the scaling of the terms in the original equations.

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial p}{\partial x} = \frac{1}{R}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

$$1 \qquad 1 \qquad \delta\,\delta^{-1} \quad 1 \qquad\qquad 1 \qquad \delta^{-2}$$

Balancing inertia and viscous terms implies $R=O(\delta^{-2})$ or $\delta=O(R^{-1/2})$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial p}{\partial y} = \frac{1}{R}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right)$$

$$\delta \qquad \delta \qquad \delta \qquad \delta^{-1} \quad \delta^2 \quad \delta \qquad 1$$

Leading orders of δ in the second equation gives ,

$$\frac{\partial p}{\partial y} = 0 \quad \Rightarrow \quad p = P(x)$$

We then get the Prandtl boundary layer equation from the first equation,

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + P_x = \frac{\partial^2 u}{\partial y^2}$$

$$v = -\int_0^y \frac{\partial u}{\partial x} d\varsigma,$$

$$u(x, y, 0) \text{ given initial values}$$

$$u(x,0,t) = 0, u(x,1,t) = U(x,t)$$

- This effective equation does not contain the small parameter 1/R. It has been used for analysis and numerical simulations. There is no rigorous derivation as the limit of the Navier-Stokes equations.
- There is a well established existence and uniqueness theory for the case that $u_y > 0$ initially.
- Other well known effective equations for the high Reynolds number limit are the various turbulence models.

Stiff dynamical systems

Analysis of certain types of stiff dynamical systems resembles that of singular perturbations above. A system of ordinary differential equations is said to be stiff if the eigenvalues of the matrix A below are of strongly different magnitude or if the magnitude of the eigenvalues are large compared to the length of interval of the independent variable,

$$\frac{du}{dt} = Au + f(t), \quad u(0) = u_0, \quad 0 < t < T, \quad u : R^1 \to R^d$$

$$\max|\sigma(A)| >> \min|\sigma(A)| \ or \ T \max|\sigma(A)| >> 1, \quad \mathrm{Re}(\sigma(A)) \le 0$$

The following nonlinear system is stiff for $0 < \varepsilon << 1$,

$$\frac{du_\varepsilon}{dt} = f(u_\varepsilon, v_\varepsilon),$$

$$\frac{dv_\varepsilon}{dt} = \varepsilon^{-1} g(u_\varepsilon, v_\varepsilon), \quad t > 0$$

$$u_\varepsilon(0) = u_0, v_\varepsilon(0) = v_0$$

If the conditions below are valid it has resemblance to the singular perturbation case,

$$\mathrm{Re}(\sigma(\frac{\partial g}{\partial v_\varepsilon})) \le \bar{\lambda} < 0, \quad \det(\frac{\partial g}{\partial u_\varepsilon}) \ne 0$$

From

$$\frac{du_\varepsilon}{dt} = f(u_\varepsilon, v_\varepsilon),$$
$$\frac{dv_\varepsilon}{dt} = \varepsilon^{-1} g(u_\varepsilon, v_\varepsilon)$$

We have the differential algebraic equations (DAE),

$$u_\varepsilon(t) \to u(t), v_\varepsilon(t) \to v(t), \quad t \geq \bar{t} > 0, as\ \varepsilon \to 0,$$
$$\frac{\partial u}{\partial t} = f(u,v), \quad u(0) = u_0$$
$$g(u,v) = 0, \quad defines\ v$$

The original functions have an exponential transient of order O(1) right after t=0 before converging to (u,v). The reduced system represents the slow manifold of the solutions of the original system.

Compare the Born-Oppenheimer approximation and the Car-Parinello method.

Oscillatory solutions

- A typical example is finite temperature molecular dynamics.
- For nonlinear problems simple averaging does not work
  $\langle f(u) \rangle \neq f(\langle x \rangle)$.
- Averaging must take resonance into account..
- KAM-theory analyses effect of perturbations.
- Simple oscillatory example,

$$\frac{du}{dt} = \varepsilon^{-1} v, \quad \frac{dv}{dt} = -\varepsilon^{-1} u, \quad \frac{dw}{dt} = u^2 + v^2,$$
$$u(0) = 0, v(0) = 1, w(0) = 0$$
$$\Rightarrow u(t) = \sin(t/\varepsilon), v(t) = \cos(t/\varepsilon), w(t) = t$$

- See also lectures by Richard Tsai and Gil Ariel

Homogenization

Homogenization is an analytic technique that applies to a wide class of multi-scale differential equations. It is used for analysis and for derivation of effective equations.

Let us start with the example of a simple two-point boundary value problem where a_ε may represent a particular property in a composite material.

$$\frac{d}{dx}(a_\varepsilon(x)\frac{du_\varepsilon}{dx}) = f(x), \quad 0 < x < 1,$$
$$u_\varepsilon(0) = u_\varepsilon(1) = 0$$
$$a_\varepsilon(x) = a(x/\varepsilon) > 0$$

The high frequencies in a_ε interact with those in $\frac{du_\varepsilon}{dx}$ to create low frequencies.

If we assume $a(y)$ to be 1-periodic then $a(x/\varepsilon)$ is highly oscillatory with wave length ε. The oscillations in a_ε will create oscillations in the solution u_ε. The oscillations in a_ε and u_ε interact to create low frequencies from these high frequencies. The effective equations can not simply be derived by taking the arithmetic average of a_ε.

This example can be analyzed by explicitly deriving the solution. After integration of the differential equation we have

$$a_\varepsilon(x)\frac{du_\varepsilon}{dx} = \int_0^x f(\xi)d\xi + C$$
$$u_\varepsilon(x) = \int_0^x (a_\varepsilon(\xi))^{-1}(\int_0^\xi f(\eta)d\eta + C)d\xi$$

The constant C is determined by the boundary conditions,

$$0 = \int_0^1 (a_\varepsilon(\xi)^{-1}(\int_0^\xi f(\eta)d\eta + C))d\xi$$

$$C = -\int_0^1 (a_\varepsilon(\xi)^{-1}\int_0^\xi f(\eta)d\eta)d\xi \,/ \int_0^1 (a_\varepsilon(\xi)^{-1}\xi d\xi$$

In this explicit form of the solution it is possible to take the limit as $\varepsilon \to 0$.

$$\lim_{\varepsilon\to 0} u_\varepsilon(x) = \lim_{\varepsilon\to 0}\int_0^x (a(\xi/\varepsilon)^{-1}(\int_0^\xi f(\eta)d\eta + C))d\xi =$$

$$= \int_0^1 a(y)^{-1}dy \left(\int_0^x F(\xi)d\xi + Cx\right)$$

$$\left(Note \quad if\ b\ 1-periodic, \quad \int_0^x b(\xi/\varepsilon)d\xi = x\int_0^1 b(y)dy + \varepsilon B(x/\varepsilon)\right)$$

The limit solution is thus,

$$u_\varepsilon(x) \to \overline{u}(x) = A^{-1}\left(\int_0^x (\int_0^\xi f(\eta)d\eta)d\xi + Cx\right) \quad as\ \varepsilon \to 0,$$

$$A = (\int_0^1 a(y)^{-1}dy)^{-1}$$

where A is the harmonic average. Differentiations yield the effective or homogenized equation,

$$\begin{cases} A\dfrac{d^2\overline{u}}{dx^2} = f(x), \quad 0 < x < 0, \\ \overline{u}(0) = \overline{u}(1) = 0. \end{cases} \qquad \left(\leftarrow \overline{F}(\overline{u}) = 0\right)$$

Elliptic homogenization problems

For most problems there is no closed form solution and the procedure in our simple example cannot be followed.

The typical approach in to assume an expansion of the solution in terms of a small parameter ε, insert the expansion into the differential equation and then to find some closure process to achieve the convergence result and the effective equation.

$$-\nabla \cdot (a(x,x/\varepsilon)\nabla u_\varepsilon(x)) + a_0(x,x/\varepsilon)u_\varepsilon(x) = f(x), \quad x \in \Omega$$
$$u_\varepsilon(x) = 0, \quad x \in \partial\Omega \; boundary\ of\ \Omega \subset R^d$$

Assume the matrix $a(x,y)$ to be positive definite and 1-periodic in y,
The function $a_0(x,y)$ is also assumed to be positive and 1-periodic in y.
The asymptotic assumption on u_ε is as follows,

$$u_\varepsilon(x) = u_0(x,x/\varepsilon) + \varepsilon u_1(x,x/\varepsilon) + \varepsilon^2 u_2(x,x/\varepsilon) + \ldots$$
$$u_j(x,y), \quad 1-periodic\ in\ y, \quad j = 1,2,\ldots$$

Introduce the variable $y=x/\varepsilon$ and equate the different orders of ε. The equation for the ε^{-2} terms is

$$-\nabla_y a(x,y)\nabla_y u_0(x,y) = 0$$

with periodic boundary conditions in y. This implies

$$u_0(x,y) = u(x)$$

The equation for the ε^{-1} terms gives a representation of u_1 in terms of u. The terms of order O(1), O(ε), etc. couple the unknown terms in the expansion of u_ε but the closure assumption that $u_2(x,y)$ is 1-periodic in y generates the effective equation as conditions on u for existence of u_2.

The effective or homogenized equations take the form,

$$-\nabla A(x)\nabla u(x) + \overline{a}(x)u(x) = f(x)$$

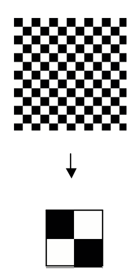
$$A: a_{ij}(x) = \frac{1}{|T|}\int_T (a_{ij}(x,y) + a_{ik}\frac{\partial \kappa^j(x,y)}{\partial y_k})dy$$

$$\overline{a}(x) = \frac{1}{|T|}\int_T a_0(x,y)dy$$

The function κ is a solution of the cell problem,

$$-(\frac{\partial}{\partial y_i}a_{ik}(x,y))\frac{\partial \kappa^j}{\partial y_k}) = -\frac{\partial a_{ij}(x,y)}{\partial y_i}$$

$$\kappa \textit{ periodic bc in } y$$



General homogenizations

- The same technique also applies to many parabolic and elliptic equations and can, for example, be used to derive the Darcy law from the Stokes equations..
- By homogenizing scale by scale several different scales can be handled ($a_\varepsilon=a(x,x/\varepsilon_1,x/\varepsilon_2,\ldots)$, $\varepsilon_1\to 0$, $\varepsilon_2/\varepsilon_1\to 0,\ldots$)
- The assumption of periodicity can be replaced by stochastic dependence.
- Compensated compactness and the theories for γ-, G-, and H-convergence are powerful non-constructive analytic technique for analyzing the limit process.

Geometrical optics

Geometrical optics equations are effective equations for high frequency wave propagation. Instead of approximating highly oscillatory functions geometrical optics gives the phase $\phi(x,t)$ and amplitude $A(x,t)$.

In this case the effective formulation were known long before the wave equation form.

New variables are introduced and not just the strong or weak limit of the original dependent variables.

Scalar wave equation

$$\frac{\partial u^2(x.t)}{\partial t^2} = c(x)^2 \Delta u(x,t)$$

$$u(x,0) = u_0(x), \quad \frac{\partial u(x,0)}{\partial t} = u_1(x)$$

The velocity is denoted by *c* and the initial values are assumed to be highly oscillatory such that the following form is appropriate,

$$u(x,t) = \exp(i\omega\varphi(x,t)) \sum_{\omega=0}^{\infty} A_j(x,t)\omega^{-j}, \quad \omega >> 1$$

Insert the expansion into the wave equation and equate the different orders of ω (=ε^{-1}). The leading equations give the eikonal and transport equations where there is no ω,

$$\frac{\partial \varphi}{\partial t} + c(x)|\nabla\varphi| = 0, \quad (|\cdot| = Euclidean\ norm)$$

$$\frac{\partial A_0}{\partial t} + c(x)\frac{\nabla\varphi \cdot \nabla A_0}{|\nabla\varphi|} + \frac{c(x)^2\Delta\varphi - \frac{\partial^2\varphi}{\partial t^2}}{2c(x)|\nabla\varphi|}A_0 = 0$$

The traditional ray tracing can be seen as the method of characteristics applied to the eikonal equation,

$$\frac{dx}{dt} = \nabla_p H(x,p), \quad \frac{dp}{dt} = \nabla_x H(x.p)$$

$$H(x.p) = c(x)|p|$$

Generalizations

- The analysis discussion above fails at boundaries. The geometrical theory of diffraction (GTD) adds correction terms for diffraction at corners and the presence of creeping waves of the shadow zone.
- The approach extends to other differential equations, for example, linear elasticity and Maxwell's equations.
- WKB - Schrödinger - frequency domain.
- If $c(x) = c(x,x/\varepsilon)$ is oscillatory, homogenization ($\varepsilon << \omega^{-1}$), geometrical optics ($\varepsilon >> \omega^{-1}$) or special expansions ($\varepsilon \approx \omega^{-1}$) apply
- See lectures by Nick Tanushev

4. Numerical methods

- These techniques are used when appropriate effective equations are not known

$$
\begin{tikzcd}
 & F_\varepsilon(u^\varepsilon)=0 \arrow[dl] \arrow[dr] & \\
\bar{F}(\bar{u})=0 \arrow[d] & & F_{\varepsilon,h}(u_{\varepsilon,h})=0 \\
\bar{F}_h(\bar{u}_h)=0 & &
\end{tikzcd}
$$

4. Numerical methods

- These techniques are used when appropriate effective equations are not known
- Fast methods resolving all scales (complexity → $O(\varepsilon^{-d})$)
  - High order methods reducing number of unknowns
  - Traditional multi-scale methods: multi-grid, fast multi-pole (using special features in operator)
  - Can not be used for extreme ε
- Numerical model reduction methods starting with all scales resolved
  - Multi-scale finite element methods (MSFEM)
  - Wavelet based model reduction
  - Can not be used for extreme ε
- Fast methods not resolving all scales (using special features in solution, i.e. scale separation)

Traditional numerical multi-scale methods

- The multigrid methods aims at solving the fully discretized problem
$$F_{\varepsilon,h}(u_{\varepsilon,h}) = 0$$
by reducing the computational complexity over direct methods for solving linear systems: r=1 in
$$flop = O((N(\varepsilon)\varepsilon^{-1})^{dr})$$
- A hierarchy of different grids is used in this iterative method. The different grids focus on different scales. The analytic properties of the differential equation is taken advantage of. Smoothing is essential.

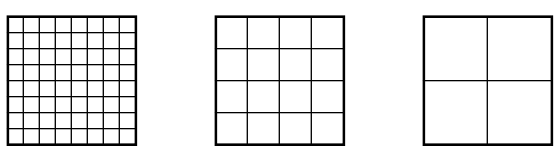
- The analytic properties of the original problem is also important for the fast multipole method (FMM). The far field behavior of analytic solution operator of importance
- Hierarchical domain decomposition is closely related to multigrid
- Conjugate gradient type of methods are algebraic in nature but can, for example, take advantage of scale separation

- For these types of problems see lectures by Lexing Ying

Example: multigrid

- Solve the system of linear equation below that comes from a discretization of an elliptic differential equation. Use a hierarchy of grids.

$$A_h u_h = f_h$$



Two-grid method

$$given\ u_h^n \rightarrow u_h^* \ by\ a\ few\ simple\ iterations$$
$$r_h = f_h - A_h u_h^* \quad residual$$
$$r_{2h} = I_h^{2h} r_h \quad restriction$$
$$A_{2h} v_{2h} = r_{2h} \quad coarse\ grid\ problem$$
$$v_h = I_{2h}^h v_{2h} \quad prolongation$$
$$u_h^{n+1} = u_h^* + v_h \quad correction$$
$$(u_h^{n+1} = u_h^* + I_{2h}^h A_{2h}^{-1} I_h^{2h} (f_h - A_h u_h^*) \approx A_h^{-1} f_h)$$

- Multigrid follows by recursively solving the coarse grid problem by the two-grid algorithm
- Different grids handle different scales → optimal computational complexity

Numerical model reduction

We will briefly mention two classes of methodologies:

- Standard model reduction of input-output systems as in control theory
- Model reduction using compression and special basis functions

Remark. The computational cost of using these methods is at least as large as the solution of the original full system. The gain comes from the potential of using the same reduced system for a large set of inputs.

Standard model reduction

Consider the input-output system

$$\frac{dx(t)}{dt} = Ax(t) + Bu(t), \quad x \in R^n, u \in R^m$$
$$y(t) = Cx(t) + Du(t), \quad y \in R^p$$

The matrix A may be the result of a spatial discretization and the dimension n is assumed to be much larger than m and p.

Transient and filtered modes are eliminated to produce an approximation with lower dimensional A. SVD of A is a possible technique. Different methods are found in the control literature.

Special basis functions

We will briefly consider two examples: the multi-scale finite element method (MSFEM) [Hou] and wavelet based homogenization [E., Runborg] - see lectures by Olof Runborg

- In MSFEM the basis functions that are used in the finite element method are chosen to satisfy the homogeneous form of the original multi-scale problem.
- The wavelets in wavelet based homogenization are used to keep the reduced operators sparse during the computation. A discretized differential equation equation in a wavelet basis is reduced by Schur complement

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} u_H \\ u_L \end{pmatrix} = \begin{pmatrix} f_H \\ f_L \end{pmatrix} \quad \rightarrow \quad (A_{22} - A_{21}A_{11}^{-1}A_{12})u_L = f_l - A_{21}A_{11}^{-1}f_H$$

II Heterogeneous multi-scale methods (HMM)

The heterogeneous multi-scale method (HMM) is a framework for developing and analyzing computational multi-scale models. A macro-scale method is coupled to a micro-scale method.

The coupling is based on related theory for analysis of effective equations. The gain in efficiency over applying the micro-scale method everywhere is the restricted use of the computational expensive technique. The micro-scale is applied only in sampled domains.

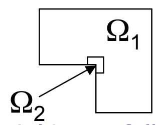
Recall computational strategies

Left: discretize homogenized or effective equation for average or expected values
Right: discretize directly in some way

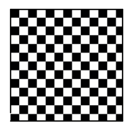
$$\begin{tikzcd}
& F_\varepsilon(u^\varepsilon)=0 \arrow[dl] \arrow[dr] & \\
\bar{F}(\bar{u})=0 \arrow[d] \arrow[drr, dashed] & & F_{\varepsilon,h}(u_{\varepsilon,h})=0 \arrow[d] \\
\bar{F}_h(\bar{u}_h)=0 & & \tilde{F}_{\varepsilon,h}(\tilde{u}_{\varepsilon,h})=0
\end{tikzcd}$$

Recall the two types of multi-scale couplings

- Type A: Macro-scale model is accurate enough in most of computational domain Ω_1. Micro-scale model used in the complement Ω_2. Compare mesh refinement.



- Type B: A Macro-scale model is not fully known throughout computational domain. Sampling the micro-scale



1. Structure of HMM

1. Design macro-scale scheme for the desired variables. The scheme may not be valid in all of the computational domain (type A) or components of the scheme may not be known in full domain (type B).
2. Use micro-scale numerical simulations to supply missing data in macro-scale model

Examples of other "better than O(ε^{-d})" multi-scale methods based on sampling

- Quasi continuum method
- Equation-free computation
- Gas kinetic schemes
- Super-parametrization
- Ultra FFTs

HMM example 1: a nonlinear conservation law is typically based on an empirical equation of state,

$$
\begin{aligned}
&\rho_t + \nabla \cdot (v\rho) = 0 \\
&(\rho v)_t + \nabla \cdot (v\rho v + p) = 0 \\
&e_t + \nabla \cdot (ve + vp) = 0 \\
&p \approx (\gamma - 1)(e - \rho v^2 / 2)
\end{aligned}
$$

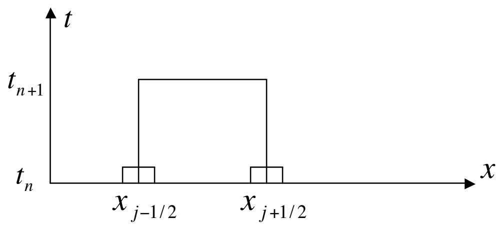
The macro-scale fluxes may, for example,be computed on the fly by micro-scale kinetic Monte Carlo or molecular dynamics simulations,

$$m_j \frac{d^2 x_j(t)}{dt^2} = -\frac{\partial V_j(x)}{\partial x_j}, \quad j = 1, \dots J$$

A generalized Godunov method: Set up approximation by a finite volume scheme for the effective nonlinear conservation law,

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0, \qquad \bar{u}_j^n = \Delta x^{-1} \int_{x_{j-1/2}}^{x_{j+1/2}} u(\xi, t_n)\, d\xi$$

$$\bar{u}_j^{n+1} = \bar{u}_j^n - \Delta t^{-1} \int_{t_n}^{t_{n+1}} \big(f(u(x_{j+1/2}, \tau)) - f(u(x_{j-1/2}, \tau)) \big)\, d\tau$$



Estimate the flux *f* by replacing the Riemann solver in the Godunov scheme by a micro-scale simulation, with appropriate initial and boundary conditions.

A generalized Godunov method: Set up approximation by a finite volume scheme for the effective nonlinear conservation law,

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0, \qquad \bar{u}_j^n = \Delta x^{-1}$$

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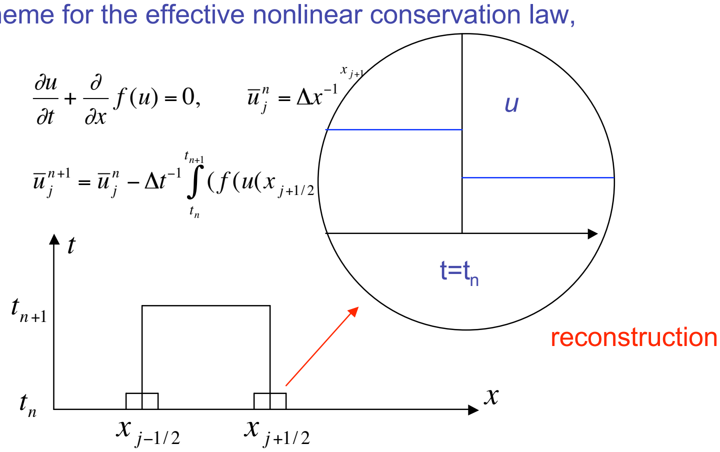

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$$\frac{\partial u}{\partial t}+\frac{\partial}{\partial x}f(u)=0, \qquad \bar{u}_j^n=\Delta x^{-1}\int^{x_{j+1}}$$

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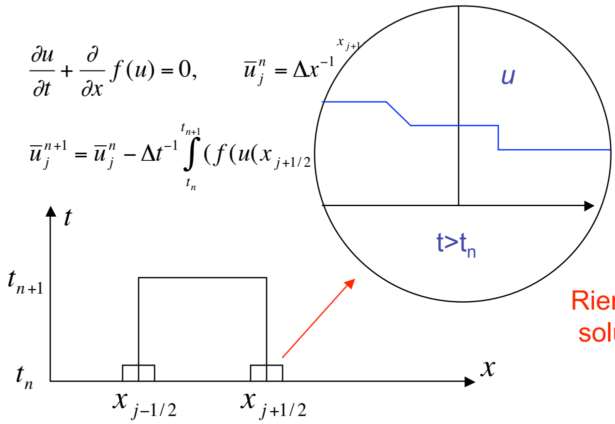

Riemann solution

Estimate the flux *f* by replacing the Riemann solver in the Godunov scheme by a micro-scale simulation, with appropriate initial and boundary conditions.

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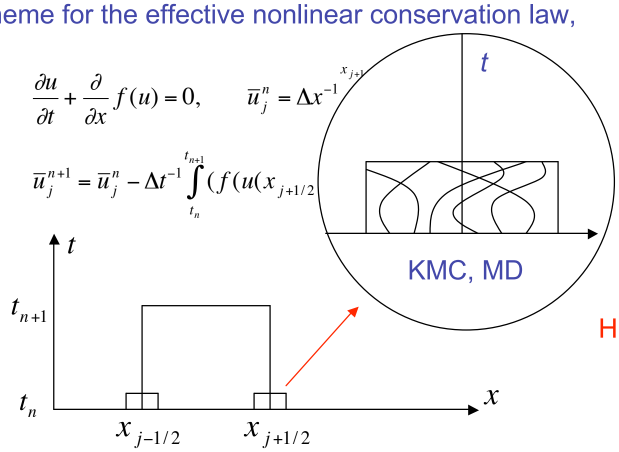

HMM

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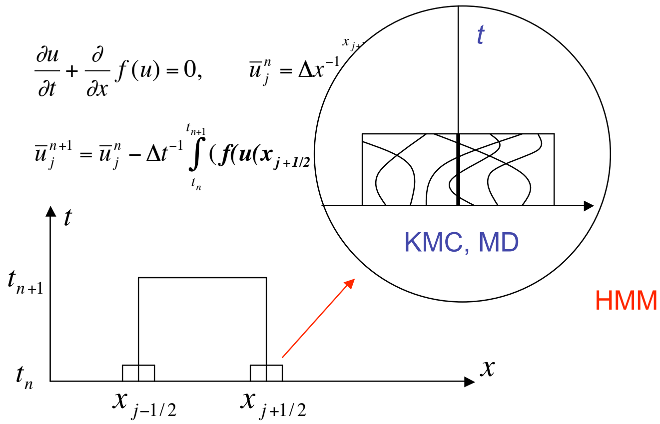

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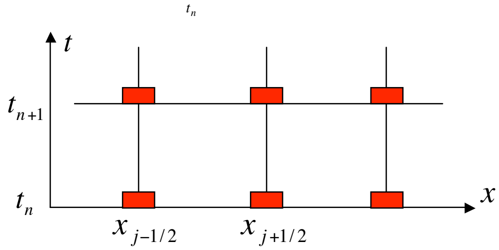

Efficiency follows from minimal use of micro-scale model (small L)

Compare QC: representative micro-scale unit >> rep atom →

→finite temperature OK.

New techniques needed

- Data estimation (from micro data to macro model)
- Boundary conditions for local micro-scale simulations
- Reconstruction techniques (from macro states to micro data)

- These techniques are also needed when when a refined simulation is used to derive fixed effective equations

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Concurrent or sequential?

- In sequential simulations, the micro-scale computations produce tables for the unknown data ahead of the macro-scale simulation (parameter passing or pre-computing)
- Concurrent also known as “on the fly”
- As described HMM is concurrent. The macro- and micro-scales are coupled throughout the simulation
- The choice is a matter of computational cost

New techniques

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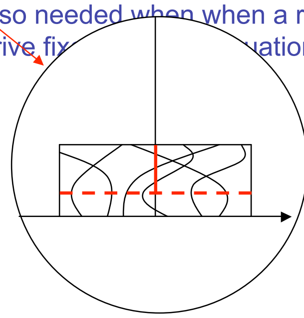
- Boundary conditions for local micro-scale simulations
- Reconstruction techniques (from macro states to micro data)

- These techniques are also needed when when a refined simulation is used to derive fix… …ations



Data estimation: micro → macro

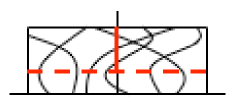
- Micro to macro operator is required: compression

$$U = Qu, \quad u = RU, \quad QR = I$$

- Often averaging in space and/or time

$$U(x,t) = \int K(x,\xi,t,\tau) Qu(\xi,\tau)\, d\xi\, d\tau$$
$$K \approx \delta, \quad K \text{ smooth}$$

- Estimation after transient and/or boundary layer (Type A, B)



New techniques

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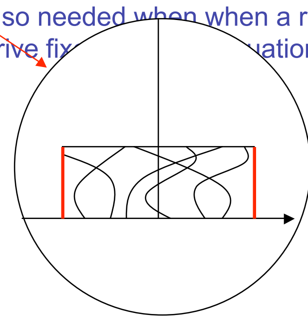


Boundary conditions: macro ↔ micro

- Use absorbing boundary conditions as much as possible,
  - Established theory for PDEs,
  - Linearize and design BC to allow for outgoing waves
- Emerging theory for MD
- Periodic BC can be modified and adjusted by thermostats.

Boundary conditions: macro ↔micro

- Use absorbing boundary conditions as much as possible,
  - Established theory for PDEs,
  - Linearize and design BC to allow for outgoing signals
    Design in phase space, continuous or discrete

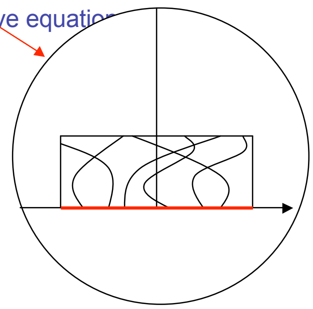
$$u_{tt} = c^2 u_{xx} \quad x > 0$$

$$u_x - c^{-1} u_t = 0 \quad x = 0$$

New techniques

- Data estimation (from micro data to macro model)
- Boundary conditions for local micro-scale simulations
- Reconstruction techniques (from macro states to micro data)

- These techniques are also needed when when a refined simulation is used to derive fixed effective equations



Reconstruction: macro → micro

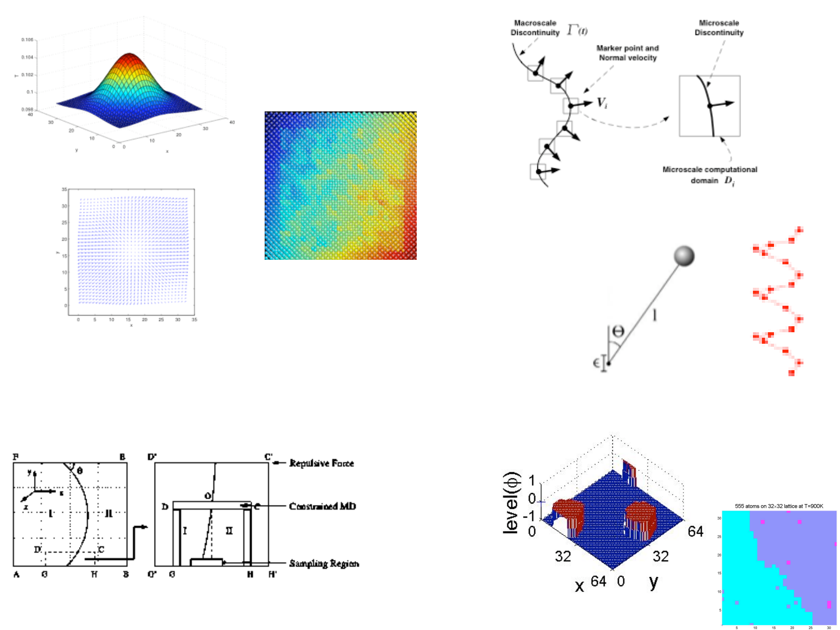
- Initial conditions: match macro-scale state

$$u = RU$$

- For extra degrees of freedoms (to reduce transient)
  - Approximate quasi-stationary state (Maxwellian)
  - Use modified distribution from previous time-steps
  - Uniform or random distribution - rely on transient
- Adaptivity can be used to find the level of matching (function value, derivative ect)

Examples of HMM simulations

- Fluid simulations: [E, Ren], contact line on multiphase fluid solid interaction. Type A example: Continuum model valid but for contact line where MD is applied.
- Solid simulation: [E, Li], thermal expansion.Type B example: Micro-scale MD model needed in full domain of elasticity continuum model.
- Combustion fronts: [Sun, Eq], micro-scale simulation with chemistry to evaluate macro scale properties at front.
- Stiff dynamical systems: [Sharp, Eq, Tsai]. intervals with short time steps to evaluate the effective force for macro time steps.
- Epitaxial growth: [Sun, Eq], atomistic kinetic Monte Carlo micro-scale simulation - diffusion and level-set models for macro-scale.



2. Analysis of HMM

- FVM for hyperbolic and parabolic equations and FEM for elliptic equations when applied to standard linear homogenization problems.
- FVM approximating the diffusion equation as by Brownian motion.
- FDM for selected dynamical systems and stochastic differential equations. Both dissipative and oscillatory problems.
- Typical error estimate (p order of macro-scale method), $e(HMM)$ error in data from micro-scale model

$$\|U_0 - U_{HMM}\| \le C(H^p + e(HMM)),$$

Structure of analysis

$$\begin{aligned} &Macro: \quad F_H(U_H, D_H(u_h)) = 0 \\ &Micro: \quad f_h(u_h, d_h(U_H)) = 0 \\ &\to \quad F_H(U_H, \tilde{D}_H(U_H)) = 0, \end{aligned}$$

$$\begin{aligned} &effective\ eqs: \quad \bar{F}(\bar{U}, \bar{D}(\bar{U})) = 0, \\ &\qquad\qquad F_H(\bar{U}_H, \bar{D}_H(\bar{U}_H)) = 0, \quad (1) \end{aligned}$$

$$\begin{aligned} &Stability\ of\ (1): \quad \|\bar{U} - U_H\| \le C(H^p + e(HMM)) \\ &\qquad e(HMM) = \|\bar{D} - \tilde{D}\|, \quad U_H \in W \end{aligned}$$

Compare Lax equivalence theorem and Strang's proof for convergence of FDM approximating nonlinear hyperbolic PDEs - implicit function theorem argument.

HMM example 2: homogenization of elliptic equation

$$-\nabla \cdot (a^{\varepsilon}(x)\nabla u^{\varepsilon}(x)) = f(x), \quad x \in D \subset R^d$$
$$u^{\varepsilon}(x) = 0, \quad x \in \partial D, \quad a_1 \ge a^{\varepsilon} \ge a_0 > 0$$

Assume there exists a homogenized equation (not known)

$$-\nabla \cdot (A(x)\nabla U(x)) = f(x), \quad x \in D \subset R^d$$
$$U(x) = 0, \quad x \in \partial D, \quad A(x) \ge A > 0$$
$$u^{\varepsilon} \to U, \quad \varepsilon \to 0$$

Ideally we want a FEM for the homogenized equation based on the bilinear form

$$A(V,W) = \int_D \nabla V(x) \cdot A(x) \nabla W(x) dx$$

$$\min_{V_H \in \boldsymbol{V_H}} \left(\frac{1}{2} A(V_H, V_H) - (f, V_H)\right)$$

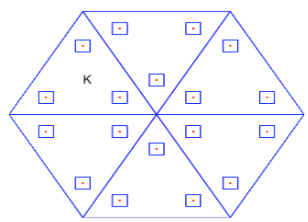
where $\boldsymbol{V_H}$ is a standard finite element space (ie. P_1, Dirichlet bc.). With T_H the corresponding triangulation of D we have the numerical approximation

$$A(V_H,V_H) \approx A_H(V_H,V_H) = \sum_{K \in T_H} |K| \sum_{x_l \in K} \omega_l (\nabla V_H \cdot A(x) \nabla V_H)(x_l)$$

The HMM strategy is now to approximate the unknown stiffness matrix (A(x) is not known) by constrained micro-scale simulations

$$(\nabla V_H \cdot A \nabla V_H)(x_l) \approx \frac{1}{\delta^d} \int_{I_\delta(x_l)} \nabla v_l^\varepsilon(x) \cdot a^\varepsilon(x) \nabla v_l^\varepsilon(x) dx$$

Where $I_\delta(x_l)$ is a cube with side length δ centered at x_l. Boundary conditions for micro-scale problem to mach gradient of V_H via Dirichlet, Neumann or periodic conditions.



Theorem, Let h→0, $a = a(x,x/\varepsilon)$

$$\|U_0 - U_{HMM}\|_s \le C(H^{p+1-s} + e(HMM)), \quad s = 1,2$$

$$e(HMM) = \max_{\substack{x_l \in K \\ K \in T_H}} |A(x_l) - A_H(x_l)|$$

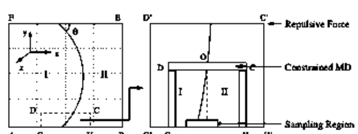
$$e(HMM) \le C((h/\delta)^q) \quad \text{if } \delta \text{ is multiple of } \varepsilon, \text{periodic}$$
$$e(HMM) \le C(\varepsilon/\delta + \delta) \quad \text{else, periodic}, \quad (h \to 0)$$
$$e(HMM) \le C(\varepsilon/\delta)^{1/2}, \quad 1-D, \text{random}, \quad (h \to 0)$$
$$e(HMM) \le C(\varepsilon/\delta)^{0.23}, \quad 3-D, \text{random}, \quad (h \to 0)$$

[Abdul, Schwab], [E, Ming, Zhang], [Abdul, Eqt]

Applications

- Continuum - molecular dynamics coupling (fluid, solid)
- Epitaxial growth
- Dynamical systems

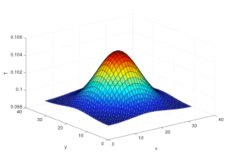
Fluid - type A

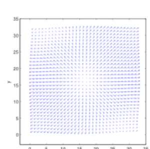


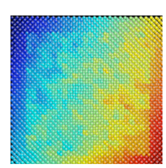
- 2 immiscible fluids and solid surface
- Macro: Navier-Stokes with curvature determined surface tension and no slip boundary condition away from slip-line.
- First order finite volume method with explicit interface tracking.

- Micro:Molecular dynamics, (y) periodic boundary conditions, (x) outer periodic boundary conditions. (z) solid and upper repulsion (from Lennard-Jone)
- Anderson thermostat velocity constraing zones.
- Time split algorithm, replaces empirical slip and contact angle.
- Micro to macro: slip-line velocity, shear stress at end point
- Macro to micro: velocity

Solid - type B



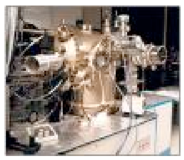


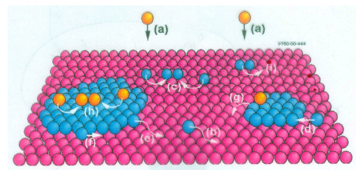


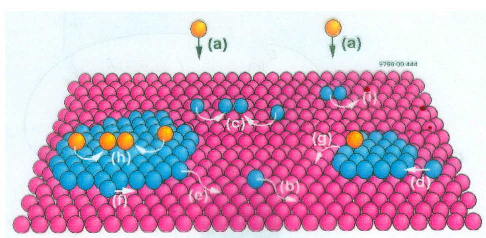
- Time split algorithm
- Macro: finite volume formulation where empirical constitutive relations replaced by data from local MD
- Micro: constrained (from macro) MD

4.2 Epitaxial growth

- Part of semiconductor production
- Layer by layer deposition of atoms
- Atoms diffuse on substrate surface, merge and nucleate islands



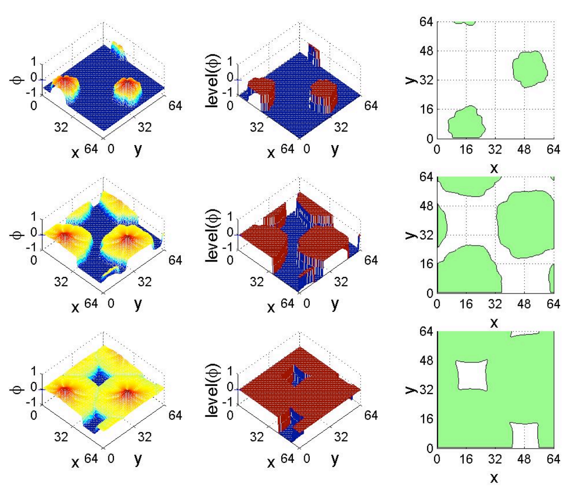




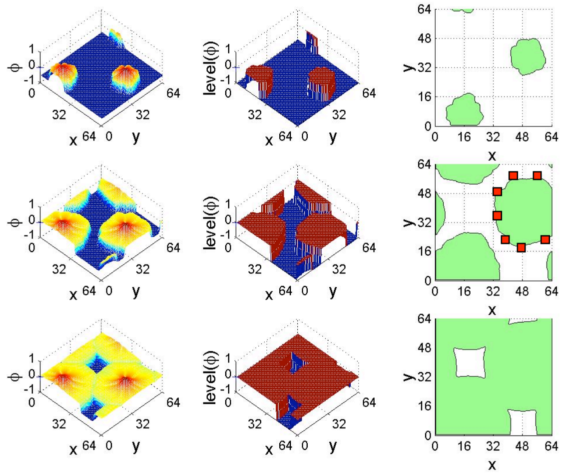
(a) Deposition (b) Diffusion (c) Nucleation (d) Attachment
(e) Detachment (f) Edge diffusion (g) Down step diffusion
(h) Nucleation on top of islands (i) Dimer diffusion

HMM strategy

- Macro-scale model: finite difference approximation of diffusion equation (ρ) coupled to levelset method for interface tracking (Γ).
- Missing data: velocity model for interface evolution and boundary conditions at interface.
- Micro-scale model: Kinetic Monte Carlo simulation of atom dynamics. Potentially based on density function computations of transition probabilities.



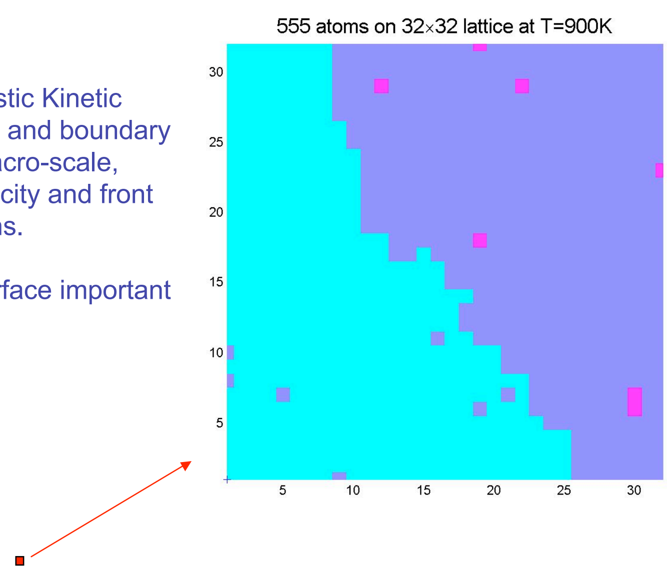
Masro-scale: diffusion equation and levelset Interface tracking



Masro-scale: diffusion equation and levelset
Interface tracking

Micro-scale: atomistic Kinetic Monte Carlo, Initial and boundary conditions from macro-scale, returning front velocity and front boundary conditions.

Roughness of interface important for front velocity

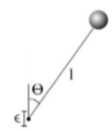


Dynamical systems

- Example: consider a stiff dynamical systems: dissipative and highly oscillatory

$$\frac{dx_\varepsilon}{dt} = f_\varepsilon(x_\varepsilon), \quad t > 0, \quad x_\varepsilon : R \to R^d$$

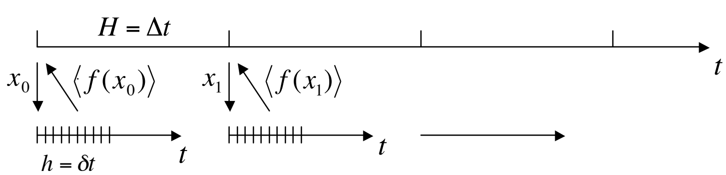
$$x_\varepsilon(0) = x_0, \quad \left\| \frac{\partial f_\varepsilon}{\partial x_\varepsilon} \right\| >> 1$$



or systems with highly oscillatory coefficients

- Potential application to molecular dynamics
- For more details, see lectures by Richard Tsai

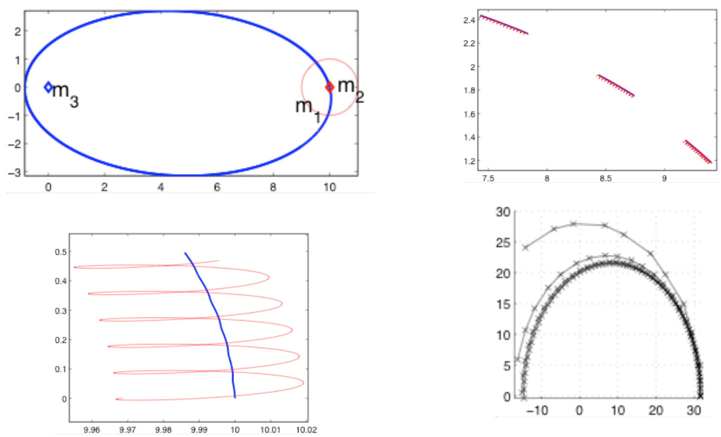
Structure of HMM-algorithm for ODEs



Effective $\langle f \rangle$ value for standard macro-scale solver from average of standard micro-scale data

Macro-scale variables the same as micro-scale variables or different for control of resonance. The choice of macro-scale variables are important

Example: sun-earth-moon, Newton’s equations



References

Bensoussan, A.,J.-L. Lions, G. Papanicolaou, Asymptotic analysis of periodic structures, Noth-Holland, 1978.

E, E., B. Engquist, Multicale modeling and computation, AMS Notices, 2003.

W. E, B. Engquist, X. Li, W. Ren and E. Vanden-Eijnden, Heterogeneous multiscale methods, Commun. Comput. Phys., 2, 367-450, 2007

Verhulst, F., Methods and Applications of Singular Perturbations, Springer-Verlag, 2005.