Multiscale Modeling

Bjorn Engquist

University of Texas at Austin

SeRC Annual Meeting, Norrköping, April 24 - 25, 2013

Outline

1. Challenges for multiscale computation and coupling of models
2. The heterogeneous multiscale method (HMM) framework
3. The issue of scale separation
4. Remarks on imaging and visualization

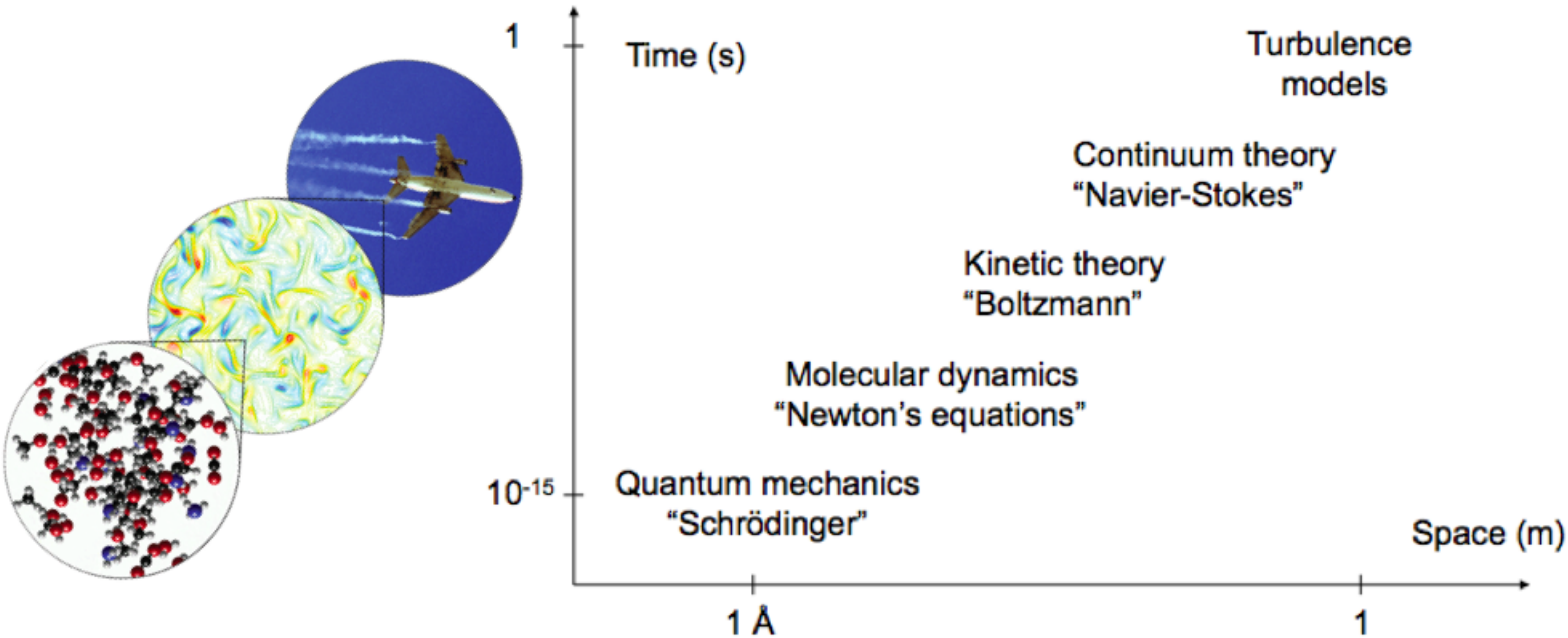
"Coupling numerical methods on different scales"

1. Challenges for multiscale computation and coupling of models

- A major e-science challenge: large amount of data – for simulations large number of unknowns and flops
- Common reason for this: multiscale phenomena
- With the size of the computational domain = *1* in each dimension, the smallest wavelength = ε and *d* dimensions, the number unknowns needed to describe a band limited function is

$$\#\ unknowns \geq O(\varepsilon^{-d}) \quad [Shannon, 48]$$

Multiscale modeling



Multiscale modeling: analytic and/or computaional

- If processes on different scales are important and

$$\# \ unknowns \geq O(\varepsilon^{-d})$$

ε << 1 $\longrightarrow$ derive effective, equations

(model reduction, homogenization theory, upscaling, averaging, boundary layer theory,)

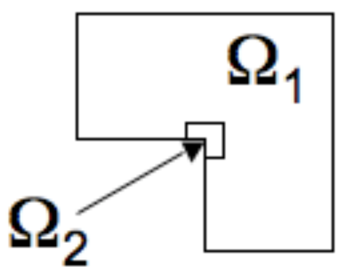
$\longrightarrow$ use the micro model in small domains and couple different models in the same simulation

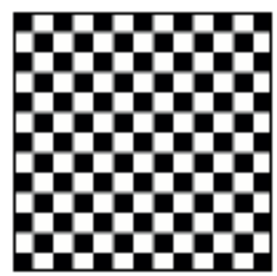
Coupling of different models (high fidelity model on small subsets)

- The goal is improved computational efficiency from only simulating the smallest scales on sub domains.

Type A: Microscale model only in sub domain Ω_2

Type B: Microscale input needed throughout computational domain from sampled sub domains

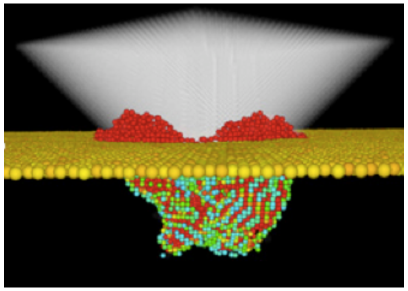


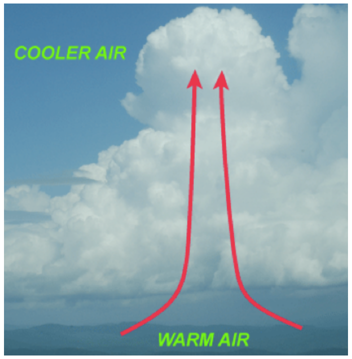


Examples of strategies

Special purpose methods

- Quasi continuum method (elasticity - molecular dynamics)
- Superparametrization (atmospheric science)





Examples of strategies

Special purpose methods

- Quasi continuum method (elasticity - molecular dynamics)
- Superparametrization (atmospheric science, see fig.)

General frameworks

- Generalized multigrid, [Brandt]
- Equation-free computation, [Kevrekides]
- Heterogeneous multiscale method (HMM) (✔)

2. The heterogeneous multiscale method (HMM) framework

1. Design macro-scale scheme for the desired variables. The scheme may not be valid in all of the computational domain or components of the scheme may not be known in full domain.

2. Use micro-scale numerical simulations locally in time or space to supply missing data in macro-scale model

$$Macro: \quad F_H(U_H, D(u_h)) = 0$$

$$Micro: \quad f_h(u_h, d(U_H)) = 0$$

$$\rightarrow \quad F_H(U_{HMM}, D_{HMM}(U_{HMM})) = 0$$

HMM: nonlinear conservation law example

- nonlinear conservation law based on an empirical equation of state,

$$\rho_t + \nabla \cdot (v\rho) = 0$$

$$(\rho v)_t + \nabla \cdot (v\rho v + p) = 0$$

$$e_t + \nabla \cdot (ve + vp) = 0$$

$$p \approx (\gamma - 1)(e - \rho v^2 / 2)$$

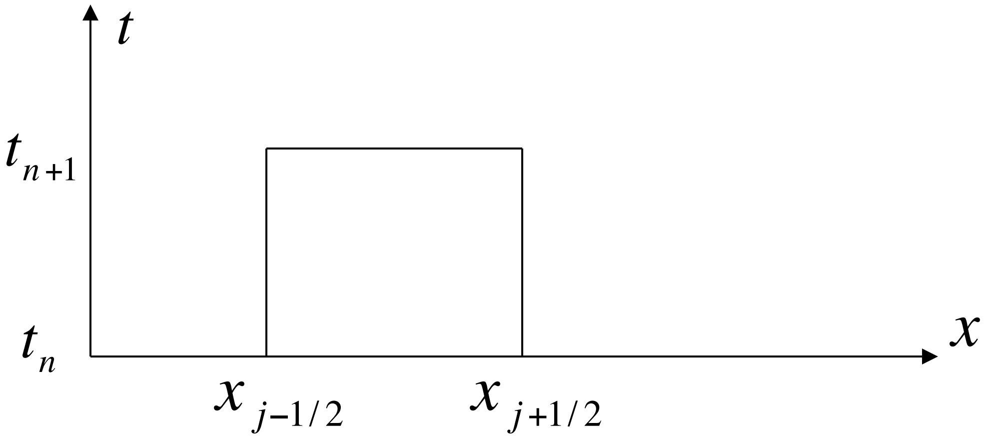
- The macro-scale fluxes could, for example, be computed on the fly by microscale molecular dynamics simulations,

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

Set up approximation by a shock capturing finite volume method (FVM) for the effective nonlinear conservation law,

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

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



Traditional numerical algorithm, for example, the Godunov scheme

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

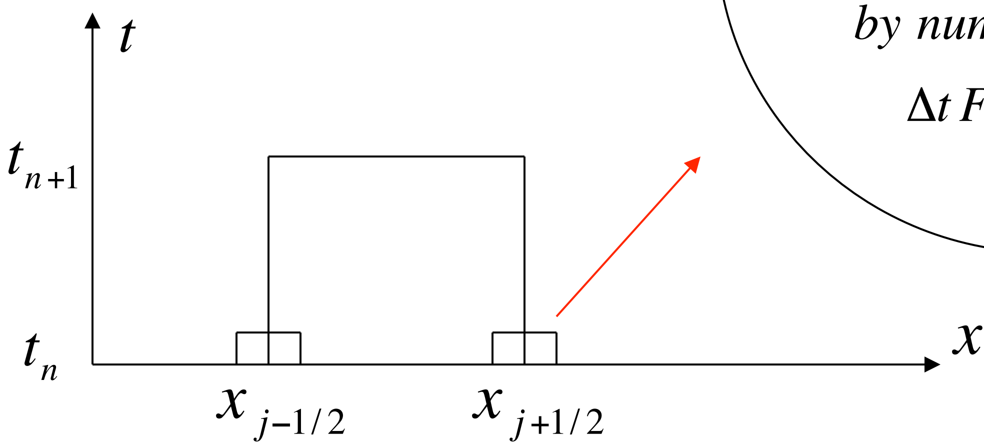
$$\overline{u}_j^{n+1} = \overline{u}_j^n - \Delta x^{-1} \int_{t_n}^{t_{n+1}} (f(u(x_{j+1/2},\tau)) -$$

If $f(u)$ *known*

$$approximate \int_{t_n}^{t_{n+1}} f(u(x_{j+1/2},\tau) d\tau$$

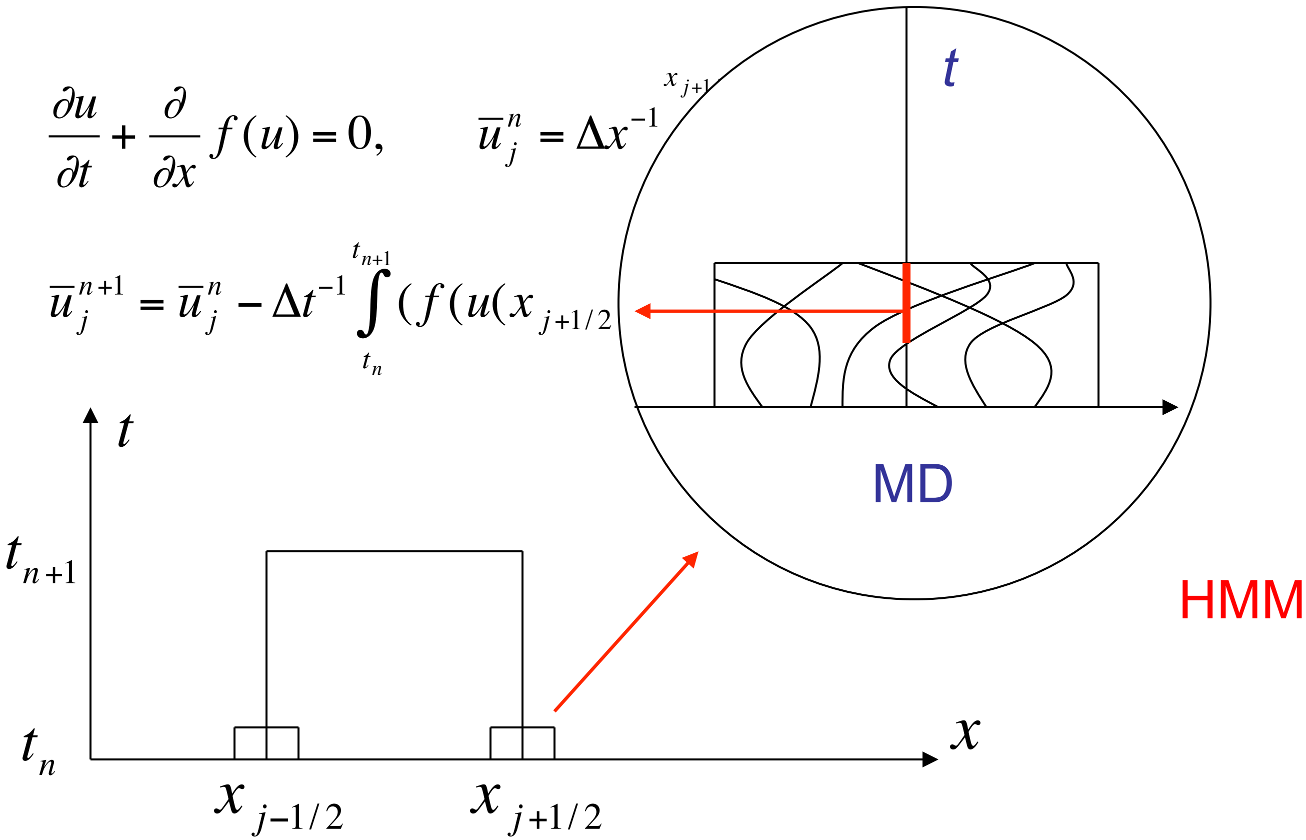
by numerical flux

$$\Delta t\, F(\overline{u}_j^n, \overline{u}_{j+1}^n)$$



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

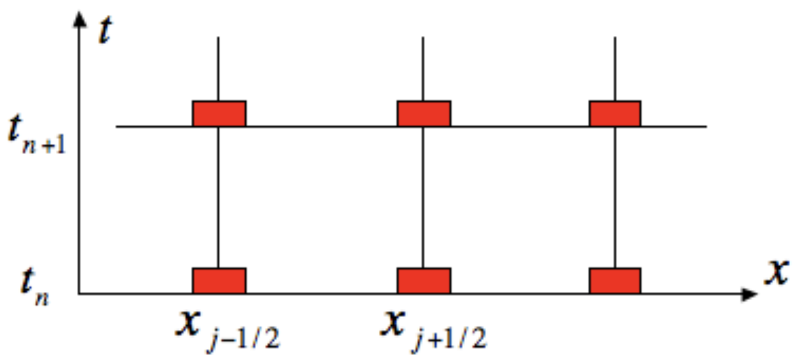
$$\bar{u}_j^{n+1} = \bar{u}_j^n - \Delta t^{-1} \int_{t_n}^{t_{n+1}} (f(u(x_{j+1/2} \ldots$$



Estimate the flux by replacing the numerical flux in the FVM by a microscale simulation, with appropriate initial and boundary conditions.

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

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



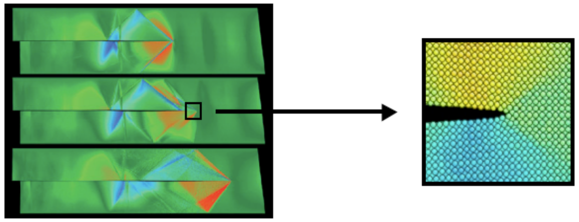
Compare homogenization

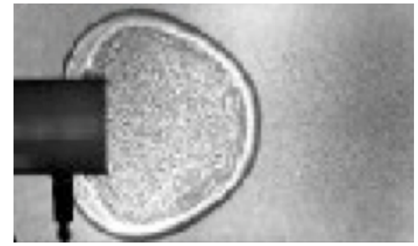
Computational complexity gain from MD in local domains

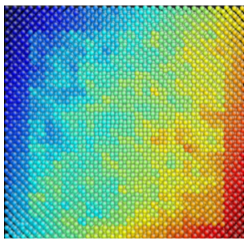
Computational issues

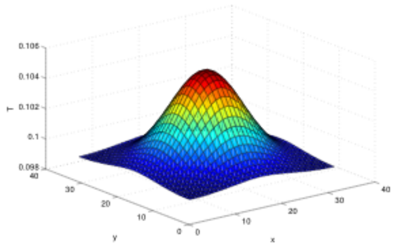
- New techniques
  - Data estimation (from micro data to macro model)
  - Reconstruction techniques (from macro states to micro data)
  - Boundary conditions for local micro-scale simulations
- Concurrent or sequential
- Choice of macro-scale variables
- Size of micro domain?
- Need for scale separation (✔)

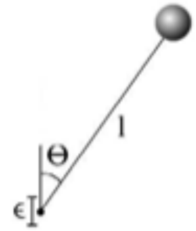
Applications

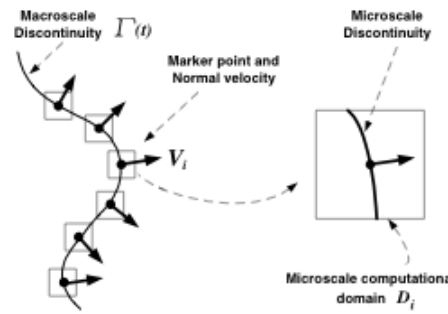


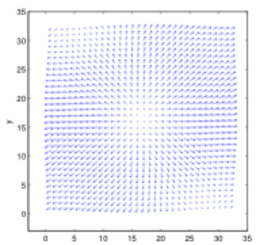


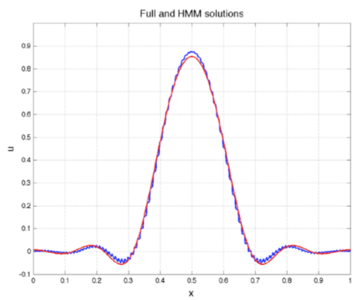


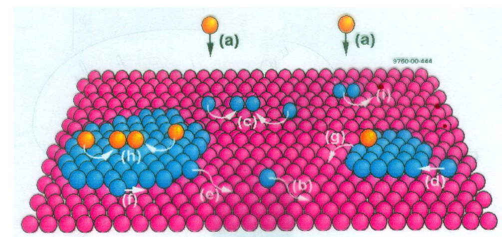


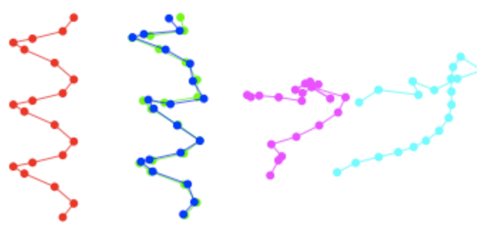


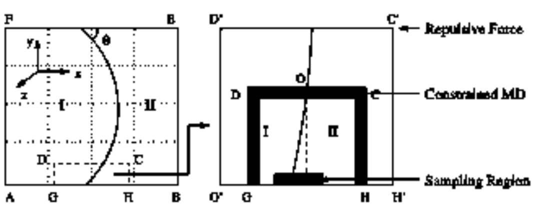


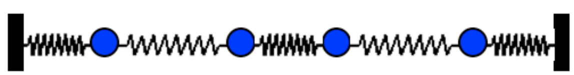


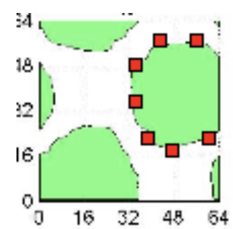


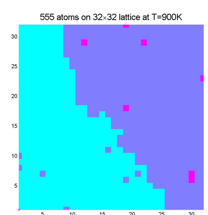






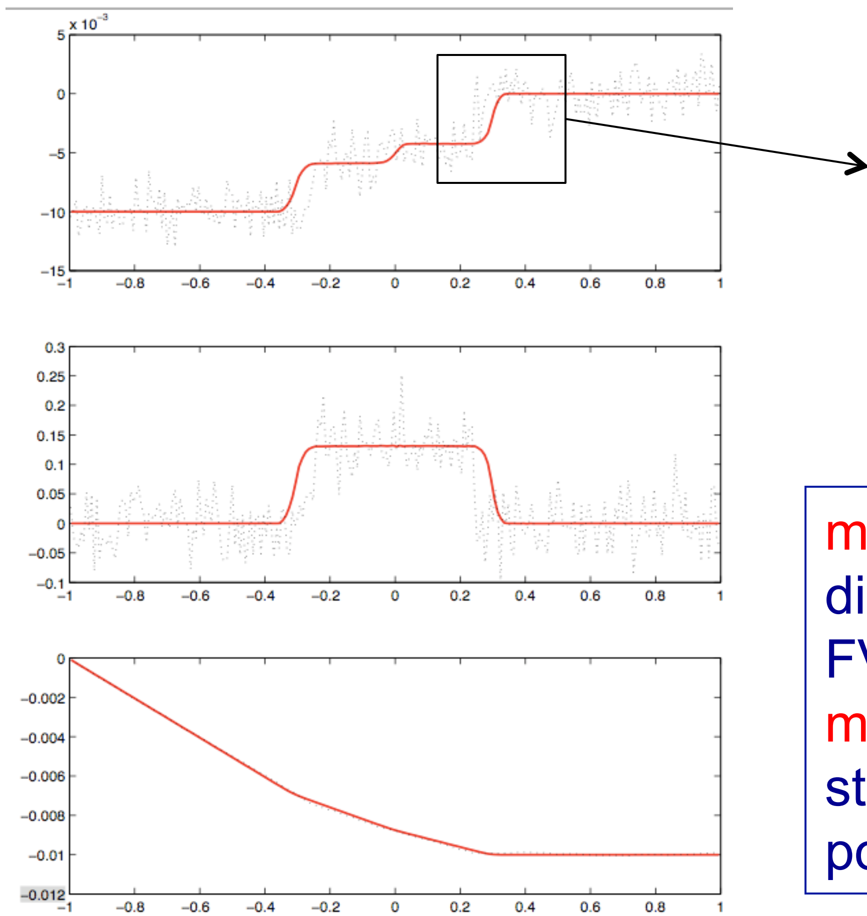


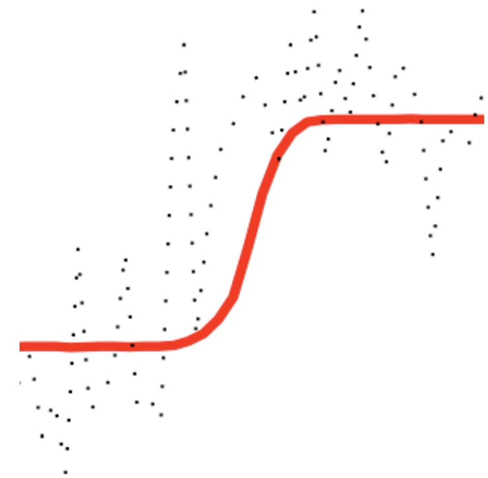




[Ariel, E, Eqt, Holst, Li, Ren, Runborg, Sharp, Sun, Tsai].

Example, shocks in solids

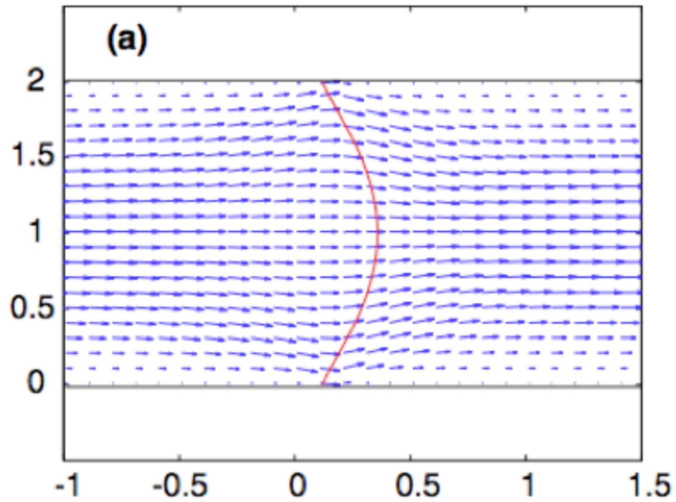




macro: strain, velocity and displacement
FVM 200 grid points, 40 steps
micro: MD 40X10 atoms,10000 steps, Lennard – Jones potential

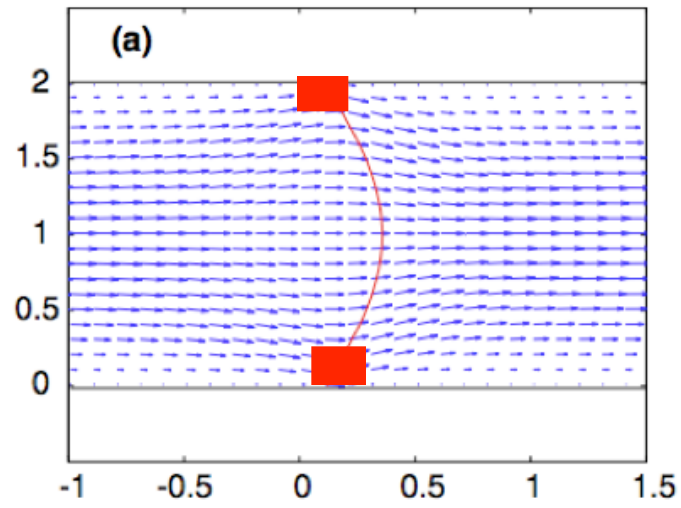
Slip line example

- No slip boundary condition for Naver-Stokes fails at slip line
- This is a type A problem (conservation law was type B)



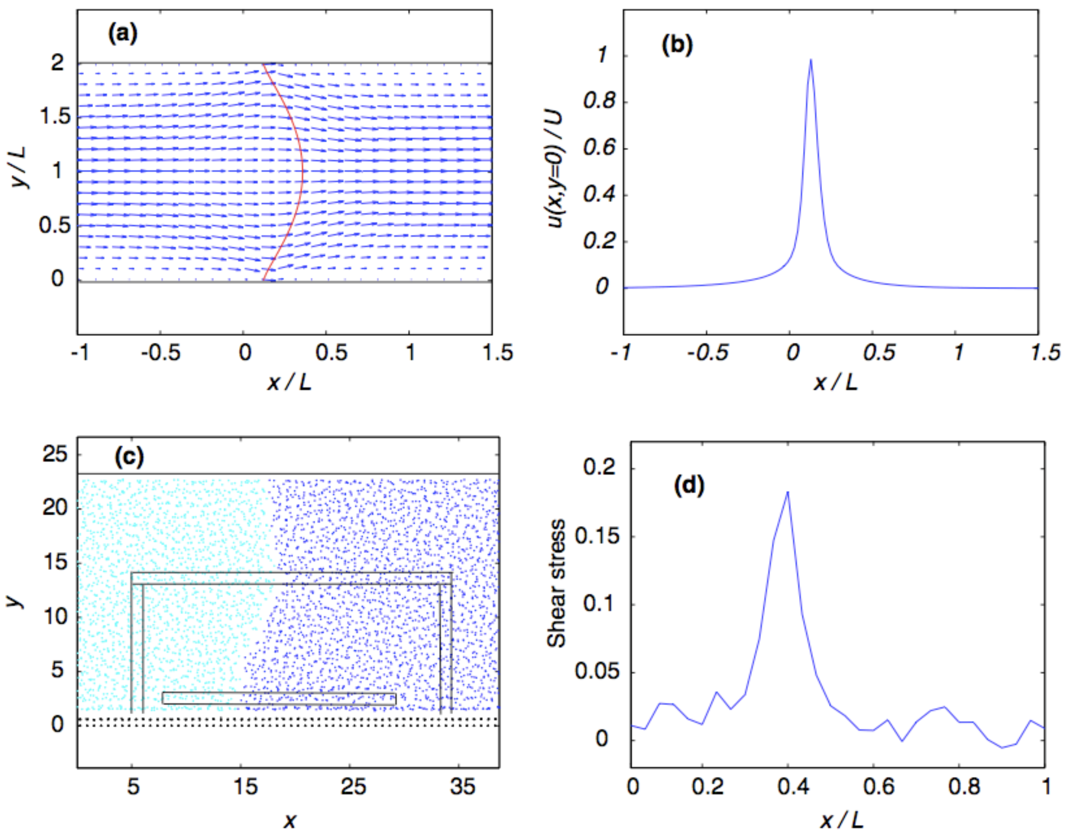
Slip line example

- No slip boundary condition for Naver-Stokes fails at slip line
- This is a type A problem (conservation law was type B)



Slip line example

- Coupling: fluid and line velocity and shear stress
- Heat bath for MD



Analysis of convergence: heat equation in composite material

- The relation between molecular dynamics and nonlinear conservation laws is not mathematically well established
- A related diffusion problem for composite media with homogenization based analysis is possible

$$f(u) \rightarrow a(x/\varepsilon)\nabla u$$

$$\frac{\partial u^{\varepsilon}}{\partial t} = \nabla \cdot (a(x/\varepsilon)\nabla u^{\varepsilon}$$

$$a(y) \ periodic$$

Steps in HMM convergence proof

- Stability and consistency of microscale problem $(u_h \to u^\varepsilon, h \to 0)$
- Convergence of computed microscale flux to homogenized flux within numerical micro domain
  - Homogenization theory
  - Eigenvalue estimates for transient

$$(-\nabla \cdot (a(x/\varepsilon)\nabla u^\varepsilon \to -\nabla \cdot A\nabla U,\ \varepsilon \to 0)$$

- Stability and consistency of macroscale algorithm $(U_H \to U, H \to 0)$

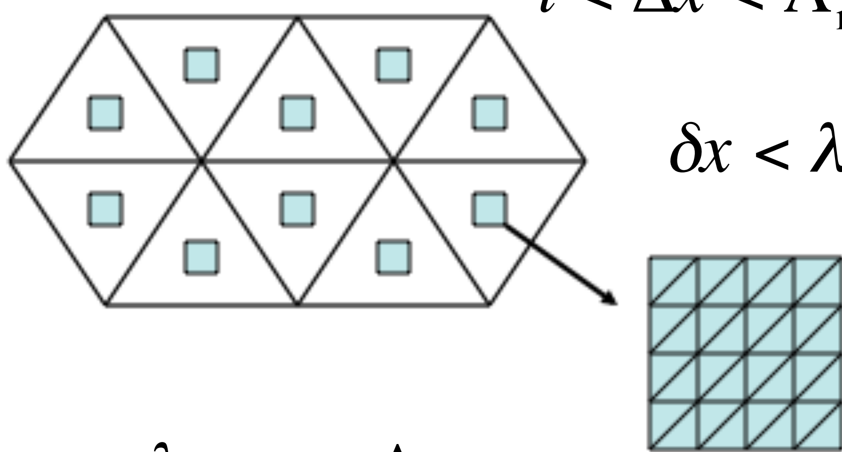
$$(U_H \to \overline{U},\ h/\varepsilon \to 0,\ \varepsilon \to 0,\ H \to 0)$$

3. The issue of scale separation

- HMM as described above require substantial scale separation

$$l < \Delta x < \Lambda_{\min}$$

$$\delta x < \lambda_{\max} < l$$



$$\longrightarrow \lambda_{\max} << \Lambda_{\min}$$

ODEs with oscillatory solutions

- Applications: dynamical systems, astrophysics,..
- Separation of fast and slow modes

$$\frac{dx}{dt} = f_\varepsilon(x) \quad \rightarrow \quad \begin{cases} \dfrac{du}{dt} = f(u,v) \\ \dfrac{dv}{dt} = \varepsilon^{-1} g(u,v) \end{cases}$$

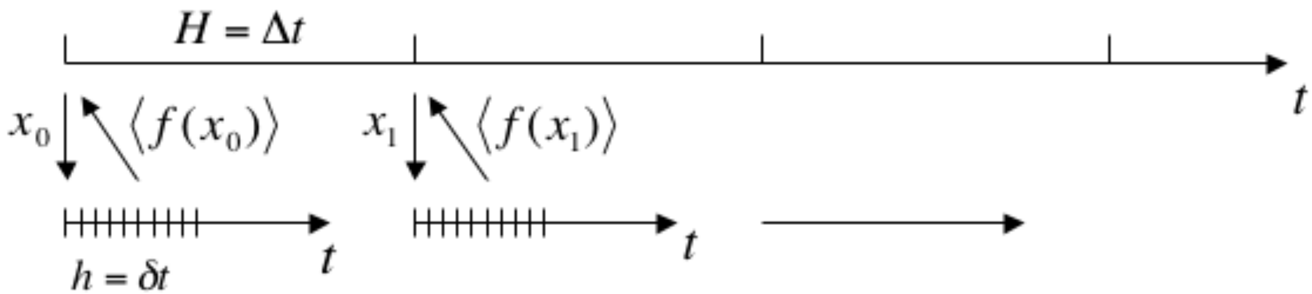
- Effective equation of ODE or SDE

$$\varepsilon \to 0 \Rightarrow u \to \bar{u}: \quad \frac{d\bar{u}}{dt} = \int f(\bar{u},v)\, d\mu_{\bar{u}}(v)$$

- Invariant measure *μ* independent of *v*(0)

HMM discretization

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



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

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

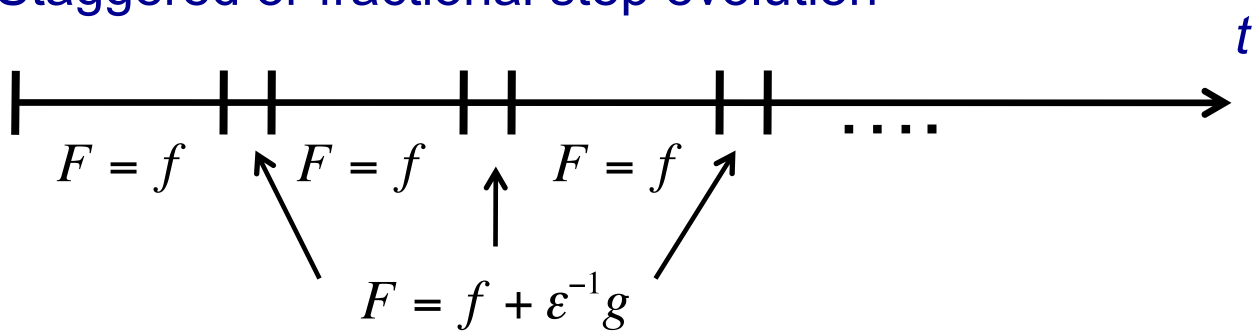
$$\left(\frac{d\overline{u}}{dt} = \int f(\overline{u}, v) \, d\mu_{\overline{u}}(v) \right)$$

A more seamless technique

- FLow AVeraging integratORS (FLAVORS) [Tao, Owhadi, Marsden, 09], also [Vanden-Eijnden, 07], VSHMM [E., Lee, 13]

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

- Staggered or fractional step evolution

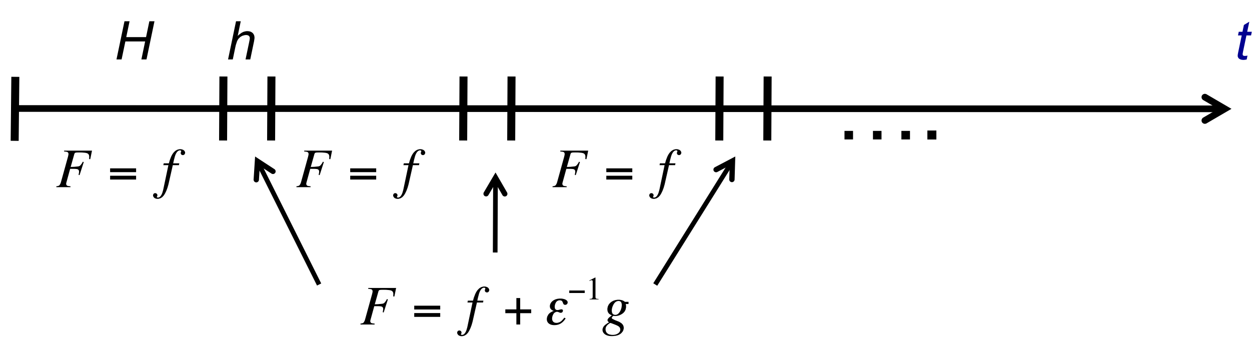


Convergence FLAVORS

- Convergence proof based on transformation to action angle formulation with ergodic fast mode
- Convergence slower than for HMM
- Compare Monte Carlo

$$\begin{cases} \dfrac{du}{dt} = f(u,v) \\ \dfrac{dv}{dt} = \varepsilon^{-1} g(u,v) \end{cases}$$

$$\frac{d\bar{u}}{dt} = \int f(\bar{u},v)\, d\mu_{\bar{u}}(v)$$



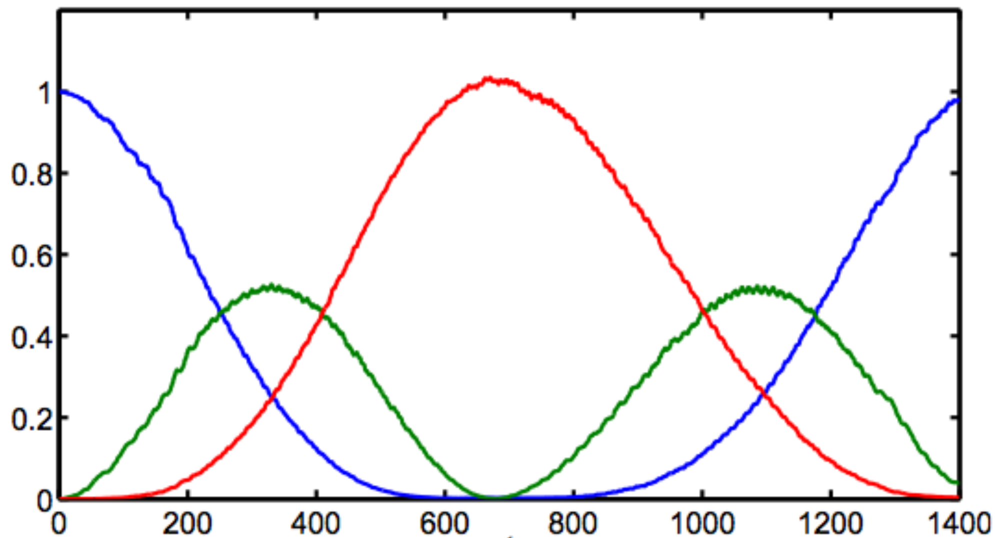
Remarks

- The Fermi-Pasta-Ulam problem is also appropriate for this technique
- Natural choice of ergodic, fast sub-system: fast linear springs (harmonic oscillators)

$$\dot{x} = f(x) + \varepsilon^{-1} g(x) \quad (\mathit{full\ system})$$

$$\dot{y} = \varepsilon^{-1} g(y) \quad (\mathit{fast\ linear\ springs})$$

Fermi-Pasta-Ulam



BF HMM Verlet-ODE45 to T = $7\varepsilon{-}1$

PDE example

- Advection enhanced diffusion in incompressible turbulent velocity field
- There exists solid convergence theory for special velocity fields

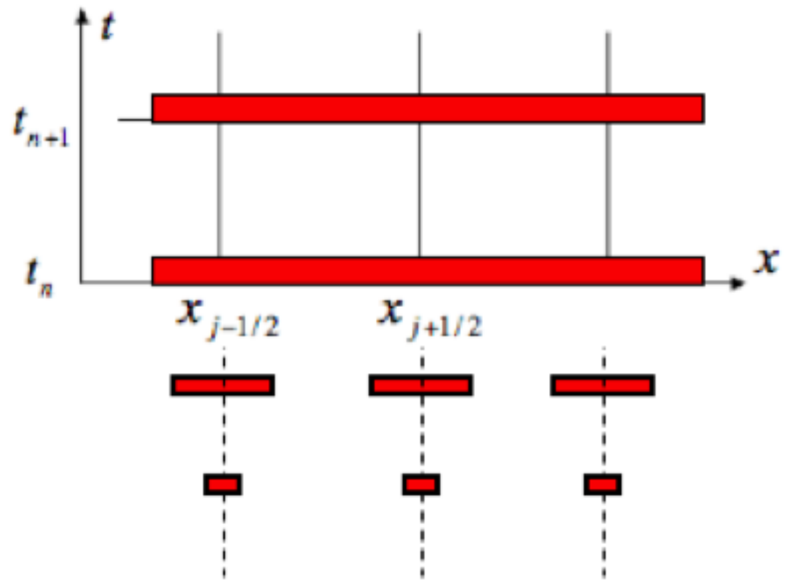
$$\frac{\partial u(x,t)}{\partial t} + v_\varepsilon(x)\cdot \nabla u(x,t) = \mu \Delta u(x,t)$$

$$\nabla \cdot v_\varepsilon(x) = 0$$

$$u(x,0) = u_0(x)$$

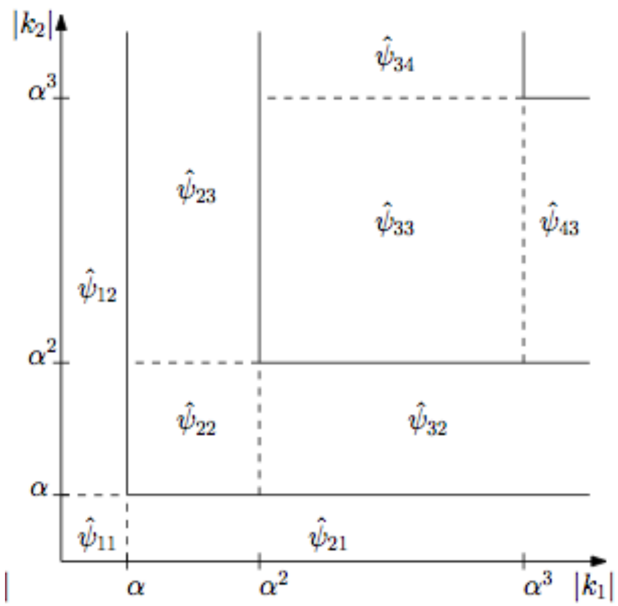
Decomposition of velocity field and solution into frequency bands

- Many locally refined grids matching the different frequency bands bands – compare multigrid
- Decomposition into frequency bands – compare LES
- Does not describe interaction between high frequency bands

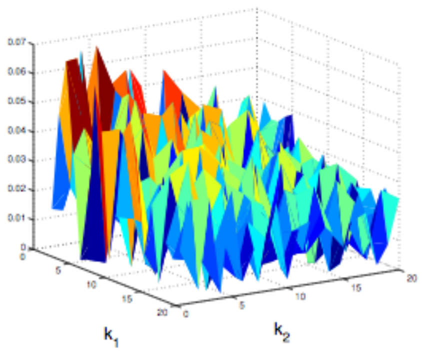


In frequency space

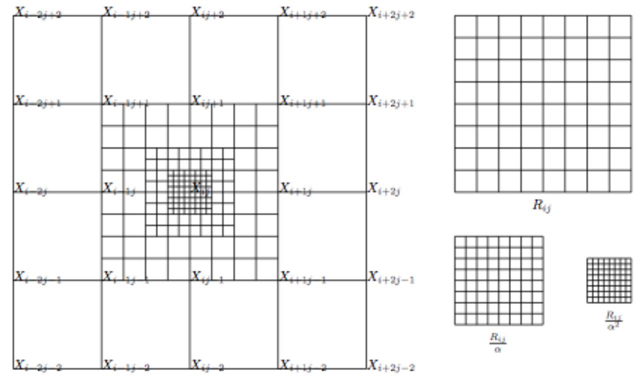
- Each diagonal box has its own grid
- Sheer flow via analytical formula

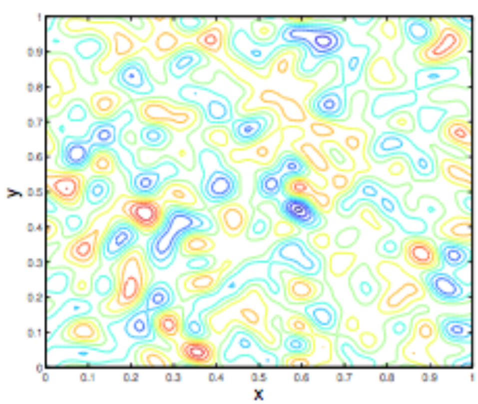


Example: passive advection (turbulent velocity field)

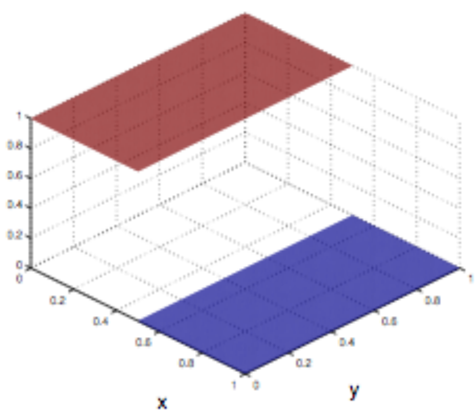


(a) Fourier spectrum of the Stream Function

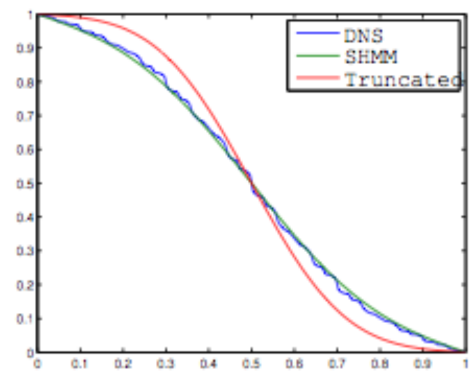




(a) Stream line of the Velocity Field **v**



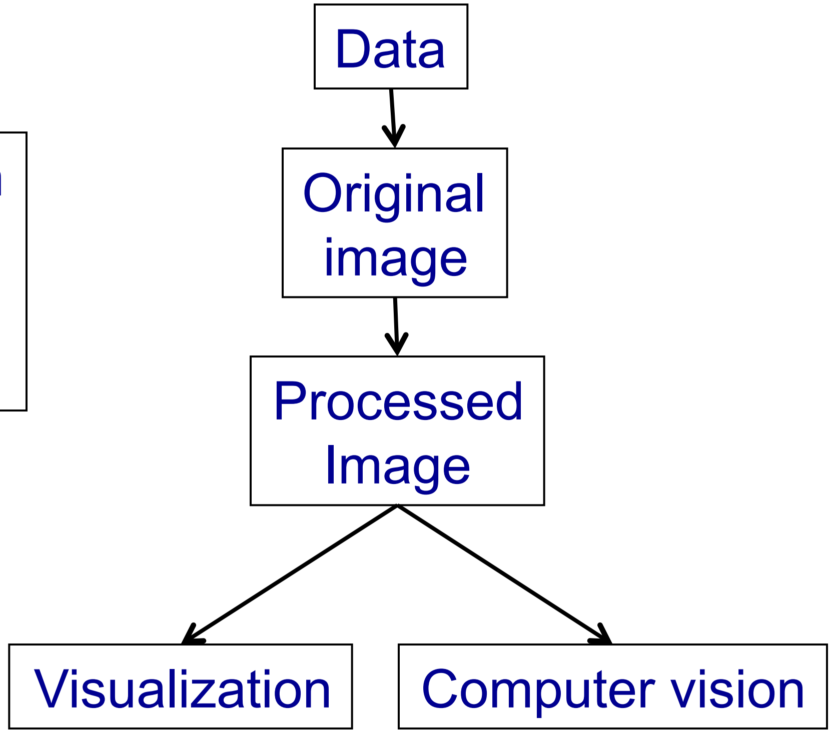
(a) Initial condition



(b) Cross section at $y = 0.5$

4. Remarks on imaging and visualization

"The imaging or visualization pipeline also contains many aspects of multiscale processes"



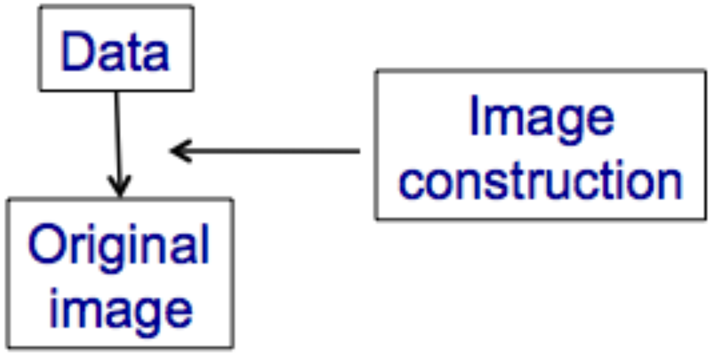
Examples of Multiscale processes in imaging pipeline

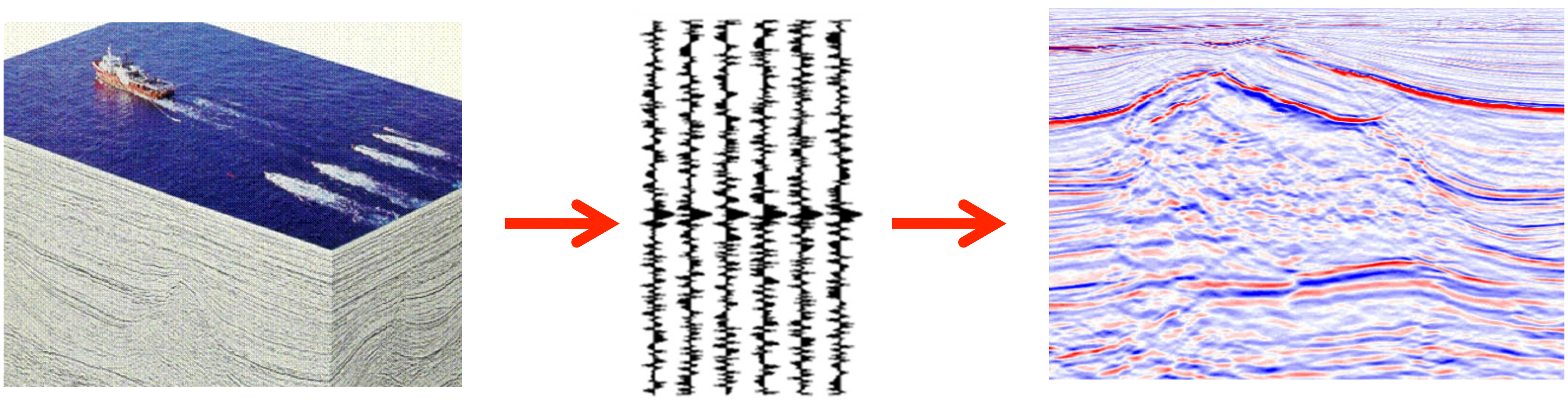
- Basic image construction (✔)
  - Build image from measured data, direct or inverse problem
- Denoising
  - Eliminate unwanted small scales
- Deblurring
  - Image correction enhancing small scales
- Inpainting
  - Correct small scale distorsions
- Image compression
  - Approximations keeping small scale features, JPEG, etc.

Examples of Multiscale processes in imaging pipeline

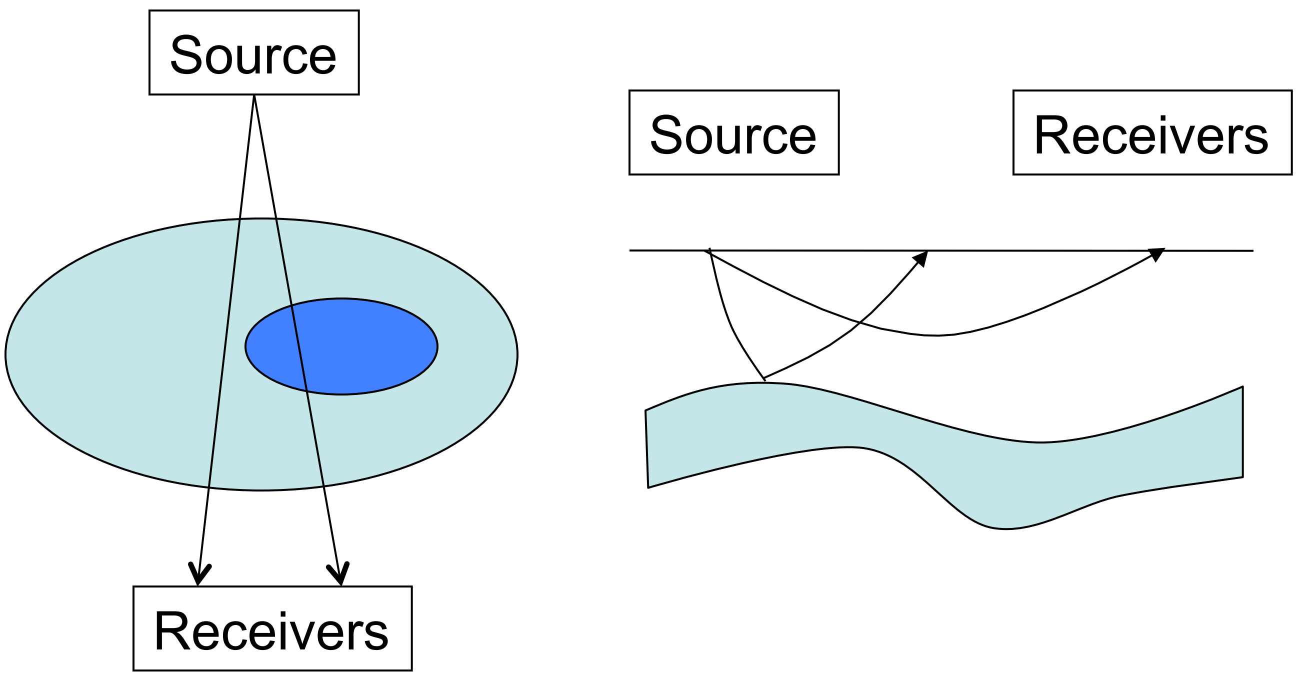
- Segmentation
  - Small scale features (curves, texture) from coarser scales
- Rendering
  - Ray equations, microscale textures
- Level of detail in visualization
  - Data structures, compression and approximation of smaller scales
- Scale-space theory in computer vision [Tony Lindeberg, 94]
  - Today linked to feature extraction and machine learning

Example: seismic Imaging





Compare tomography



Tomography – Radon transform

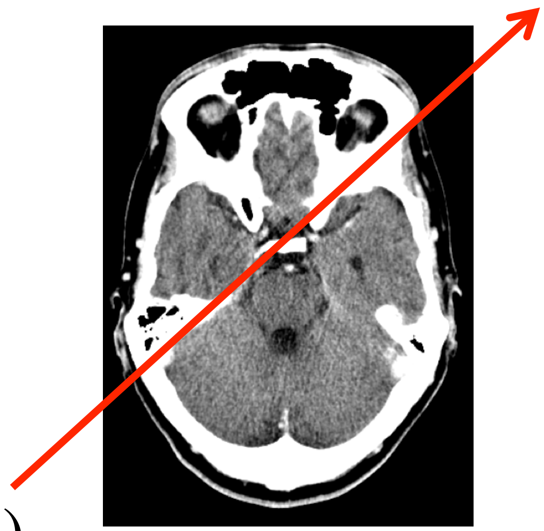
- The Radon transform (f_R) - Inversion: measure f_R find f
- Computer assisted tomography: Allan M. Cormack, Godfrey N. Hounsfield Nobel prize 1979

$$f_R(\alpha,\omega) = \int_{L(\alpha,\omega)} f(x(s),y(s))ds$$

$$f(x,y) = \int T(\alpha,s)d\alpha\, d\omega$$

$$T = \hat{f}_R(\alpha,\omega)\left|\omega\right|e^{i2\pi\omega(x\cos\alpha + y\alpha)}$$

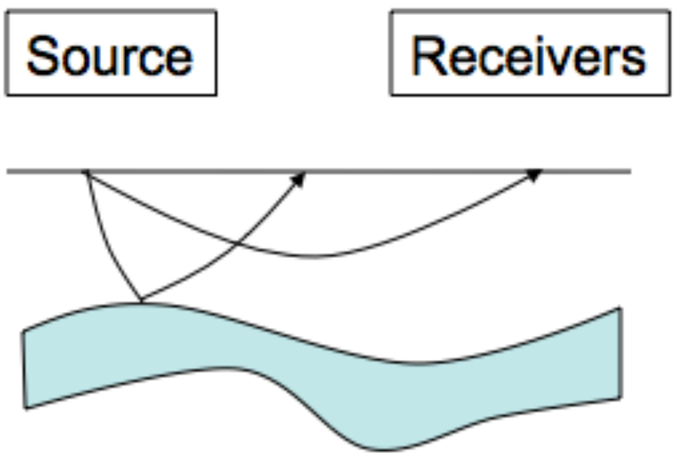
$$\hat{f}_R : \quad Fourier\ transform$$



$L(\alpha,\omega)$

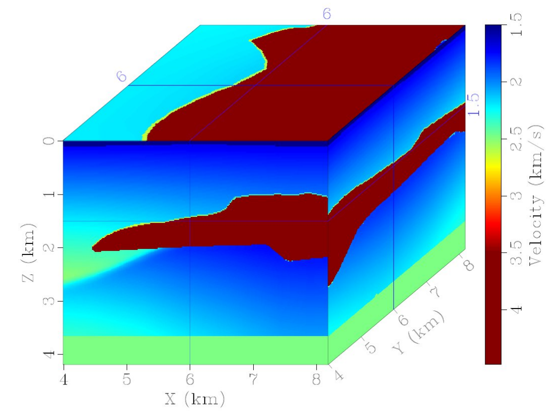
Seismic imaging

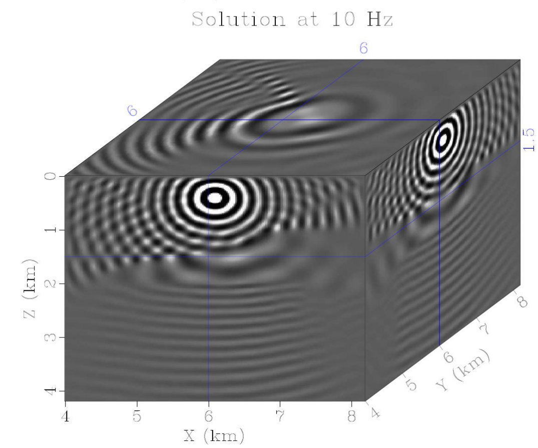
- Find velocity and reflectivity (or low and high frequency part of velocity field) separately
  - First velocity estimation: similar to tomography but harder: bending “rays”, wave action
  - Then reflectivity: details too small for velocity estimation, compare ultrasound imaging
- Full waveform inversion in frequency domain (Helmholtz)

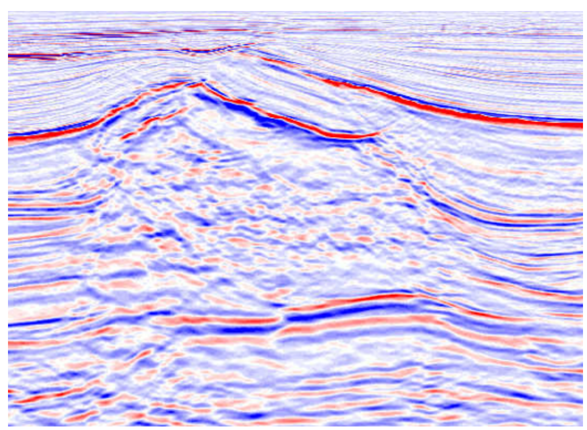


Multiscale aspects

- Fast Helmholtz solver: preconditioning based on compression rather than multigrid
- HMM style representation of microscale features layers etc. for effective equation

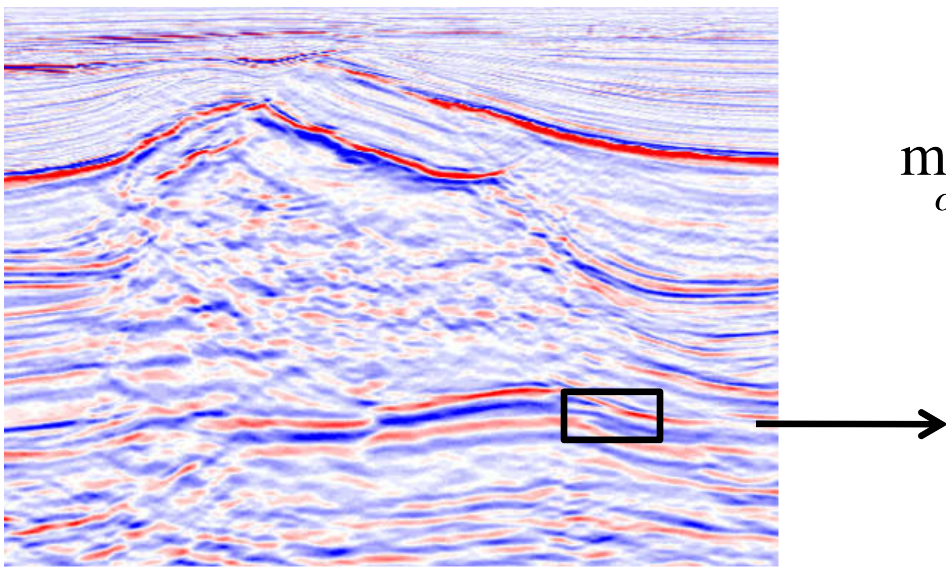




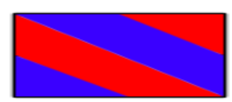


Multiscale aspects

- HMM style techniques can be used in the inverse process
- Parameterization of local properties



$$\min_{\alpha}\left(\| data - u_{\alpha} \| + \lambda \| u_{\alpha} \|_{*}\right)$$



Conclusions

- There are frameworks guiding simulations coupling models of different scales
- Realistic applications emerging
- Convergence theory possible in some cases
- Recent development to reduce need for scale separation