Macroscopic Newton-Krylov methods for multiscale systems

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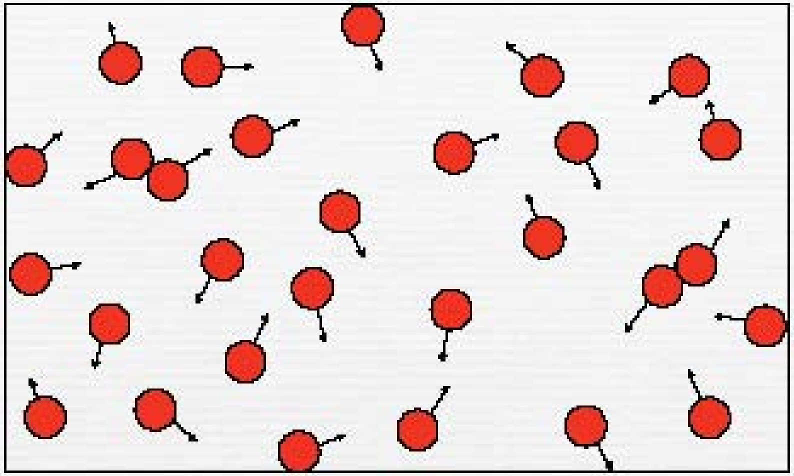
Modeling of multiscale phenomena

Microscopic models and coarse-graining

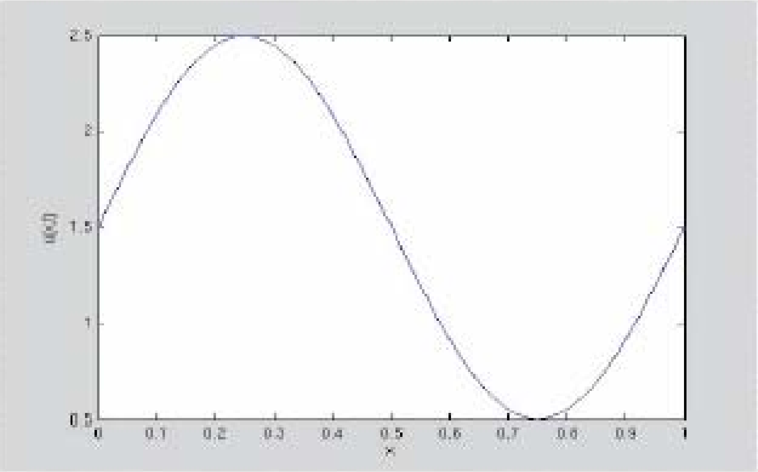


- Microscopic description
- E.g. molecular dynamics

  $$\forall i \ : \ m_i \ddot{x}_i = \sum_{j=1}^{N} F_{ij}$$

  - Expensive
  - (Too) much detail

Coarse-graining



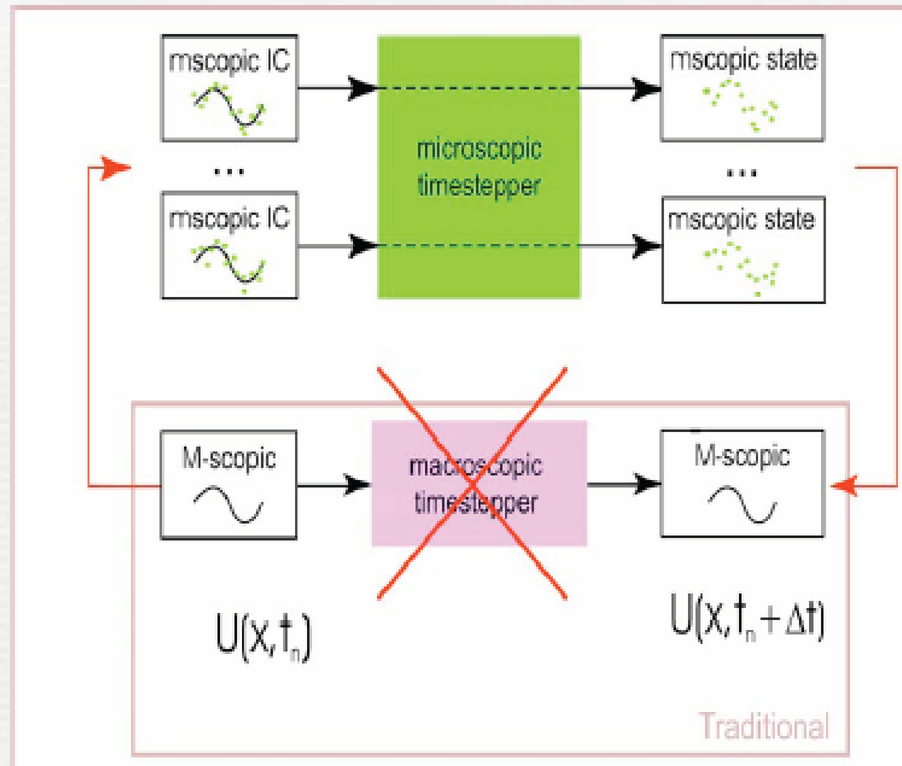
- Macroscopic description
  - PDE for particle densities

    $$\partial_t U(x,t) = D \partial_{xx} U(x,t)$$

  - Only averaged quantities
- Often not possible analytically

Numerical coarse-graining
Coarse time-stepper

- A macroscopic model **should exist**, but is unavailable
- Approximate time-stepper for the **macroscopic** variables using **microscopic** simulations
- **Lifting** $u(x,t) := \mathcal{L}(U)(x,t)$
  - need to fill in "implied" data
- Microscopic **simulation**
  - possibly of an ensemble
- **Restriction** $U(x,t+\Delta t) := \mathcal{R}(u)(x,t+\Delta t)$

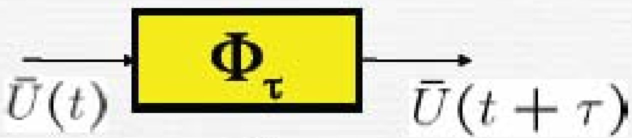


Outline

- Newton-Krylov methods and preconditioning
- Preconditioning with an approximate macroscopic model
  - lattice Boltzmann model
  - coarse traveling wave solutions
- Patch dynamics and multi-grid preconditioning
  - homogenization problems

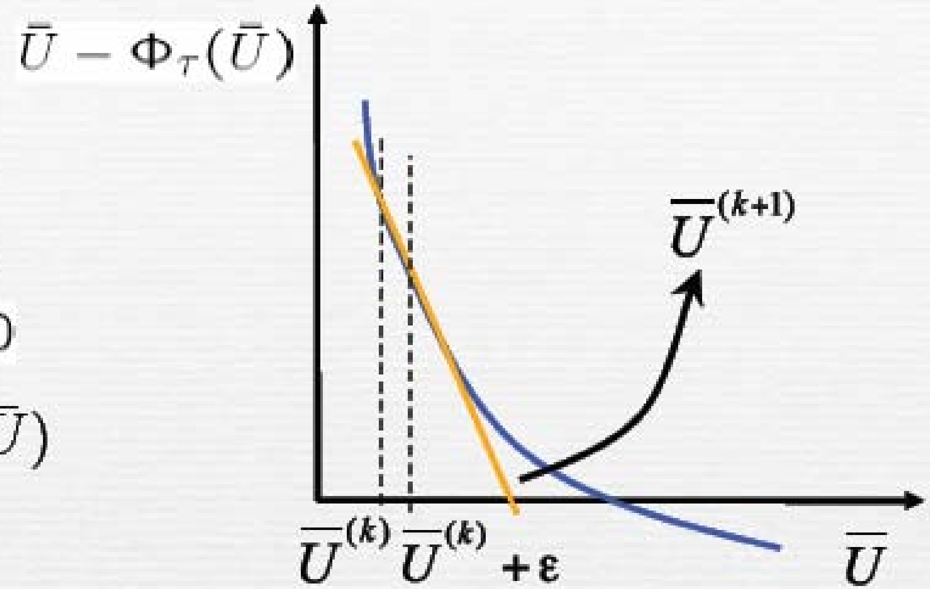
Timestepper-based bifurcation analysis

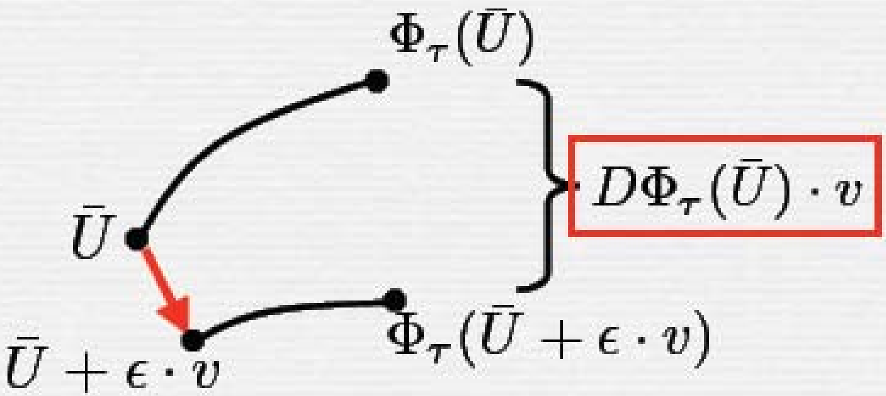
$$\partial_t \bar{U} = F(\bar{U})$$



$$\bar{U} - \Phi_\tau(\bar{U}) = 0$$

$$D\Phi_\tau(\bar{U})$$



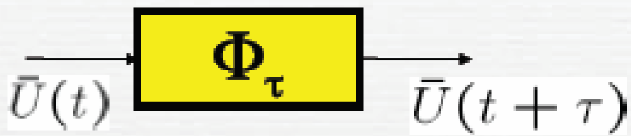


Newton — Krylov

Newton — Picard

Tuckerman and Barkley, Bifurcation analysis for timesteppers.
Lust and Roose, Computation and bifurcation analysis of periodic solutions of large-scale systems.
Both in IMA Volumes in Mathematics and its Applications 119 (2000)

Coarse bifurcation analysis



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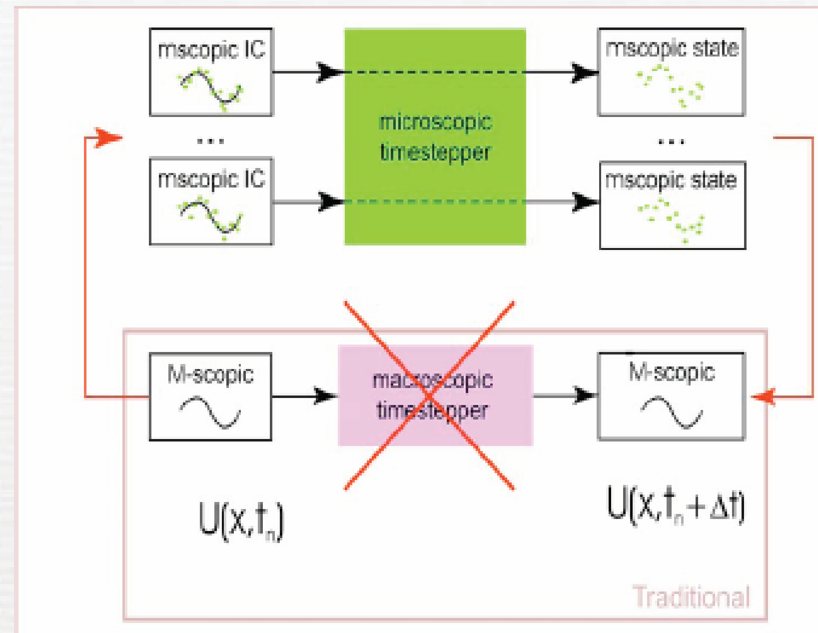

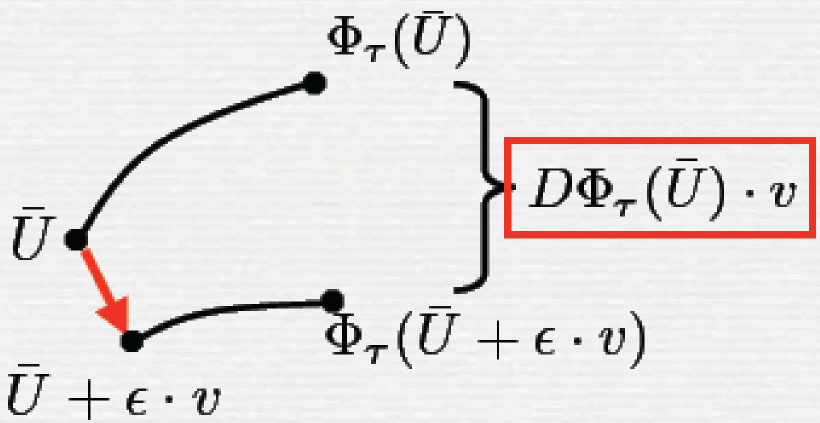

Newton — Krylov

Newton — Picard

I.G. Kevrekidis et al. 2000 - ...

Newton – GMRES and preconditioning

- Nonlinear system $\bar{U} - \Phi_\tau(\bar{U}) = 0$
- Newton-Raphson procedure
  - iterative method $\bar{U}^{(k+1)} = \bar{U}^{(k)} + \boxed{d\bar{U}^{(k)}}$
  - in each step, solve a linear system

$$\left(I - D\Phi_\tau(\bar{U}^{(k)})\right) d\bar{U}^{(k)} = -\left(\bar{U}^{(k)} - \Phi_\tau(\bar{U}^{(k)})\right)$$

- We only have matrix-vector products
  - iterative method, such as GMRES
  - performance depends on spectrum => precondition

$$M^{-1}\left(I - D\Phi_\tau(\bar{U}^{(k)})\right) d\bar{U}^{(k)} = -M^{-1}\left(\bar{U}^{(k)} - \Phi_\tau(\bar{U}^{(k)})\right)$$

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  - lattice Boltzmann model
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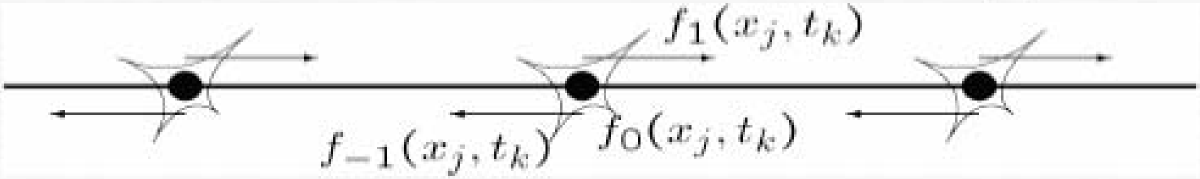
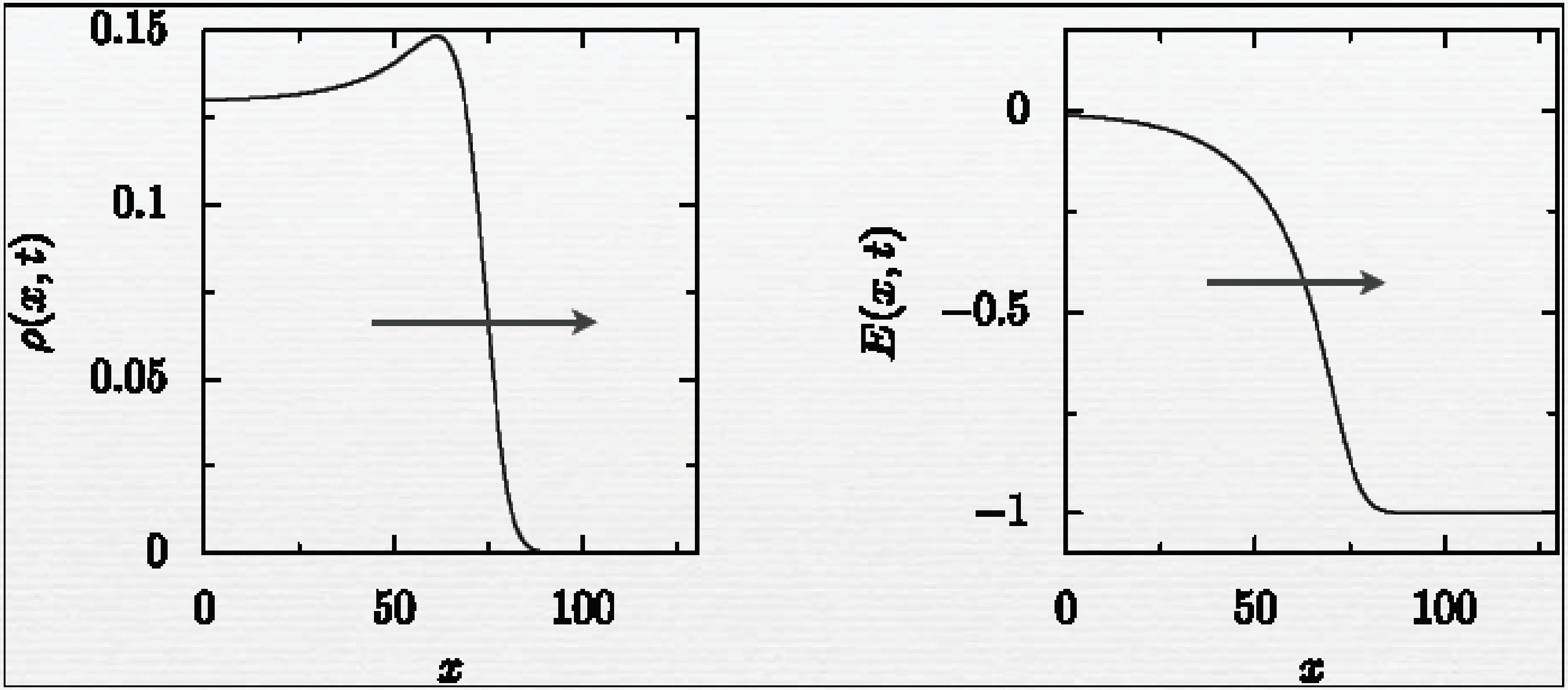
Lattice Boltzmann model problem



$$\begin{cases} f_i(x + c_i dx, t + dt) &= (1-\omega) f_i(x,t) - \omega f_i^{eq}(x,t) \\ & \quad - E(x,t) \sum_j V_{ij} f_j(x,t) + R_i(x,t), \\ \partial_t E(x,t) &= -\bar{\rho}(x,t) E(x,t) - a \partial_x \bar{\rho}(x,t) \end{cases}$$

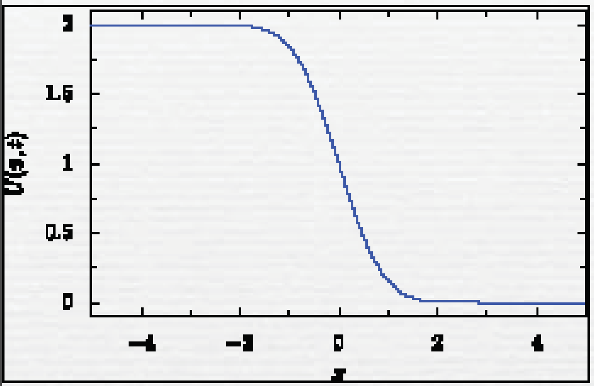
- Modeling of ionization waves
- Position **and velocity** of electrons are important
  - fast particles collide with (immobile) ions (which are not modeled)
  - collision generates 2 slow electrons, which are accelerated
- Time-scale separation
  - an effective reaction-diffusion equation exists for density
  - the reaction term cannot be obtained in closed form

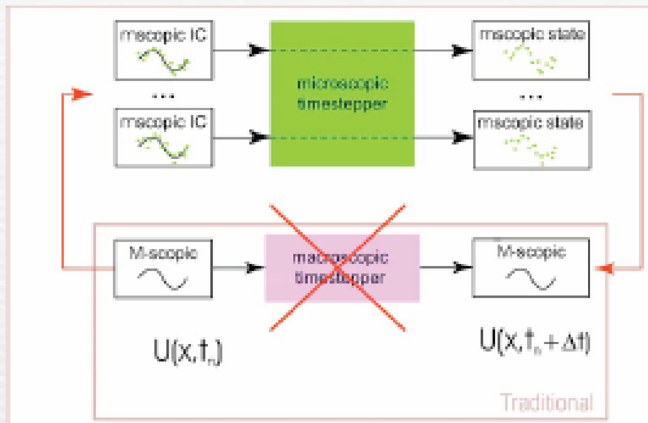
Lattice Boltzmann model problem

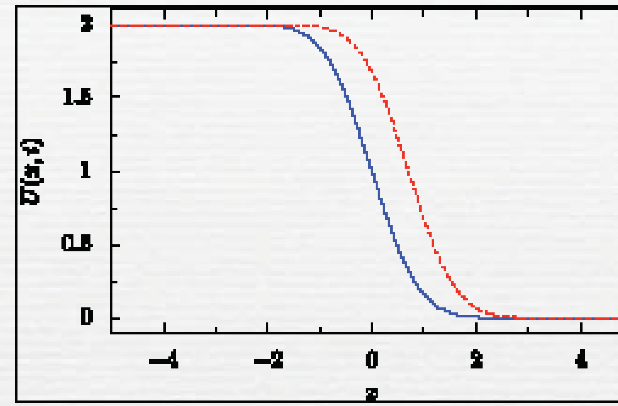


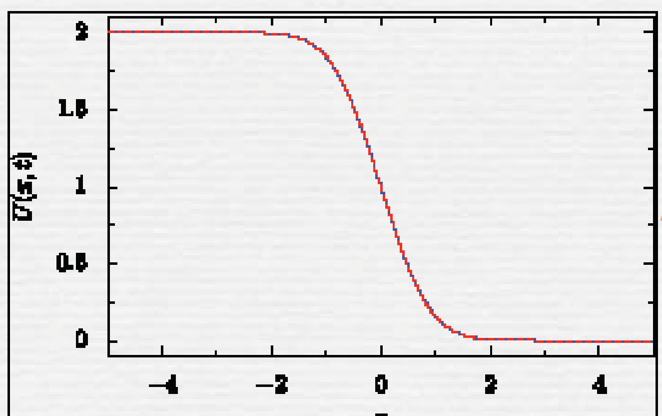
- Traveling waves, which move with constant speed
- Avalanche of electrons, which shield the electrical field

Traveling wave solutions as fixed points



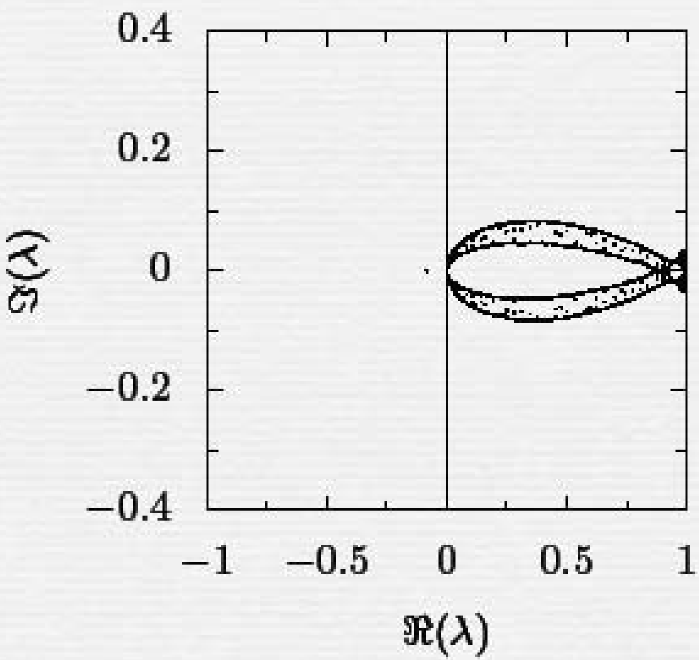


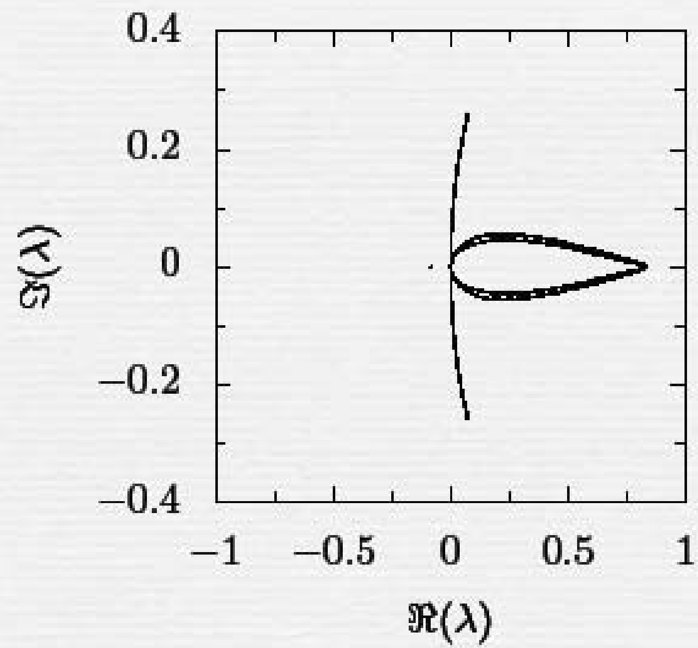




Numerical example

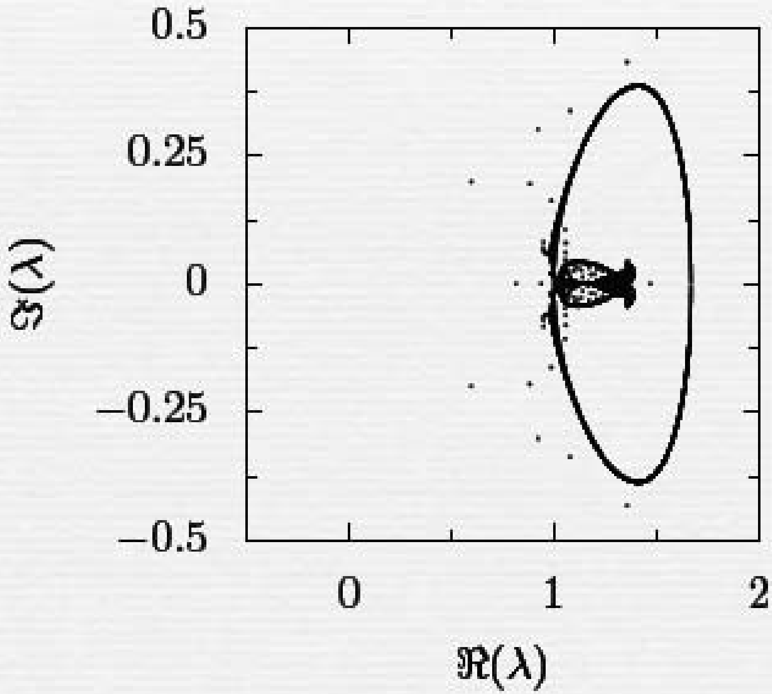
- Coarse time-stepper
  - lifting is done with constrained runs (see PVL)
  - runs LBM for 20 steps
- Preconditioner
  - "sloppy" Chapman-Enskog to get an approximate PDE
  - implicit Euler time-stepper

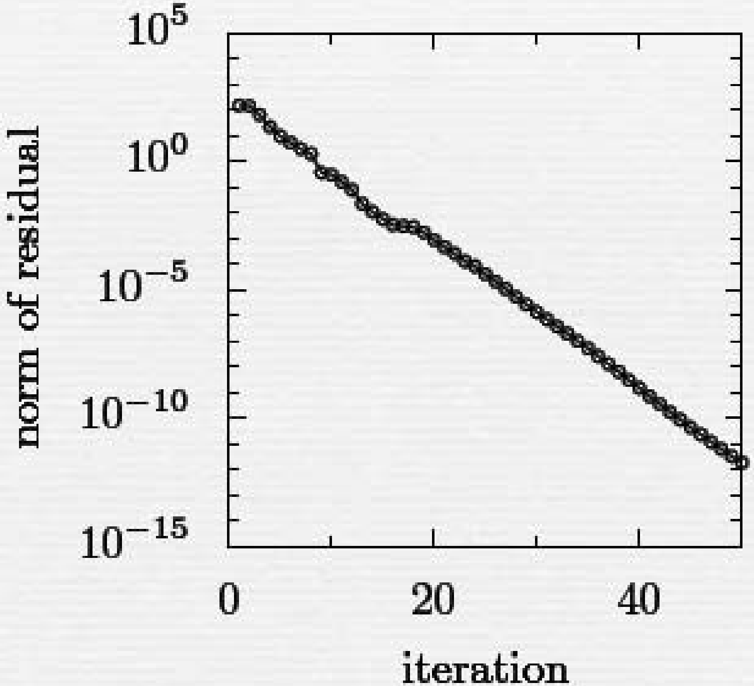




Convergence and performance

- System size: 2601 mesh-points
- Spectrum bounded away from zero
- GMRES converges in 30-40 iterations





S, Vanroose, Roose, Kevrekidis, Equation-free computation of traveling waves of lattice Boltzmann models with Newton-Krylov solvers, 2007, Preprint.

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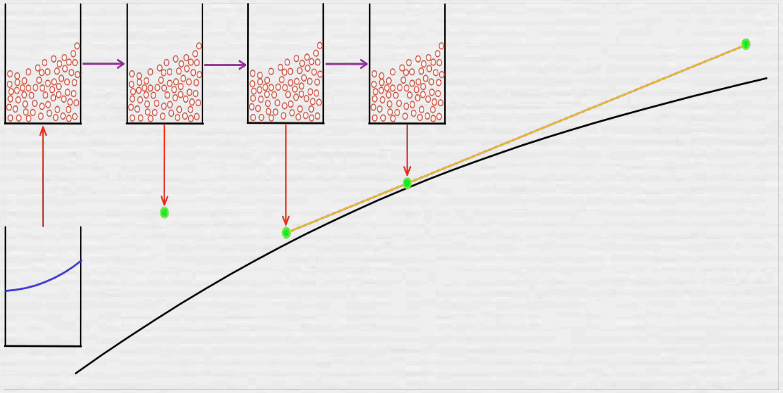
- Preconditioning with an approximate macroscopic model
  - model problem: lattice Boltzmann
  - coarse traveling wave solutions
- Patch dynamics and multi-grid preconditioning
  - patch dynamics
  - multi-grid
  - model problem: homogenization

Coarse time-stepper
Increasing efficiency

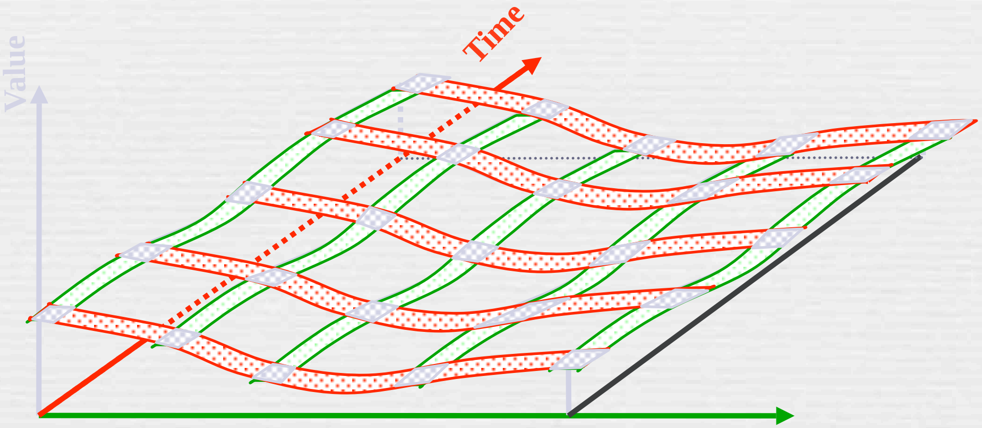
Microscopic simulations over whole domain: too expensive!

- Compute only in small fraction of space-time domain

Projective integration



Patch dynamics

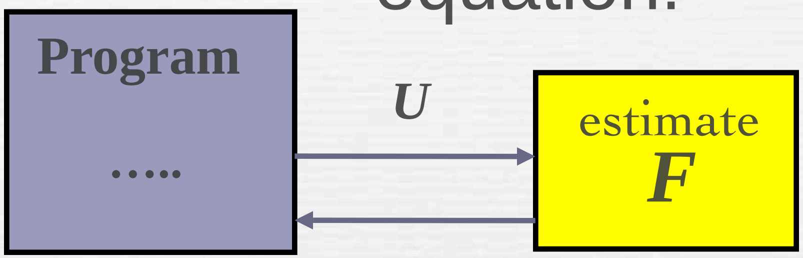


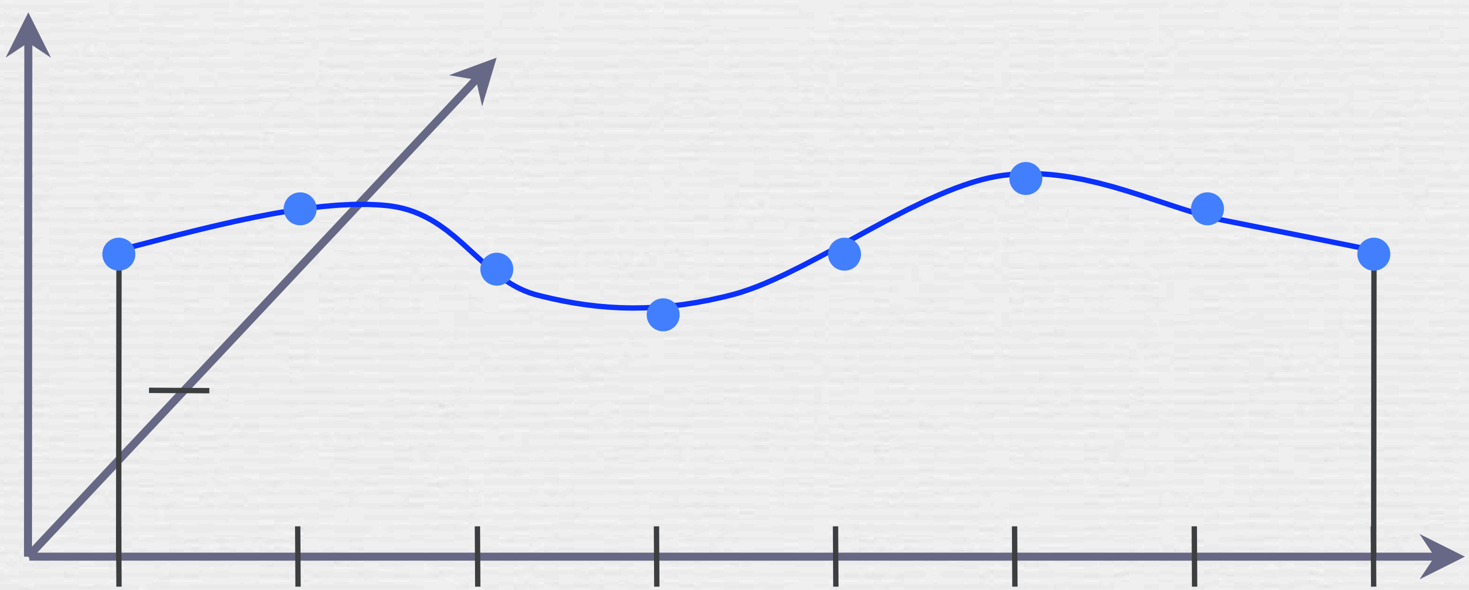
Gear and Kevrekidis, Projective integration for stiff differential equations, SISC 24:1091-1106, 2004
Kevrekidis et al., Equation-free computation, Comm. Math. Sci 1(4), 2003

Finite Difference Patch Dynamics

Unknown partial differential equation:

$$\partial_t U = F(U, \partial_x U, \ldots, \partial_x^d U)$$





S, Kevrekidis, Roose, Patch dynamics with buffers for homogenization problems, JCP 213: 264-287, 2006

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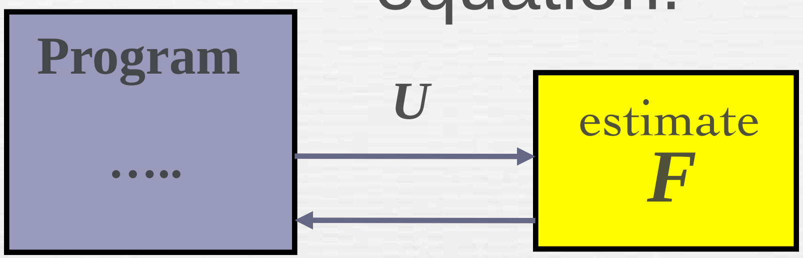

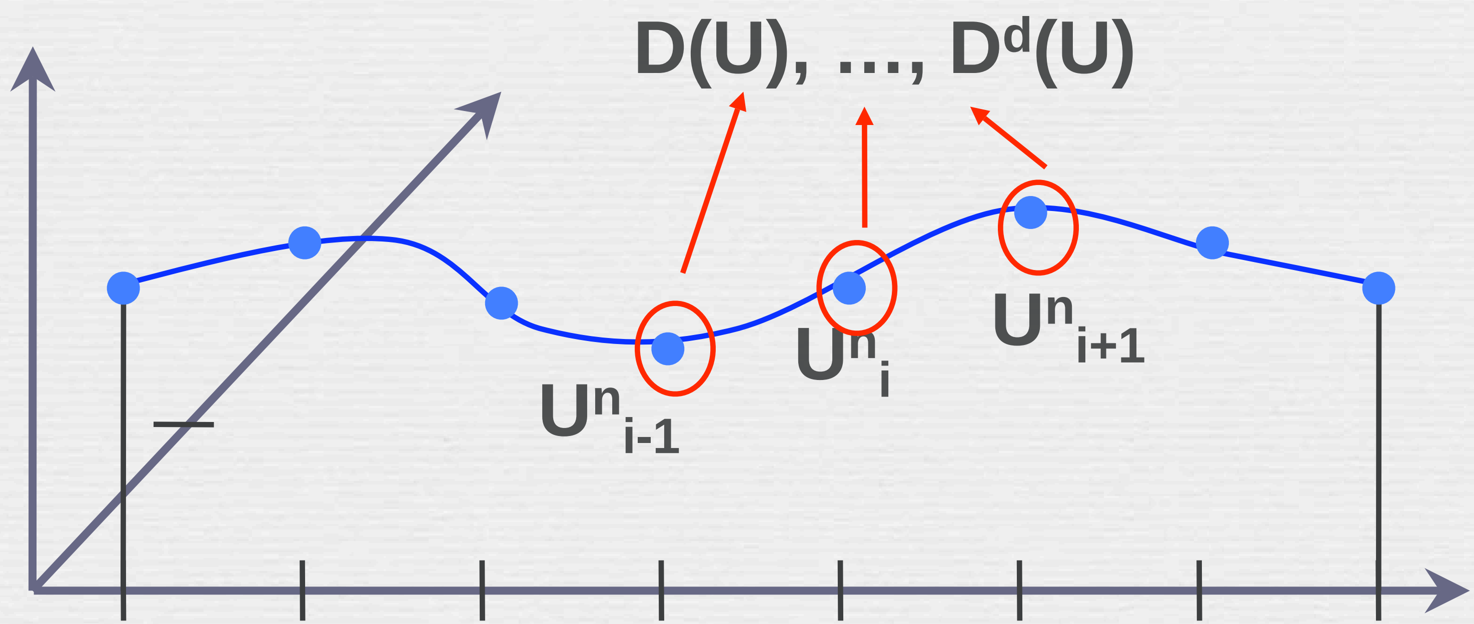

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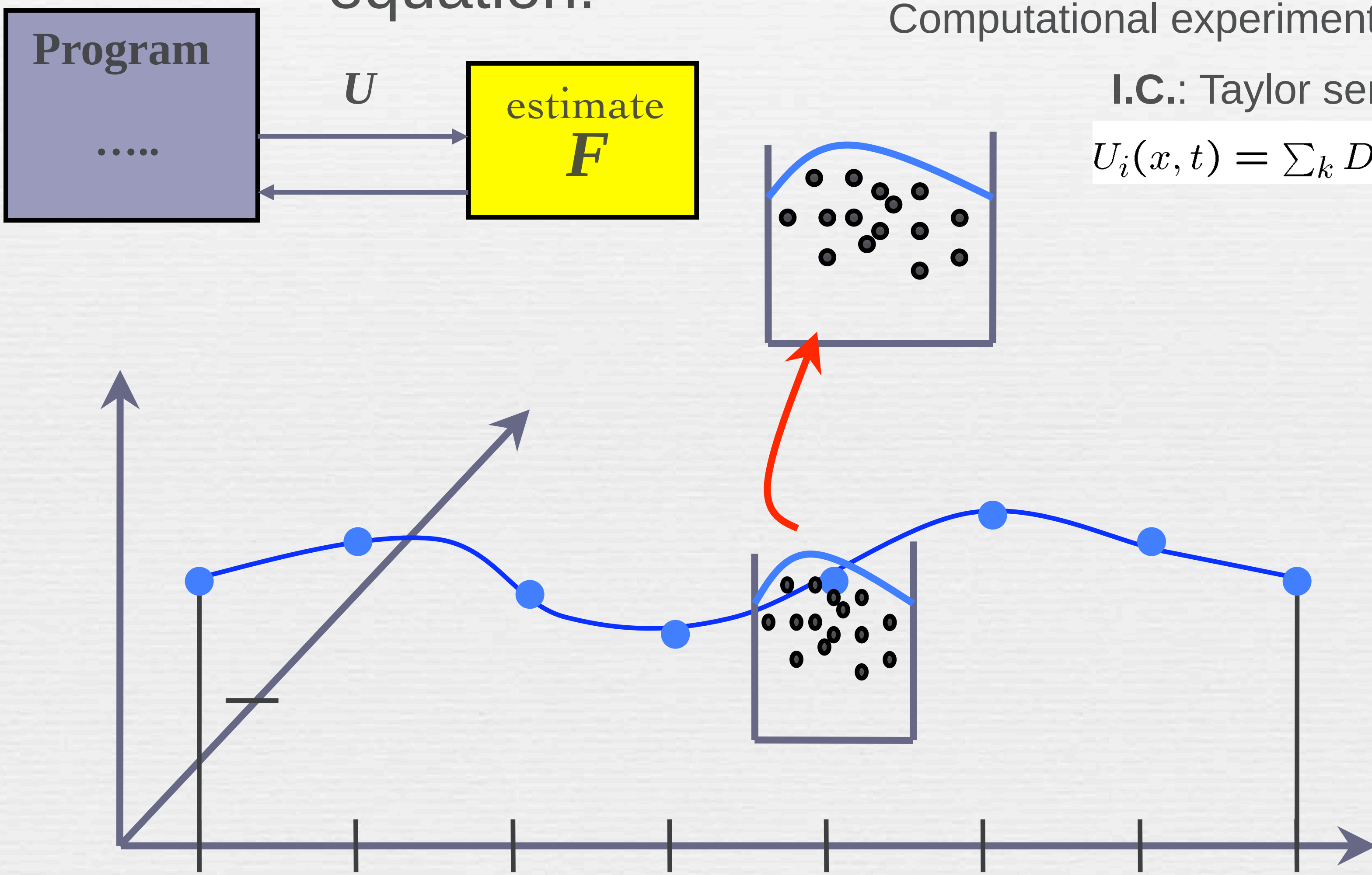
Computational experiment

I.C.: Taylor series

$$U_i(x,t) = \sum_k D^k(U) \frac{(x-x_i)^k}{k!}$$



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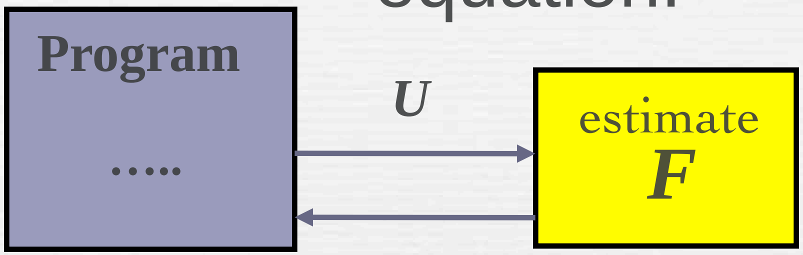

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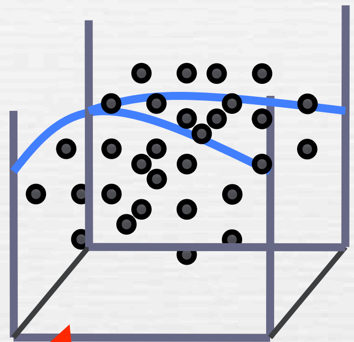

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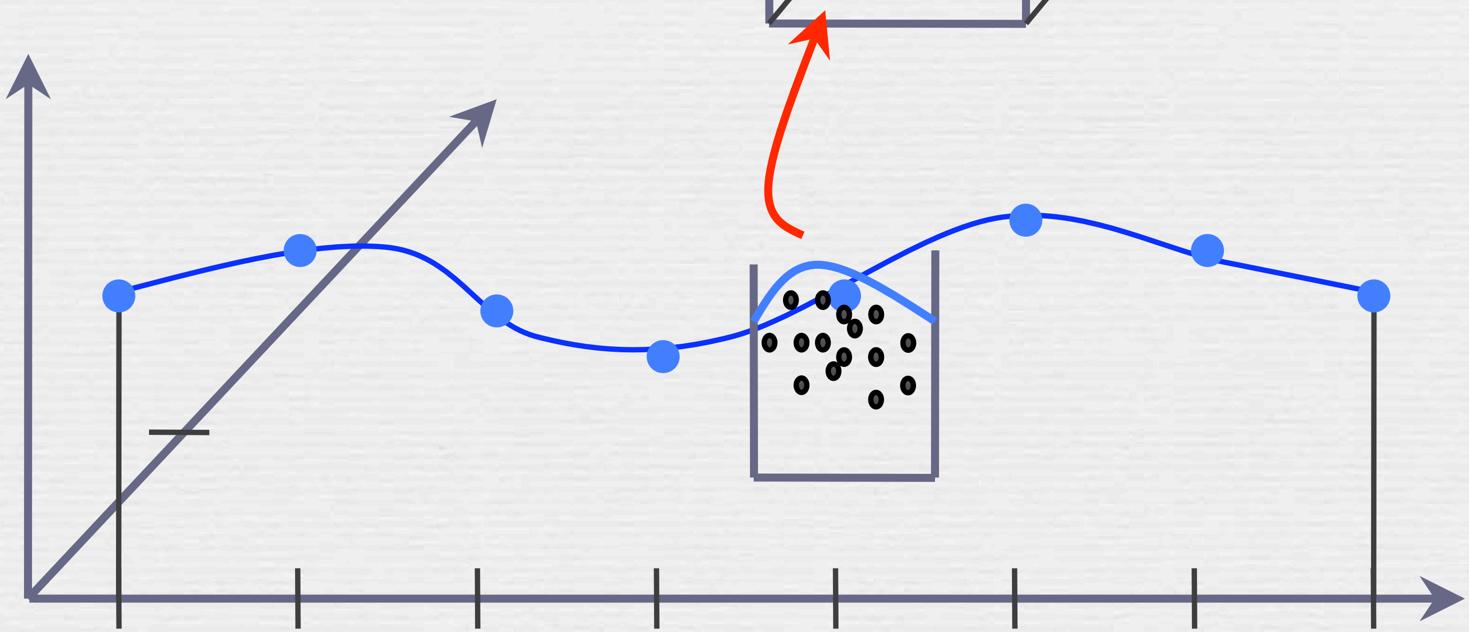
Run for a time δt



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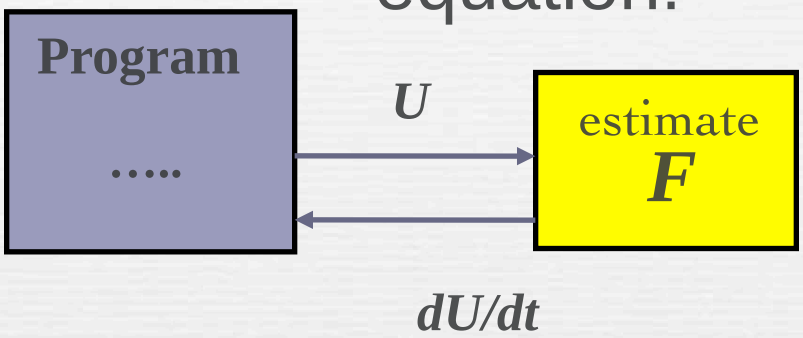
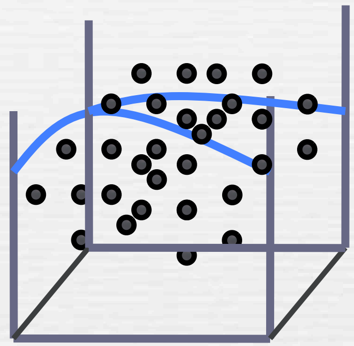


Computational experiment



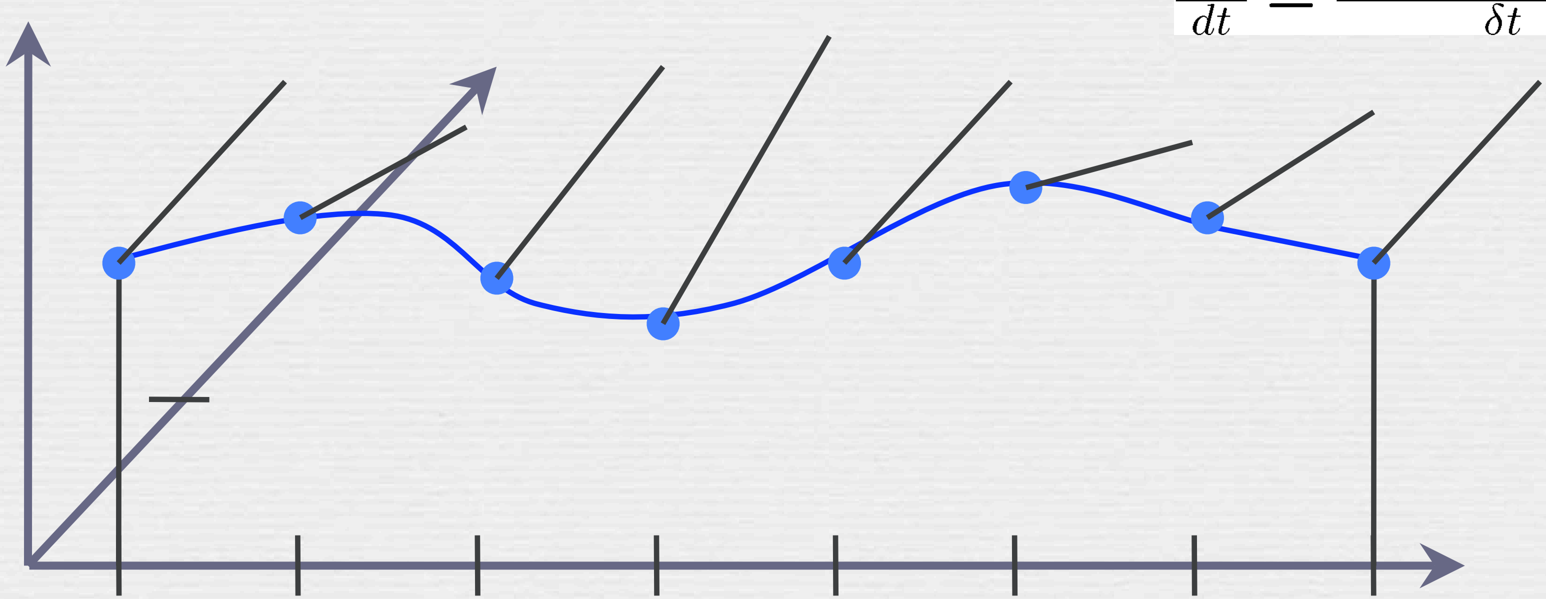
I.C.: Taylor series

$$U_i(x,t) = \sum_k D^k(U)\frac{(x-x_i)^k}{k!}$$

Run for a time δt

Estimate

$$\frac{dU_i}{dt} = \frac{U_i(t+\delta t) - U_i(t)}{\delta t}$$



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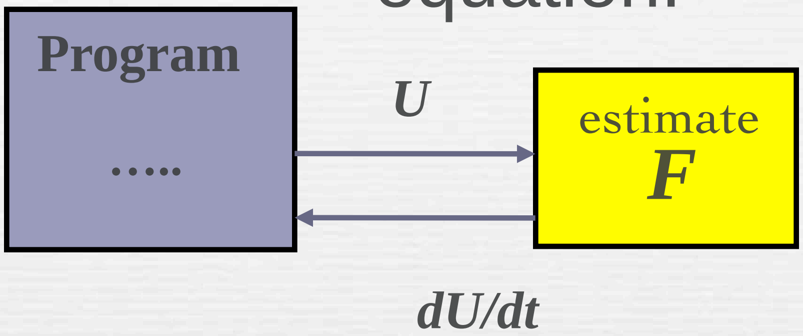

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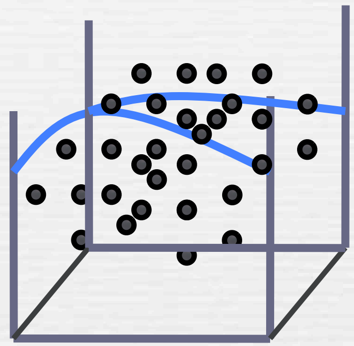

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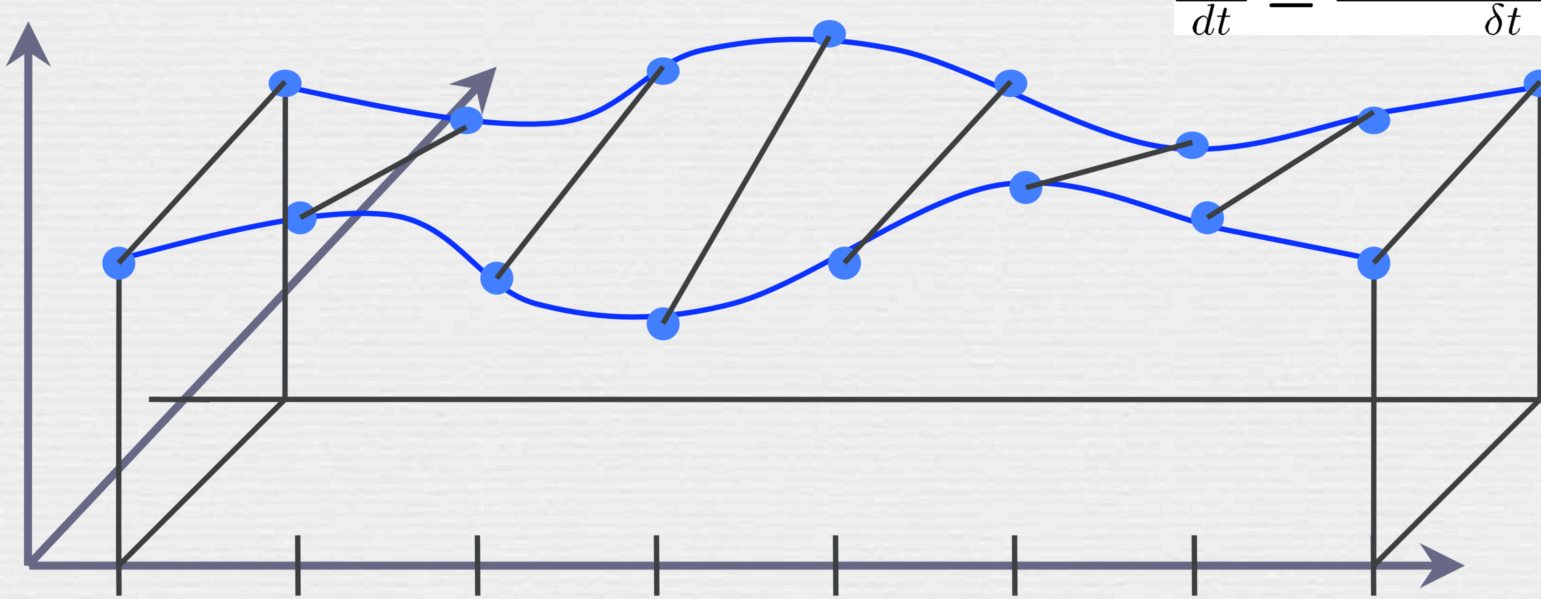

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Multi-grid preconditioning

- Nonlinear system $\bar{U} - \Phi_\tau(\bar{U}) = 0$
- Linear system in each Newton step

$$\left(I - D\Phi_\tau(\bar{U}^{(k)})\right) d\bar{U}^{(k)} = -\left(\bar{U}^{(k)} - \Phi_\tau(\bar{U}^{(k)})\right)$$

- We only have matrix-vector products => GMRES
- Precondition with a few (1) iterations of a **different** solver

$$M^{-1}\left(I - D\Phi_\tau(\bar{U}^{(k)})\right) d\bar{U}^{(k)} = -M^{-1}\left(\bar{U}^{(k)} - \Phi_\tau(\bar{U}^{(k)})\right)$$

  - Here M^{-1} represents a single multi-grid cycle
  - Can be inaccurate ; has to be cheap

Multi-grid idea 1
Smoothing

Multi-grid idea 1
Smoothing

- Linear system $\left(I - D\Phi_\tau(\bar{U}^{(k)})\right) d\bar{U}^{(k)} = -\left(\bar{U}^{(k)} - \Phi_\tau(\bar{U}^{(k)})\right)$

Multi-grid idea 1
Smoothing

- Linear system $\left(I - D\Phi_\tau(\bar{U}^{(k)})\right) d\bar{U}^{(k)} = -\left(\bar{U}^{(k)} - \Phi_\tau(\bar{U}^{(k)})\right)$

$$A \quad x \quad = \quad b$$

Multi-grid idea 1
Smoothing

- Linear system $Ax = b$
- We assume to have an iterative method of the form

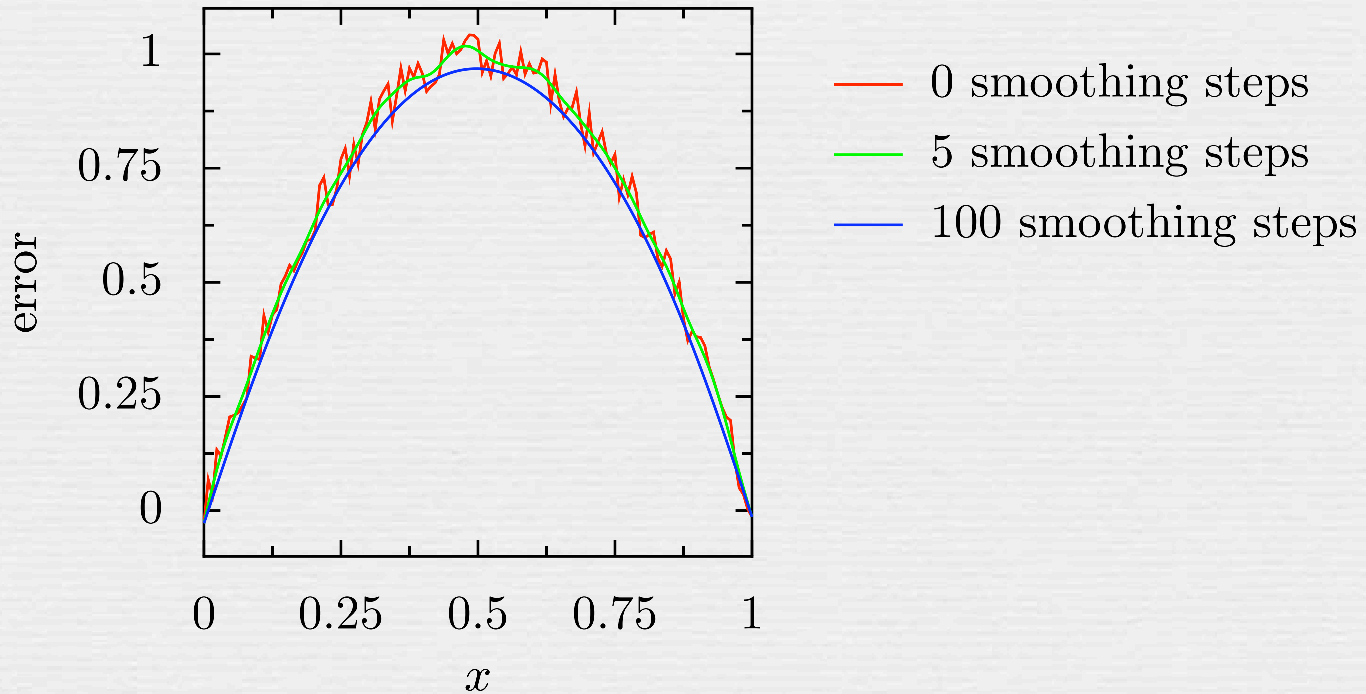
$$x^{(m+1)} = x^{(m)} + p(A)\left(b - Ax^{(m)}\right)$$

Multi-grid idea 1
Smoothing

- Linear system $Ax = b$
- We assume to have an iterative method of the form

$$x^{(m+1)} = x^{(m)} + p(A)\left(b - Ax^{(m)}\right)$$

- Good error smoothing, but slow convergence



Multi-grid idea 2
Coarse-grid correction

- Do a few iterations until error is smooth: **smoothing**
- Solve **for the error** on a coarser grid

Presmoothing: $\bar{x}_h^{(m)} = S(x_h^{(m)}, b, \nu_1)$

Coarse grid correction

Compute defect: $d_h^{(m)} = b - A_h \bar{x}^{(m)}$

Restrict defect: $d_{2h}^{(m)} = I_h^{2h} d^{(m)}$

Coarse grid solve: $A_{2h} v_{2h} = d_{2h}^{(m)}$

Interpolate correction: $v_h^{(m)} = I_{2h}^h v_{2h}^{(m)}$

Update fine-grid solution: $\hat{x}_h^{(m)} = \bar{x}_h^{(m)} + v_h^{(m)}$

Postsmoothing: $x_h^{(m+1)} = S(\hat{x}_h^{(m)}, b, \nu_1)$

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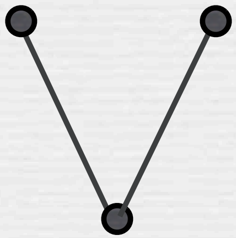

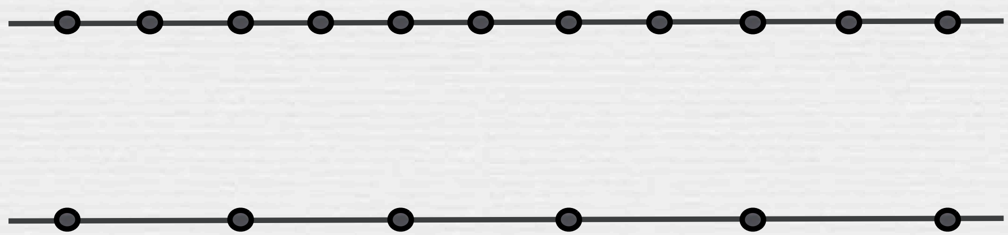

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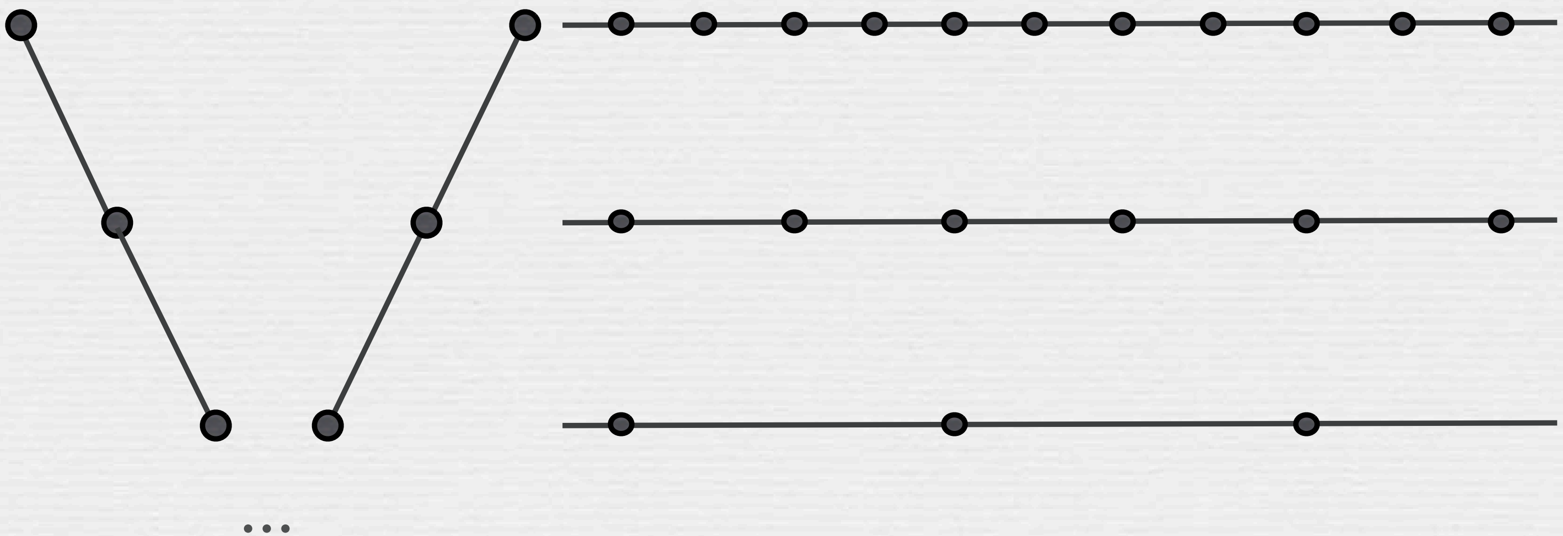
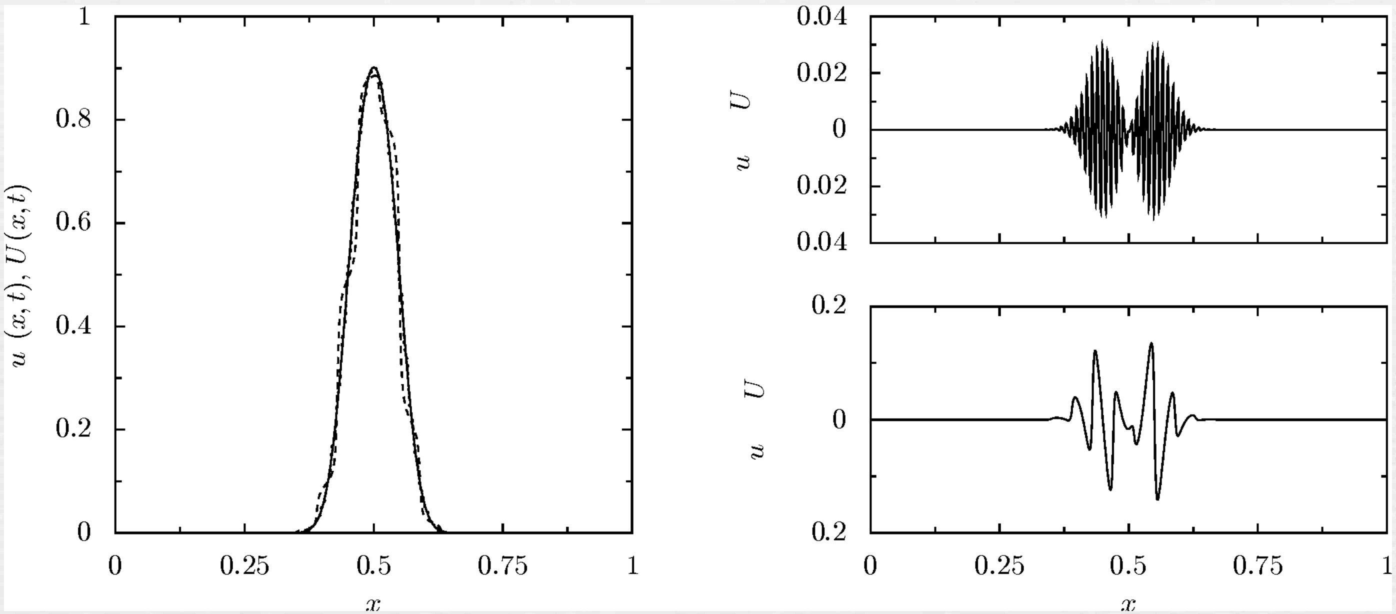


Model homogenization problem

- "Microscopic" equation: $\partial_t u(x,t) = \partial_x \left(a\left(x/\epsilon\right) \partial_x u(x,t) \right) + r(u(x,t))$
- Macroscopic equation: $\partial_t U(x,t) = \partial_x \left(a^* \partial_x U(x,t) \right) + r(U(x,t))$



Model problem for convergence **analysis**

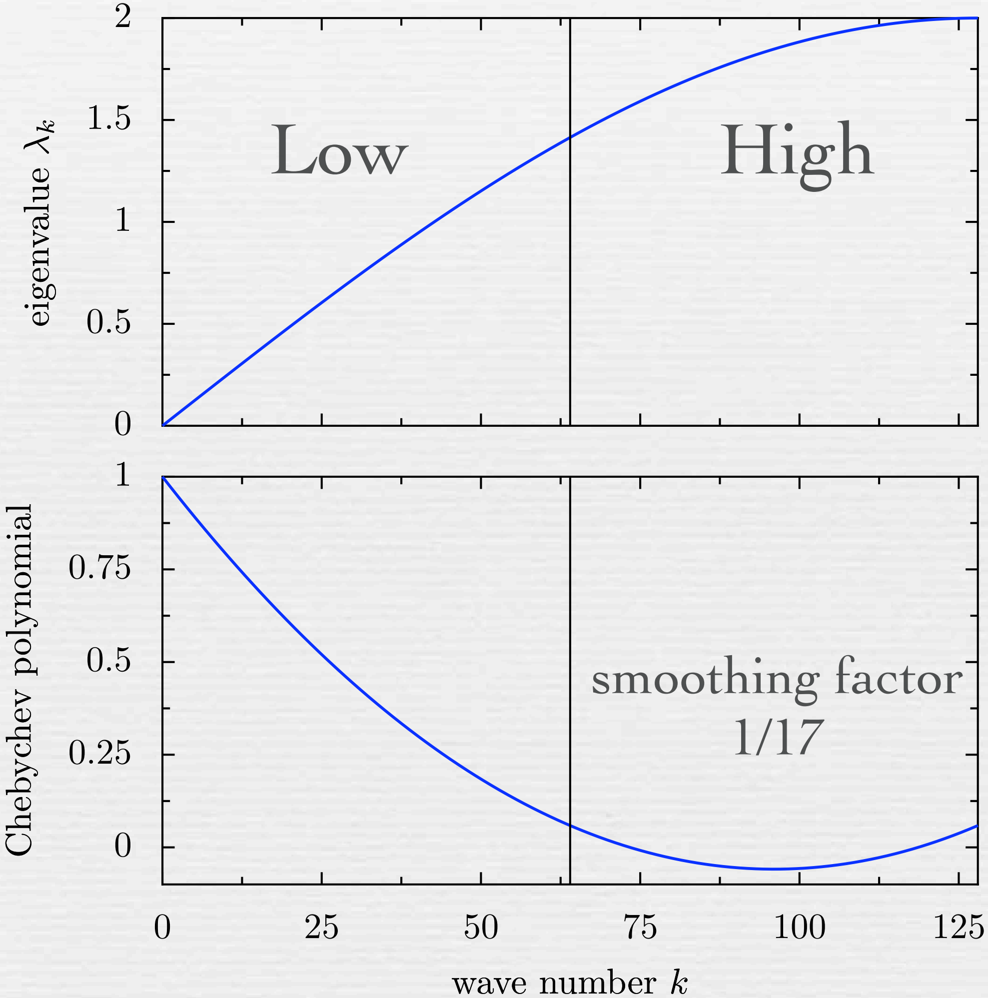
PDE at both levels => possible to analyze convergence analytically

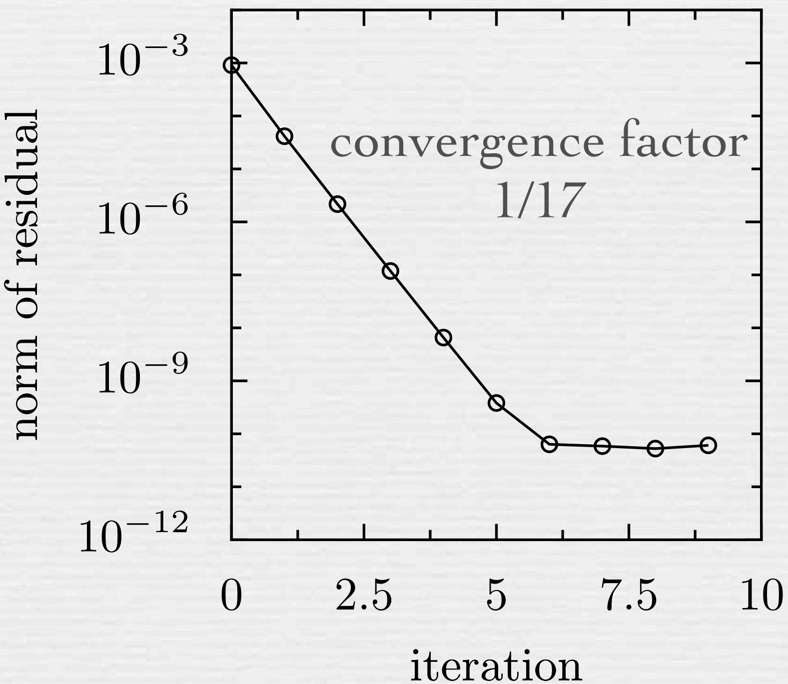
Elimination of additional effects (e.g. initialization of microscopic model)

Numerical results
Multigrid as solver

Pure diffusion model problem

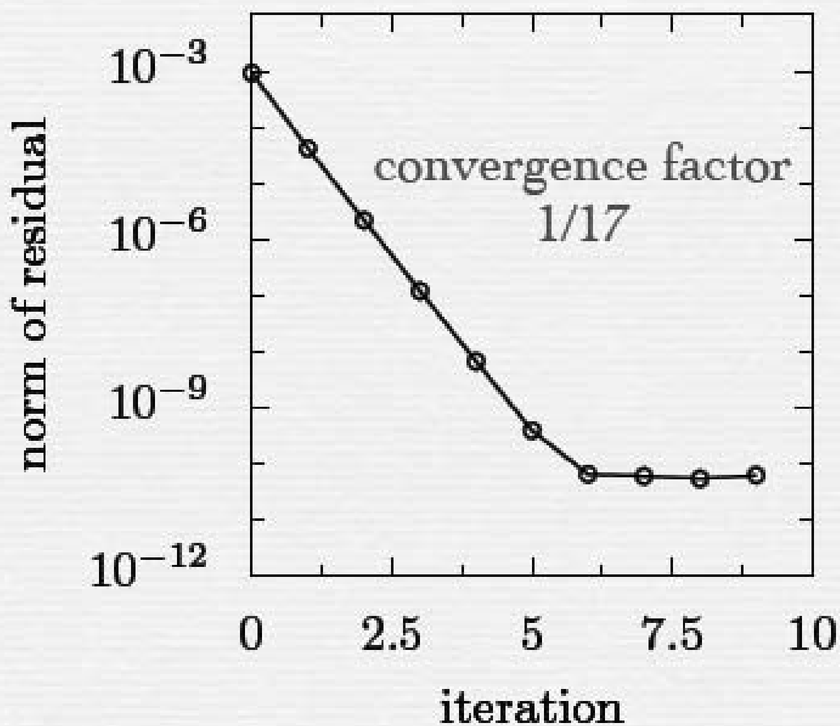
Chebychev polynomial smoother

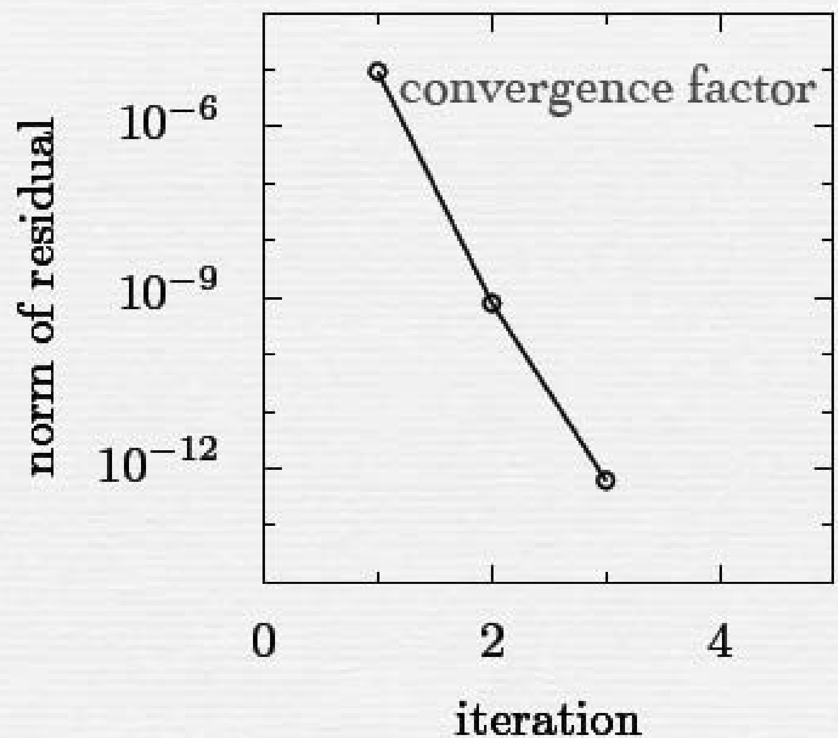




Numerical results
Multigrid as preconditioner

- Multigrid as preconditioner for GMRES is more efficient
- Behaviour identical to standard multigrid for PDEs





Conclusions and current work

- Newton-GMRES for coarse fixed points
- Preconditioning is necessary for fast convergence
  - Based on a “sloppy” macroscopic model
  - If patch dynamics: multi-grid
- Currently investigating:
  - Decreasing accuracy of the macroscopic model
  - Extend multi-grid ideas to hyperbolic problems