Equation-free computing:
A lattice Boltzmann case study

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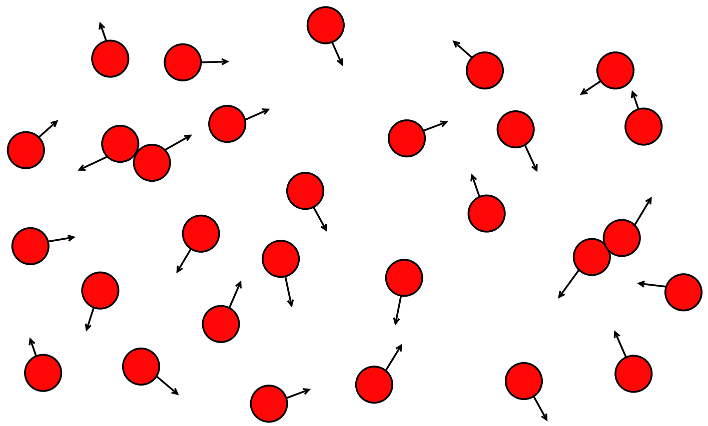
Outline

Mathematical Models

Microscopic/Mesoscopic models

- Relations between micro. variables



- particles (e.g. fluid molecules) ...
- ...collide and propagate

Macroscopic models

- Relations between macro. variables

$$\frac{\partial v}{\partial t} + v \cdot \nabla v = -\frac{\nabla P}{\rho} + \nu \nabla^2 v$$

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2} + F(\rho^a, \rho^b, \ldots)$$

- ρ: density
- v: flow velocity

Microscopic/Mesoscopic models

- Evolution of individual particles, distributions
- Detailed microscopic behavior
  - Fine space/time scales
  - Modeling flexibility (physics)
- Computationally expensive

Macroscopic models

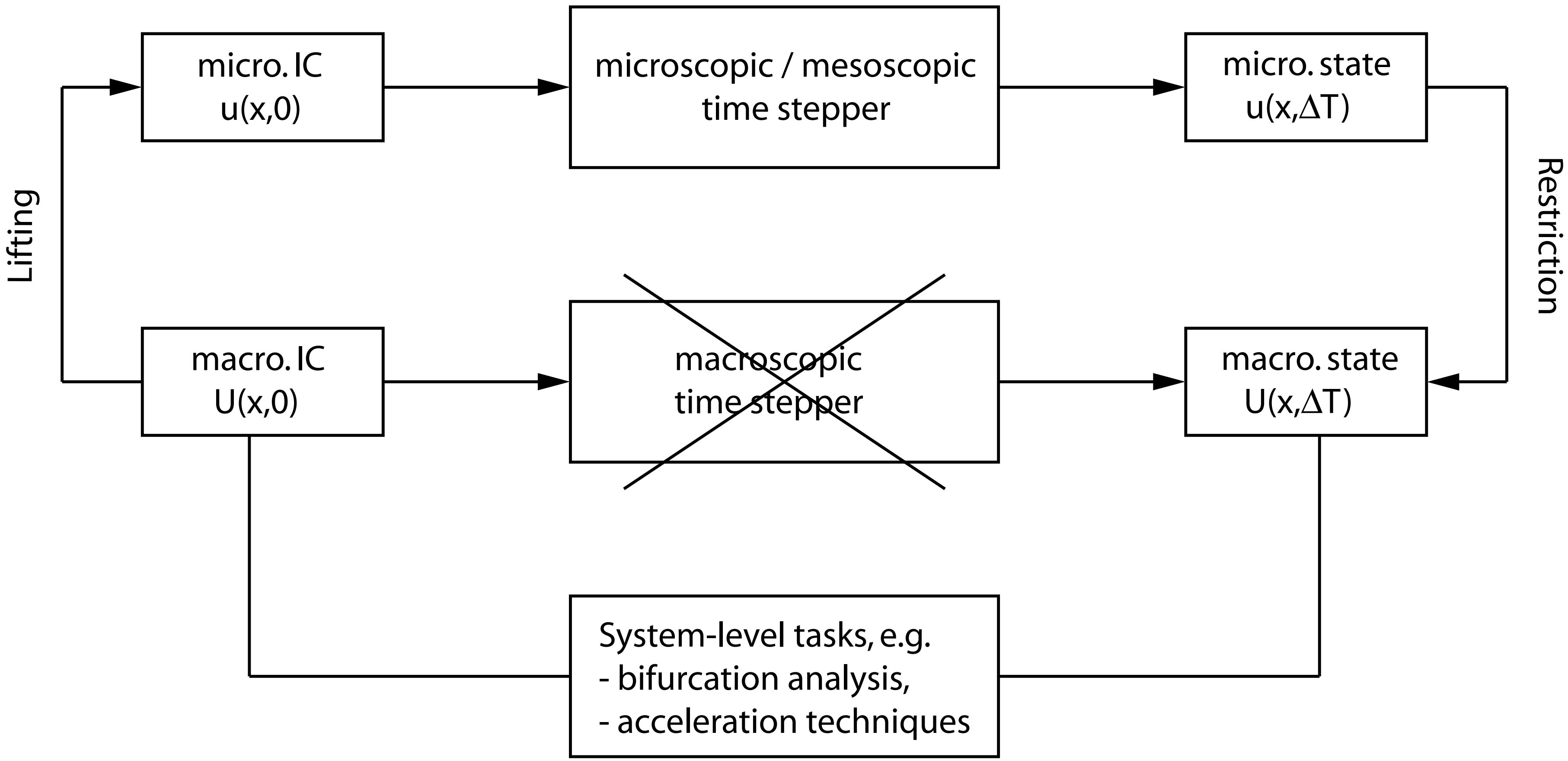
- Evolution of e.g. moments (density, momentum, . . .)
- Averaged macro-scale behavior
  - Macroscopic space/time scales
  - Mathematical abstraction
- Efficient algorithms exist
- System tasks, e.g. bifurcation analysis

$\longrightarrow$

Coarse equation-free computing

- Simplifying assumptions, closures, . . . are not always analytically possible
- Bypass the derivation of a macroscopic model

Equation-Free Computing



[Kevrekidis et al., 2000 — . . .]

Mesoscopic lattice Boltzmann models are deterministic $\Rightarrow$ no stochastic effects

Scale Separation

U: lower order moments: macroscopic variables

V: higher order moments

Conceptually in moment space:

$$\frac{\partial u}{\partial t} = p(u) \quad \Leftrightarrow \quad \frac{\partial U}{\partial t} = \bar{P}(U,V) \tag{1}$$

$$\frac{\partial V}{\partial t} = \bar{Q}(U,V) \tag{2}$$

After short simulation with (1)-(2), slaving relations are attained

$$V = S(U) \quad \text{or} \quad u = s(U) \tag{3}$$

Substitute (3) in (1) to obtain reduced equation (PDE) which describes evolution on a slow manifold

$$\frac{\partial U}{\partial t} = \bar{P}(U, S(U)) = P(U) \tag{4}$$

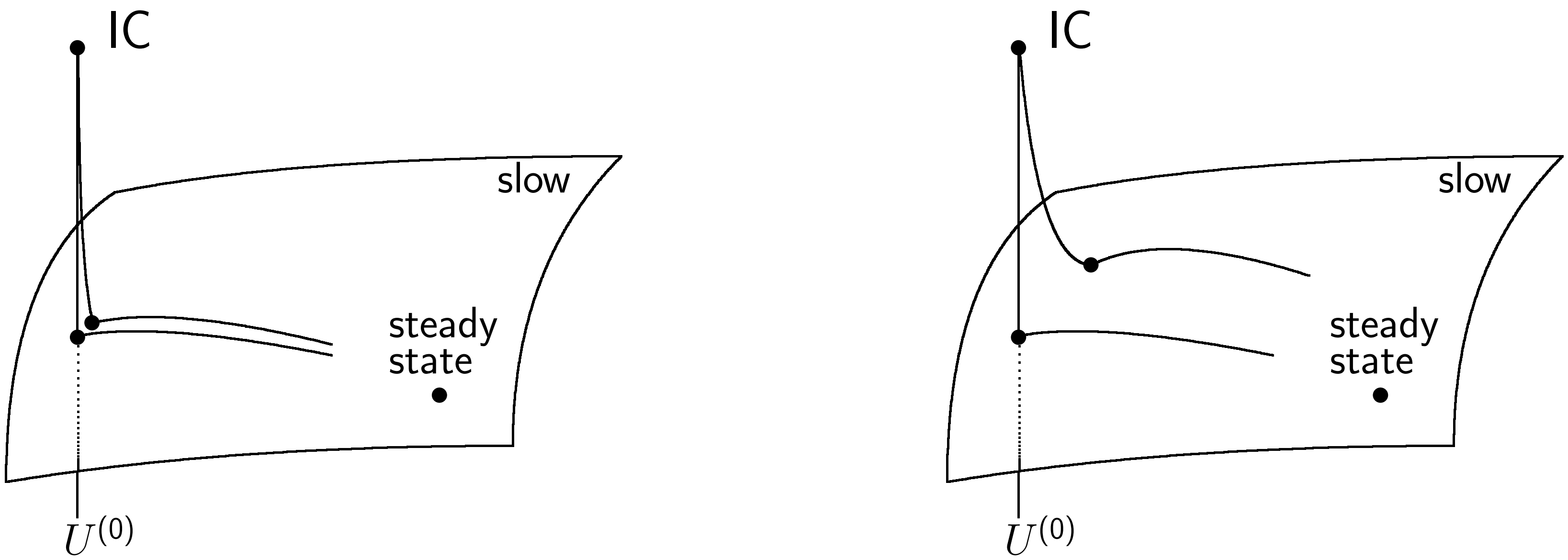
Equation-free: (3)-(4) unavailable, only microscopic time stepper $\frac{\partial u}{\partial t} = p(u)$

In singularly perturbed form:

$$\frac{\partial U}{\partial t} = \bar{P}(U, V)$$
$$\frac{\partial V}{\partial t} = \frac{1}{\epsilon}\bar{Q}(U, V)$$

small $\epsilon \Rightarrow$ large gap in time scales between U and $V \Rightarrow$ fast slaving

Does not necessarily result in a small error (pure slow/fast variables, mixed)



Outline

Lattice Boltzmann Model (LBM)

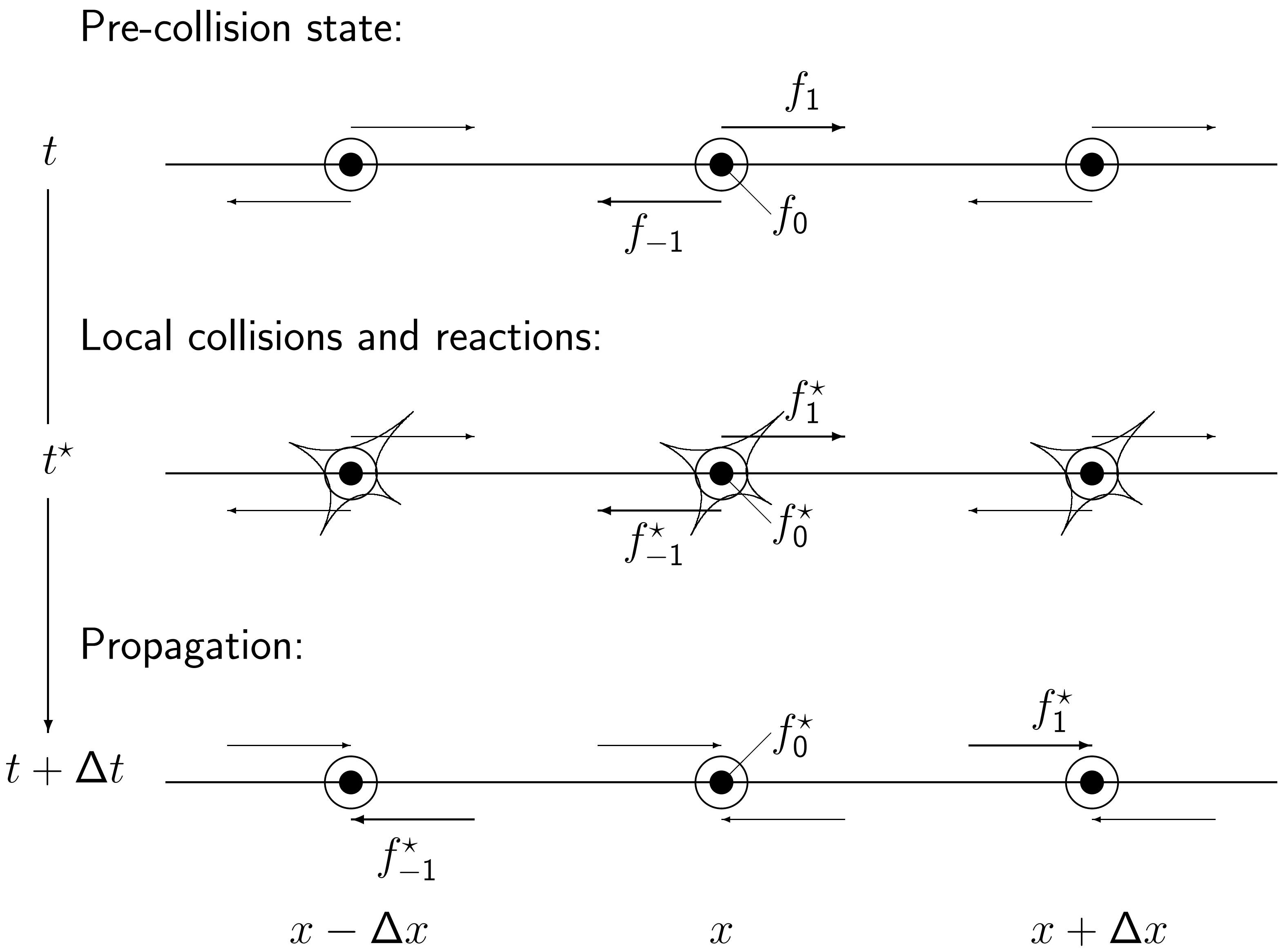
- For one-dimensional reaction-diffusion systems
- Discretize space x and time $t \Rightarrow \Delta x$, Δt
- Only 3 "particle" velocities (D1Q3 scheme)

$$v_i = i\,\frac{\Delta x}{\Delta t} \quad \text{with} \quad i = -1, 0, 1$$

- "Microscopic" variables u: distribution functions $f_i(x,t)$. They relate to the probability that a particle enters a lattice site x at time t with velocity v_i
- $\frac{\partial u}{\partial t} = p(u)$: LBM time stepper describes evolution:

$$f_i(x + i\Delta x, t + \Delta t) - f_i(x,t) = -\omega \left(f_i(x,t) - f_i^{eq}(x,t)\right) + \frac{\Delta t}{3} F\left(\rho(x,t)\right)$$

with local diffusive equilibrium distribution $f_i^{eq}(x,t) = \frac{1}{3}\,\rho(x,t)$
and relaxation parameter ω (which depends on D, Δx and Δt)



Pre-collision state:
t
f_1
f_0
f_{-1}
Local collisions and reactions:
$t^\star$
$f_1^\star$
$f_0^\star$
$f_{-1}^\star$
Propagation:
$t+\Delta t$
$f_1^\star$
$f_0^\star$
$f_{-1}^\star$
$x-\Delta x$
x
$x+\Delta x$

- Macroscopic variables U: densities ρ defined as zeroth order velocity moments

$$\rho(x,t) = \sum_{i=-1}^{1} f_i(x,t)$$

- Higher order moments V: "momentum" ϕ and "kinetic energy" ξ

$$\phi(x,t) = \sum_{i=-1}^{1} i\, f_i(x,t) \qquad \xi(x,t) = \frac{1}{2}\sum_{i=-1}^{1} i^2\, f_i(x,t)$$

- State of the LBM at (x,t) is completely described by either
  - the distributions $\boldsymbol{f} = [f_{-1}\ f_0\ f_1]'$ or
  - the moments $\boldsymbol{m} = [\rho\ \phi\ \xi]'$.

$$\begin{bmatrix} \rho \\ \phi \\ \xi \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix} \begin{bmatrix} f_{-1} \\ f_0 \\ f_1 \end{bmatrix} \quad \Leftrightarrow \quad \boldsymbol{m} = M\,\boldsymbol{f}$$

and vice versa $\boldsymbol{f} = M^{-1}\boldsymbol{m}$ (one-to-one relationship)

Slaving Relations

Chapman-Enskog expansion of the LBM (when density $\rho(x,t)$ varies smoothly)
$\Rightarrow$ Slaving relations
The distributions can be written as a functional of the macro. variable $\rho(x,t)$ only

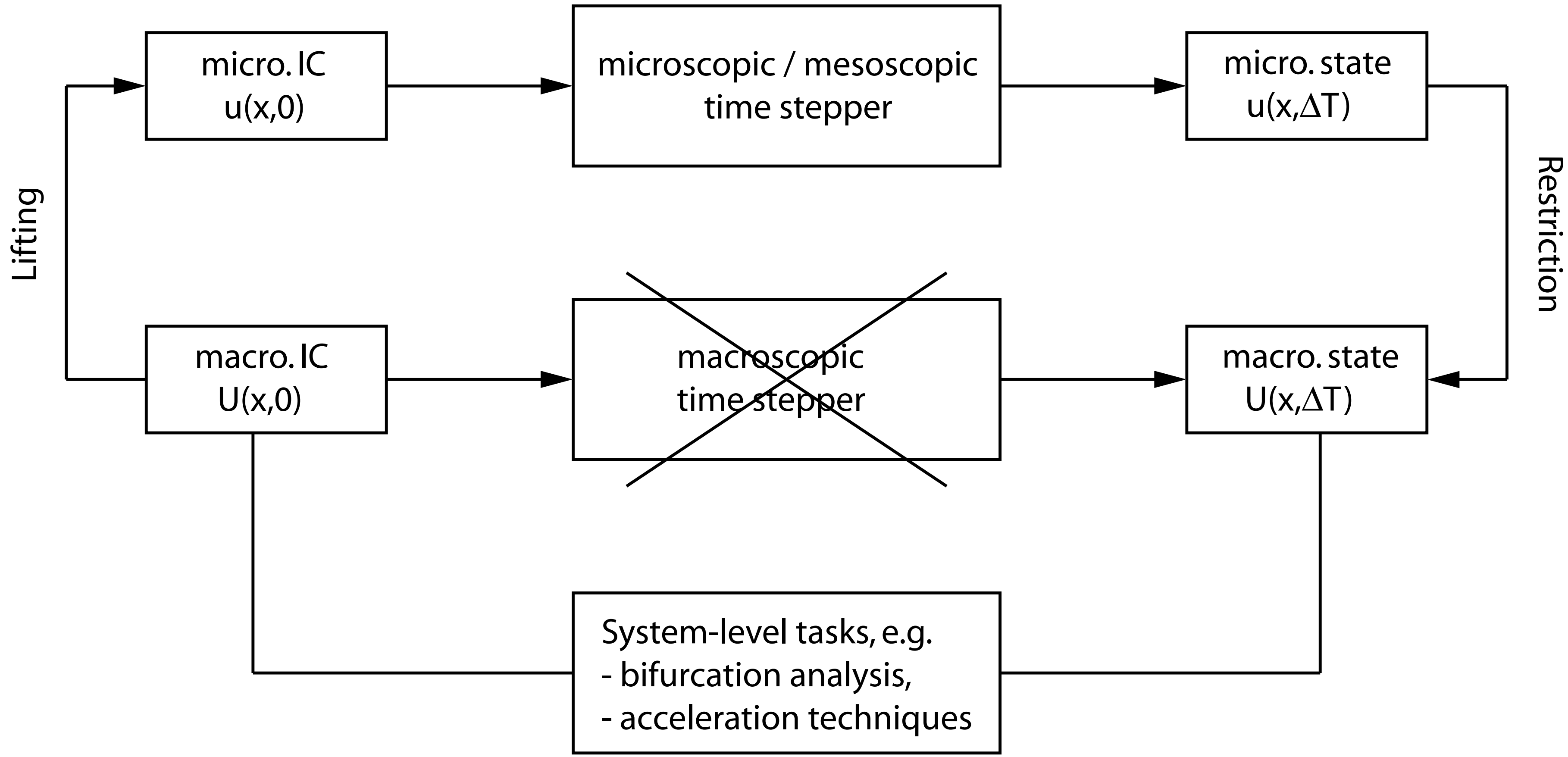
$$u = s(U) \qquad \Leftrightarrow \qquad f_i = \frac{1}{3}\rho - \frac{i\Delta x}{3\omega}\frac{\partial \rho}{\partial x} + \mathcal{O}(\Delta x^2) \quad ; i = -1, 0, 1$$

The corresponding higher order moments $\phi(x,t)$ and $\xi(x,t)$ are

$$V = S(U) \qquad \Leftrightarrow \qquad \begin{aligned} \phi &= -\frac{2\Delta x}{3\omega}\frac{\partial \rho}{\partial x} + \mathcal{O}(\Delta x^3) \\ \xi &= \frac{1}{3}\rho + \mathcal{O}(\Delta x^2) \end{aligned}$$

$\Rightarrow$ Reduced equation is the standard reaction-diffusion PDE:

$$\frac{\partial U(x,t)}{\partial t} = P(U(x,t)) \quad \Leftrightarrow \quad \frac{\partial \rho(x,t)}{\partial t} = D\frac{\partial^2 \rho(x,t)}{\partial x^2} + F(\rho^a(x,t), \rho^b(x,t), \ldots)$$



[Kevrekidis et al., 2000 — . . .]

Mesoscopic lattice Boltzmann models are deterministic $\Rightarrow$ no stochastic effects

Coarse Time Stepper for the LBM

Determine the macroscopic variables U: concentration $\rho(x,t)$ (cf. PDE)

(the microscopic variables u are the distributions $f_i(x,t)$)

One coarse time step ΔT:

1. Lifting: initialization is a one-to-many problem

$$\rho(x,0) \mapsto f_i(x,0)\ ; \quad \text{for} \quad i=-1,0,1 \quad \text{with} \quad \rho(x,0) = \sum_{i=-1}^{1} f_i(x,0)$$

   Or: How to initialize the missing higher order moments $\phi(x,0)$ and $\xi(x,0)$?

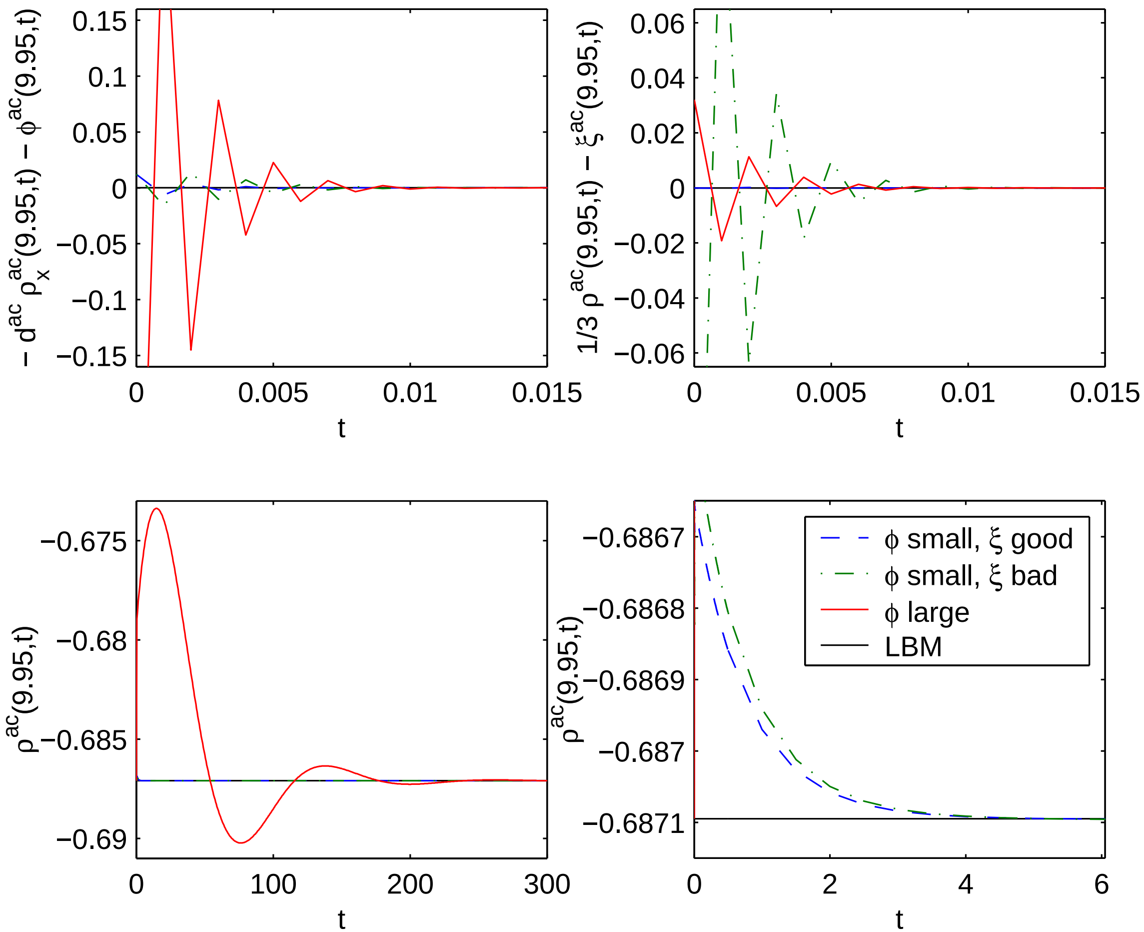
2. Mesoscopic simulation using the LBM over a time interval ΔT
3. Restriction:

$$\rho(x,\Delta T) = \sum_{i=-1}^{1} f_i(x,\Delta T)$$

Successively repeat procedure within time integration interval $[0,T]$

Outline

Very fast slaving of higher order moments: $\Delta T_{healing} \approx 20\Delta t$



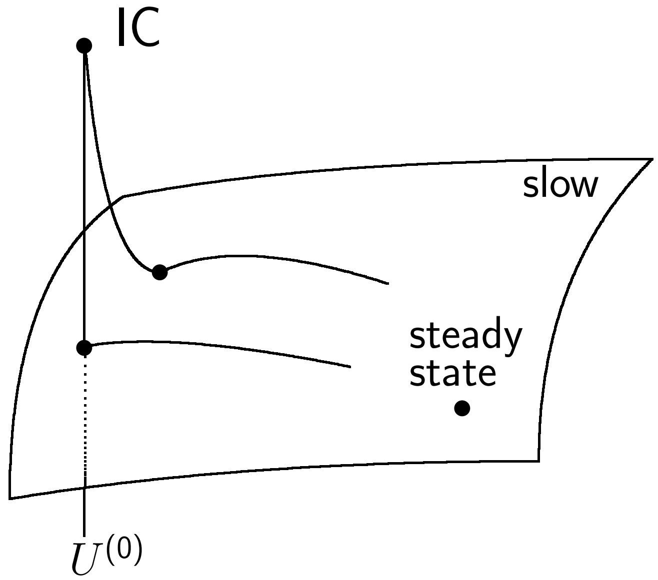
Lifting scheme:

$$f_i = w_i \rho\ ; \quad \sum_i w_i = 1$$

$$w_i = 1/3;\ i = -1, 0, 1\ (\text{blue})$$

$$w_{-1} = w_1 = 0.01\ (\text{green})$$

$$w_{-1} = 0.75,\ w_1 = 0.01\ (\text{red})$$



But lower order moment ρ also changes $\Rightarrow$ different trajectory $\Rightarrow$ $\Delta T \gg 20\Delta t$

[VL, Lust and Kevrekidis, Physica D (2005)]

- Inaccurate lifting can induce significant and persistent errors
- Time trajectory described by erroneous reaction-diffusion PDE [Vandekerckhove, VL and Roose, submitted (2007)]

$$\frac{\partial \rho(x,t)}{\partial t} = D \frac{\omega}{2-\omega} \frac{\partial^2 \rho(x,t)}{\partial x^2} + F(\rho^a(x,t), \rho^b(x,t), \ldots)$$

- Initialize micro. state $u^{(0)} = f_i(x,0)$ from the macro. variables $U^{(0)} = \rho(x,0)$ such that initial state is consistent with $U^{(0)}$ and lies on the slow manifold
- Accurate initialization possible using
  - known analytical slaving relations: Chapman-Enskog
  - numerical alternative: Constrained runs scheme
- Note: Results also useful in the context of LBM simulation itself (because a LBM is deterministic). E.g. one should not initialize with the BGK equilibrium (as is mostly done now)

$$f_i(x,0) = f_i^{eq}(x,0) = \frac{1}{3}\rho(x,0)$$

Analytical Slaving Relations

Chapman-Enskog expansion of the LBM (when density $\rho(x,t)$ varies smoothly)
$\Rightarrow$ Slaving relations
The distributions can be written as a functional of the macro. variable $\rho(x,t)$ only

$$u = s(U) \qquad \Leftrightarrow \qquad f_i \approx \frac{1}{3}\rho - \frac{i\Delta x}{3\omega}\frac{\partial \rho}{\partial x} + \mathcal{O}(\Delta x^2) \quad ; i = -1, 0, 1$$

The corresponding higher order moments $\phi(x,t)$ and $\xi(x,t)$ are

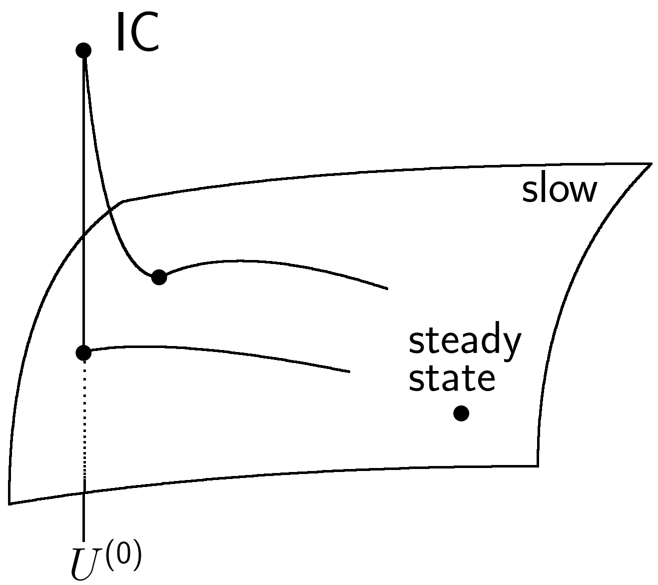
$$V = S(U) \qquad \Leftrightarrow \qquad \begin{aligned} \phi &\approx -\frac{2\Delta x}{3\omega}\frac{\partial \rho}{\partial x} + \mathcal{O}(\Delta x^3) \\ \xi &\approx \frac{1}{3}\rho + \mathcal{O}(\Delta x^2) \end{aligned}$$

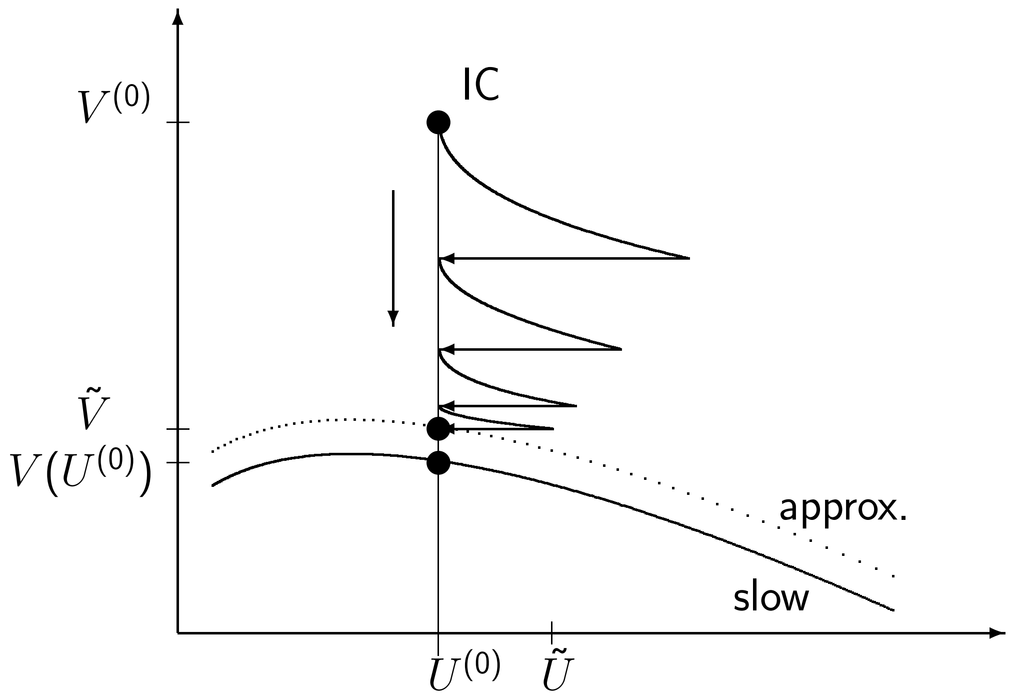
slaved to (are functionals of) the macroscopic variable $\rho(x,t)$ only

Needs analytical derivation, correct discretization, ...

Numerical Approximation: Constrained Runs (CR) Scheme

- Slaving relations difficult to compute analytically → numerical approximation
- [Gear and Kevrekidis, J. Sci. Comp. (2005)]
- Short simulations and 'resetting' of U to $U^{(0)}$





Constrained Runs Scheme for the LBM

Require: $\rho^{(0)} = \rho(x, 0)$

$f_i^{(0)} = w_i\, \rho^{(0)}$ e.g. $w_i = 1/3$

repeat

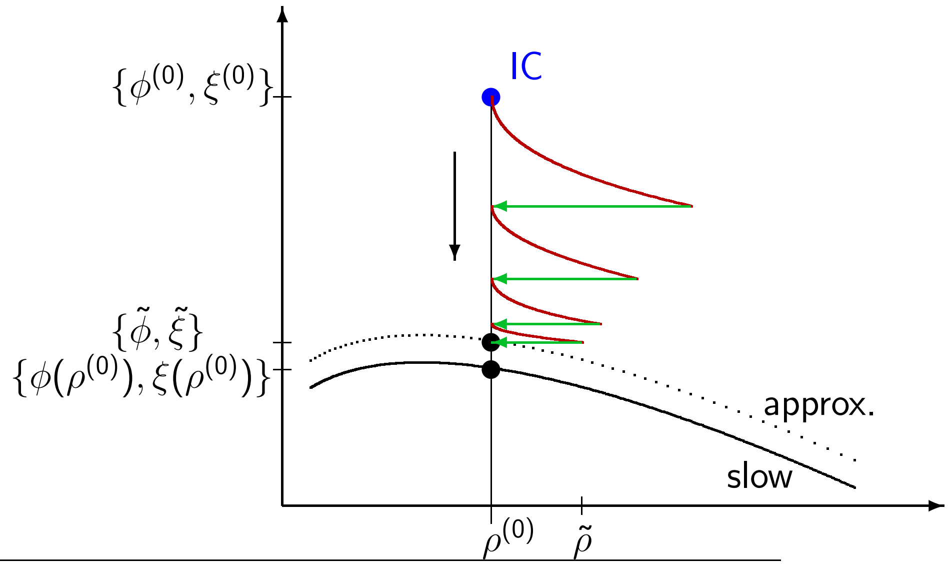
$\boldsymbol{f}^{(k+1)} = \mathsf{LBM}_{\delta t}(\boldsymbol{f}^{(k)})$

$\boldsymbol{m}^{(k+1)} = M\boldsymbol{f}^{(k+1)}$

$\rho^{(k+1)} = \rho^{(0)}$

$\boldsymbol{f}^{(k+1)} = M^{-1}\boldsymbol{m}^{(k+1)}$

until convergence heuristic $< \epsilon$, with $\epsilon \ll 1$



Fixed point iteration for the higher order moments ϕ and ξ, given $\rho^{(0)}$

$$\boldsymbol{m}^{(k+1)} = [\rho^{(0)}\ \phi^{(k+1)}\ \xi^{(k+1)}]' = \mathcal{C}_{\delta t}(\boldsymbol{m}^{(k)}) \quad k = 0, 1, 2, \ldots$$

with fixed point $\{\rho^{(0)}, \tilde{\phi}, \tilde{\xi}\}$

Proven: CR scheme is unconditionally stable with convergence rate $|1 - \omega|$

Convergence to Approximation of Slaved State

Fixed point $\{(\rho^{(0)}), \tilde{\phi}, \tilde{\xi}\}$ (given here for pure diffusion)

$$\tilde{\phi} = -\frac{2\Delta x}{3\,\omega}\frac{\partial \rho^{(0)}}{\partial x} + \frac{\Delta x}{\omega^2}\frac{(-2\omega+2)}{(\omega-2)}\frac{\partial(\tilde{\rho}-\rho^{(0)})}{\partial x}$$

$$\tilde{\xi} = \frac{1}{3}\rho^{(0)} + \frac{1}{2\omega}(\tilde{\rho}-\rho^{(0)})$$

is a first order approximation of the unknown slaved state (Chapman-Enskog)

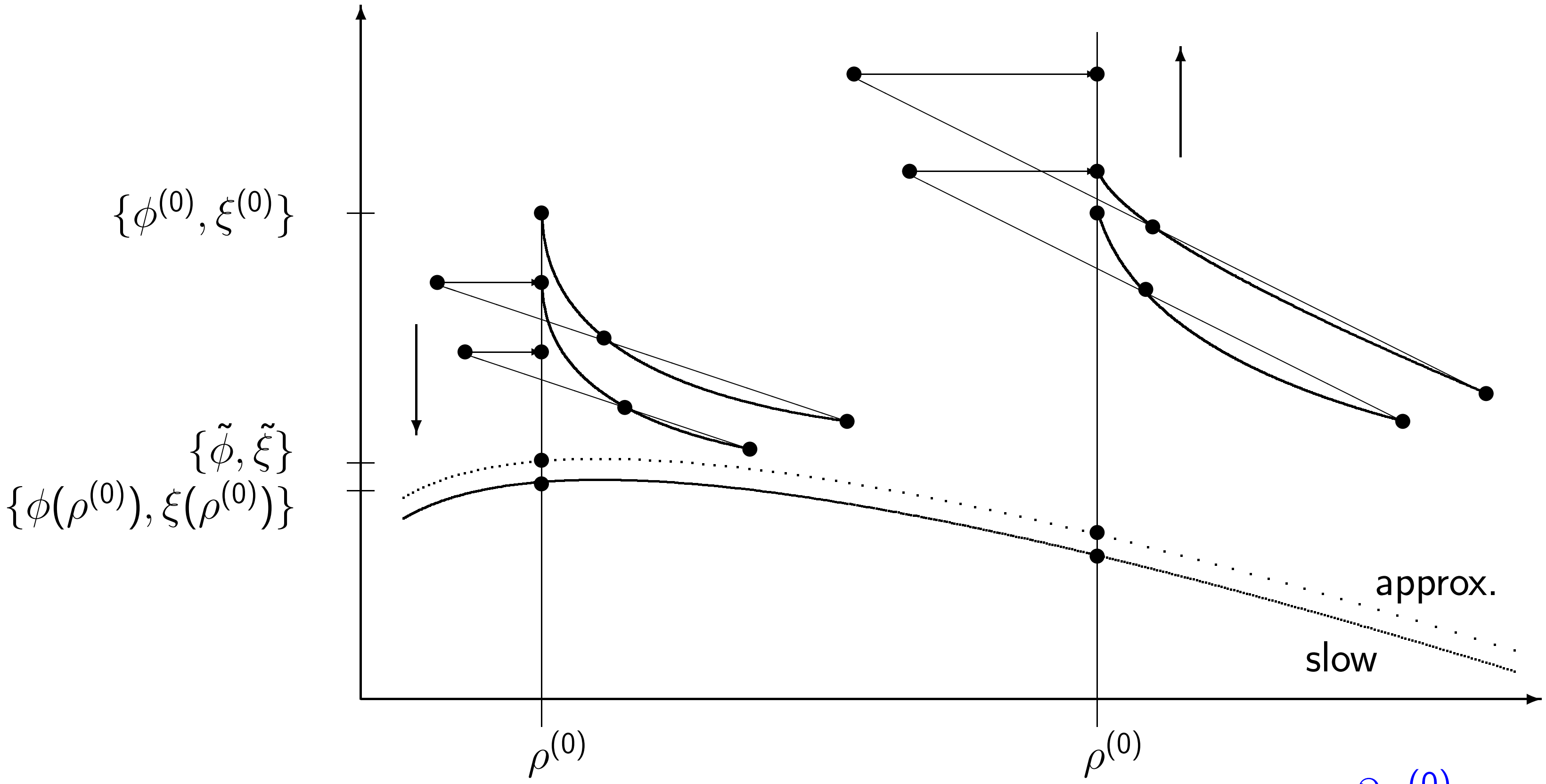
$$\phi(\rho^{(0)}) = -\frac{2\Delta x}{3\,\omega}\frac{\partial \rho^{(0)}}{\partial x} + \frac{\Delta x \Delta t}{3\omega^2}\frac{(-2\omega^2+2\omega-2)}{(\omega-2)}\frac{\partial^2 \rho^{(0)}}{\partial x \partial t} + \dots$$

$$\xi(\rho^{(0)}) = \frac{1}{3}\rho^{(0)} + \frac{\Delta t}{6\omega}\frac{\partial \rho^{(0)}}{\partial t} + \dots$$

Approximation error depends on $\tilde{\rho}-\rho^{(0)}$, i.e. the error made by constraining (resetting) the macro. variables

Because $(\tilde{\rho}-\rho^{(0)}) \sim \Delta t \frac{\partial \rho^{(0)}}{\partial t}$ $\Rightarrow$ Use smallest possible simulation time $\delta t = \Delta t$

[VL, Vanroose and Roose, TW444, submitted (2005)]

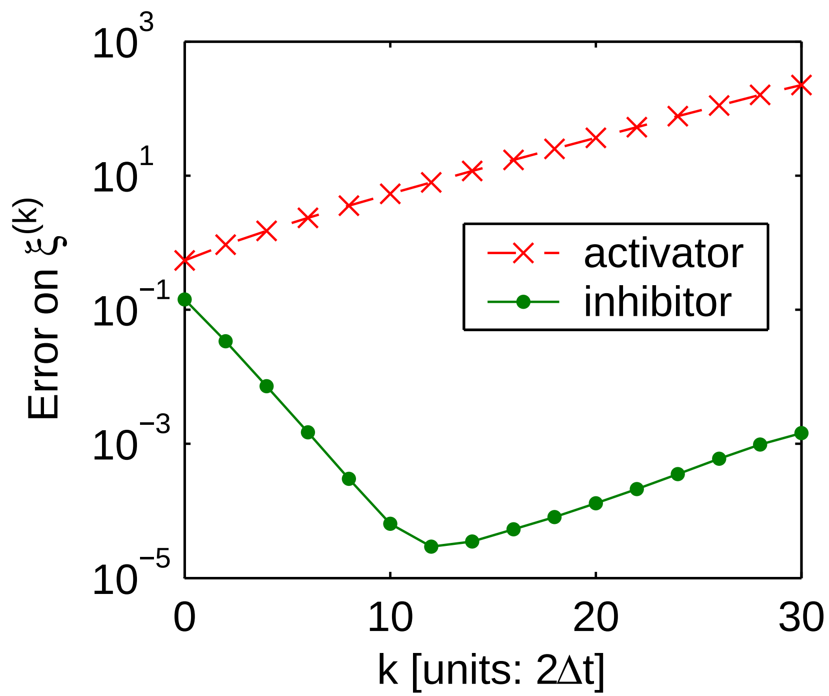


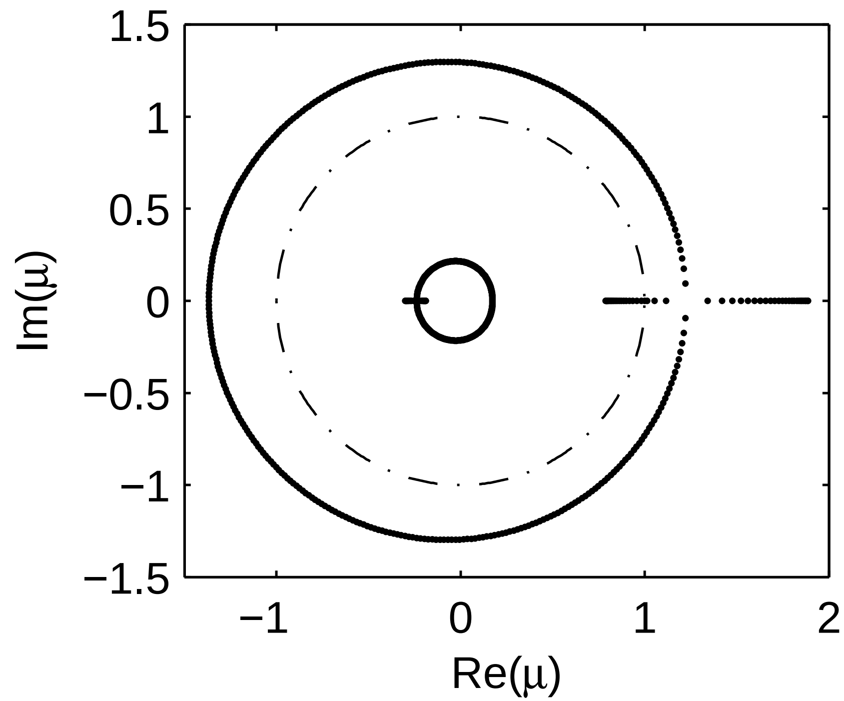
Error of regular constrained runs scheme related to $(\tilde{\rho} - \rho^{(0)}) \sim \Delta t \frac{\partial \rho^{(0)}}{\partial t}$

Interpolate higher order moments and reset lower order ones:

$$\xi^{(k+1)} = \xi_1 - \Delta t \frac{\partial \xi_1}{\partial t} = \xi_1 - \Delta t \frac{\xi_2 - \xi_1}{\Delta t} = 2\xi_1 - \xi_2 \quad \text{and} \quad \rho^{(k+1)} = \rho^{(0)}$$

Rely on slaving and attraction towards slow manifold: $\xi(\rho^{(0)}) = \frac{1}{3}\rho^{(0)} + \mathcal{O}(\Delta x^2)$



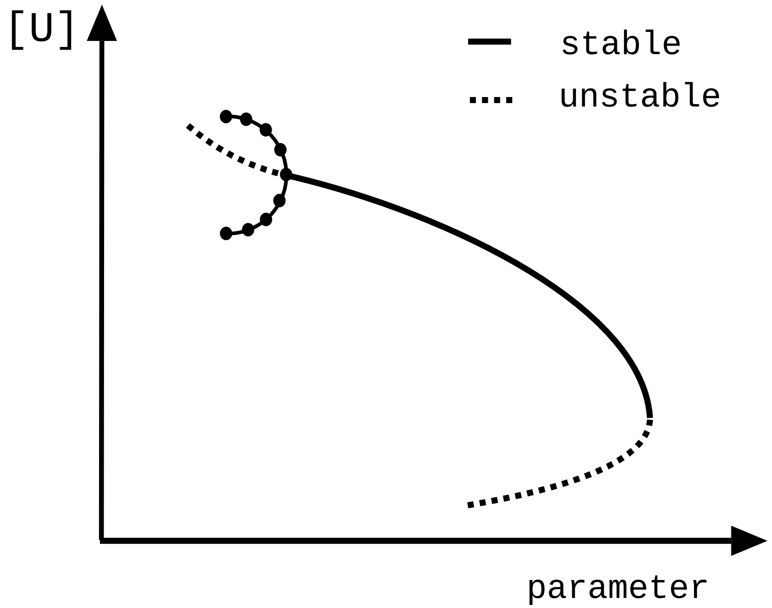


- Fixed point closer to slow manifold $\Rightarrow$ higher accuracy
- But possibly unstable: restricted range of ω-values, e.g. $\omega \in (0.69, 1.29)$
- Analysis of CR schemes for stiff singularly perturbed ODEs
  [Gear, Kaper, Kevrekidis and Zagaris, SIADS (2005) & submitted (2007)]
- Compute fixed point numerically with e.g. Newton-Krylov, GMRES
  [Vandekerckhove, Kevrekidis and Roose, submitted (2007)]

Outline

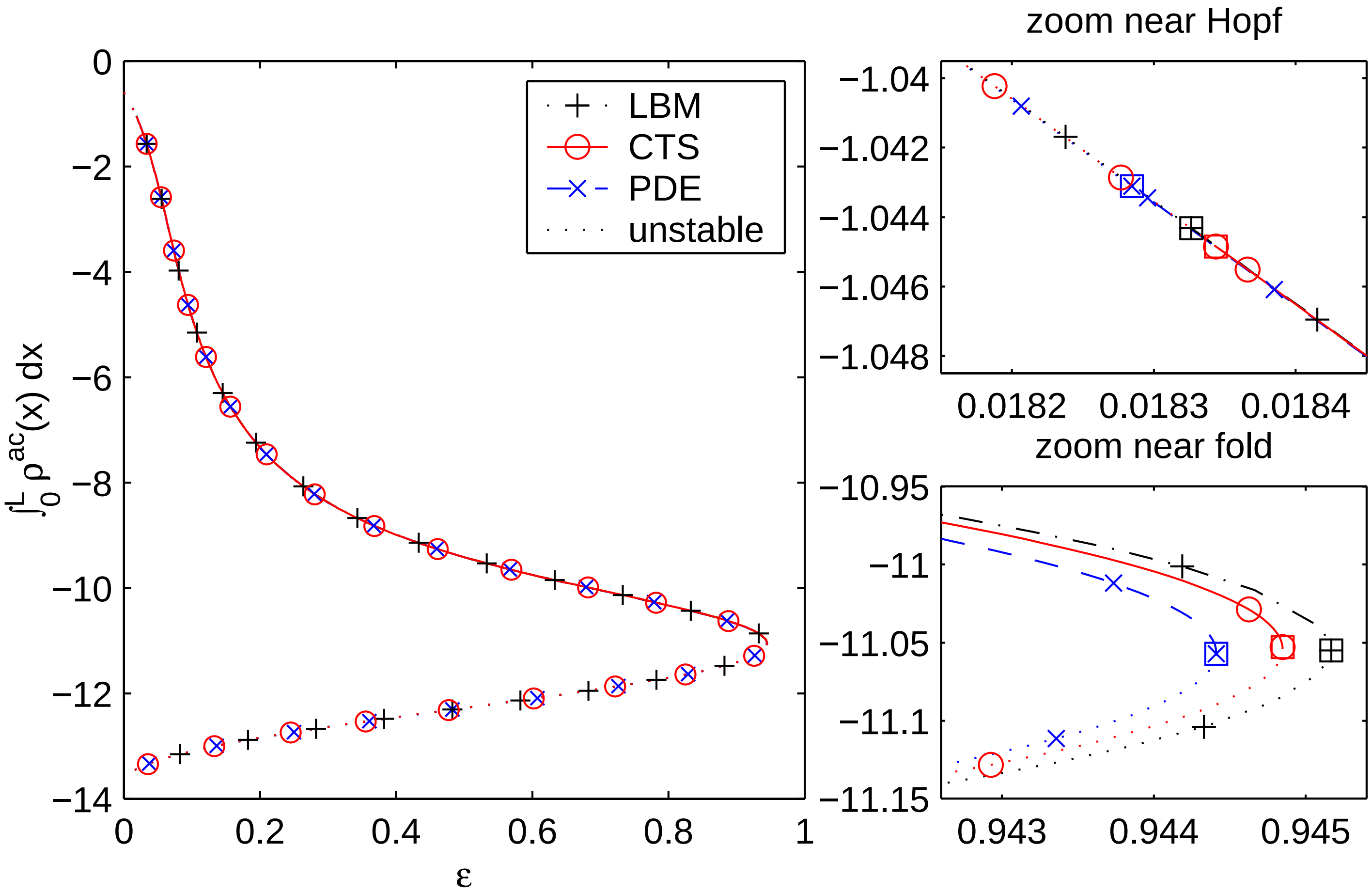
System-Level Tasks: Numerical Bifurcation Analysis

Non-linear models: Evolution of asymptotic states of macro. variables (steady states, periodic solutions) and their stability as function of system parameters



- Classical bifurcation analysis: requires linearization, Jacobian matrix, ...
- Time stepper based bifurcation analysis: 'matrix-free'
  - Condition on time stepper: few dominant eigenvalues at fixed point solution
  - Given only a truly microscopic model: use coarse time stepper

Steady state bifurcation diagram for large $\Delta T = T = 5 = 5000\Delta t$



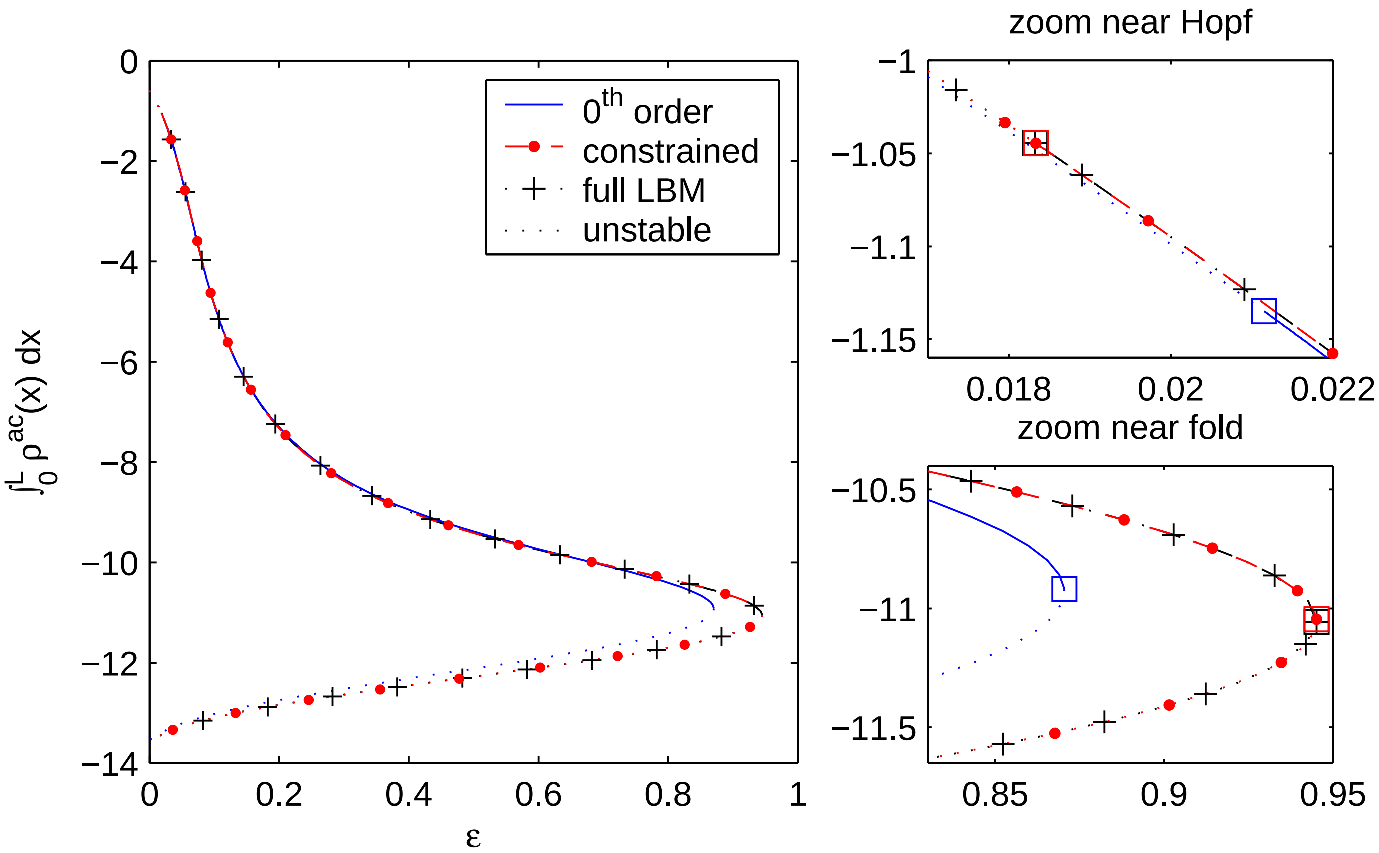
Newton-Picard method — FitzHugh-Nagumo reaction-diffusion system

Accurate bifurcation and stability information for all models (eigenvalues!)

[VL, Lust and Kevrekidis, Physica D (2005)]

Steady state bifurcation diagram for small $\Delta T = 20\Delta t$

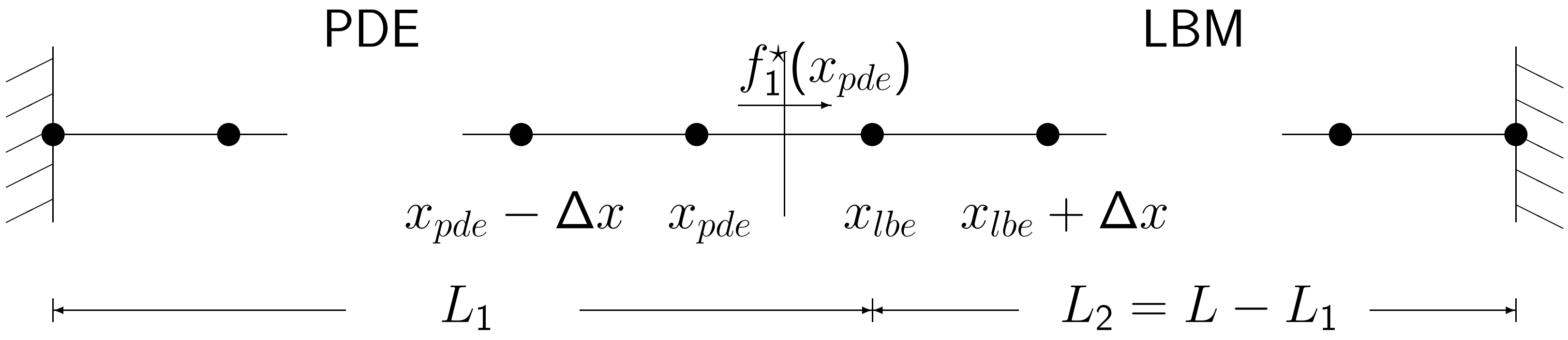
- Zeroth order lifting: $f_i = \dfrac{1}{3}\rho$ (blue)
- First order lifting: constrained runs (red)



No computational gain; to be combined with projective integration

Outline

Hybrid Spatial Coupling

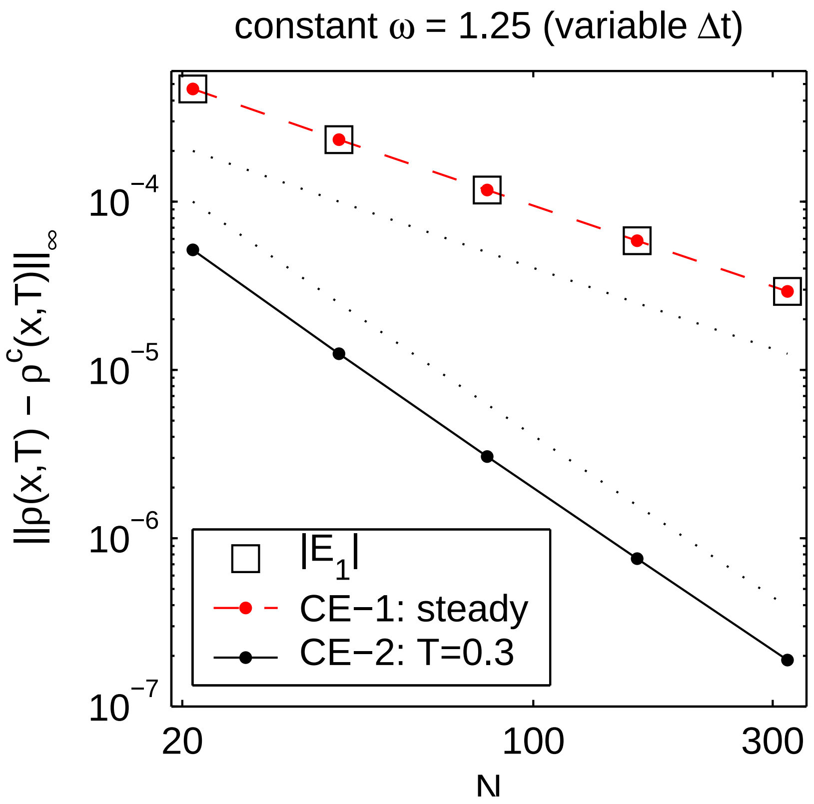


- LBM domain: Unknown post-collision distribution $f_1^\star(x_{pde}, t)$:

$$f_1(x_{pde}, t) = \frac{\rho(x_{pde}, t)}{3} - \frac{\Delta x}{3\,\omega} \frac{\rho(x_{lbe}, t) - \rho(x_{pde} - \Delta x, t)}{2\Delta x} + \mathcal{O}(\Delta x^2) \qquad (*)$$

- LBM local collisions and reactions to obtain $f_1^\star(x_{pde}, t)$
- Propagate this value to x_{lbe}, i.e. $f_1(x_{lbe}, t + \Delta t) = f_1^\star(x_{pde}, t)$
- Variant with overlap [Albuquerque, LNCS (2004), I. J. Mult. Comp. Eng. (2006)]

Alternative to above CE-1 coupling scheme: Replace $(*)$ with constrained runs



Spatial discretization error $E(x)$ at steady state: $E(x) = \rho(x) - \rho^c(x)$

Maximal $E(x)$ for CE-1 coupling scheme (and constant reaction term):

$$E_1 = E(x_{lbe}) = \frac{L_1 L_2}{L}(1-\omega)\frac{\Delta x}{6\omega}(\omega - 2)\left(2\frac{\partial^2 \rho^c(x_{lbe})}{\partial x^2} - \frac{\partial^2 \rho^c(x_{lbe}+\Delta x)}{\partial x^2}\right)$$

[VL, Vandekerckhove, Vanroose and Roose, to appear in MMS (2007)]

Outline

Conclusions

- LBM test case for multiscale and equation-free computing (no stochastic effects!)
- Lifting/Initialization is critical step in equation-free/LBM simulation
- Influence on size ΔT / significant errors
- Constrained runs scheme for LBM for 1D reaction-diffusion
  - Unconditionally stable with convergence factor $|1 - \omega|$
  - Converges to a first order approximation of the slaved state
- Higher order constrained runs schemes: more accurate, possibly unstable
- Time stepper based bifurcation analysis of LBM is feasible
  - Steady states and periodic solutions
  - Both full LBM and coarse equation-free time stepper for LBM
- Hybrid spatial coupling of LBM and discretized PDE
  - Use slaving relations or constrained runs at the interface
  - Spatial discretization error one order less accurate than local interface error