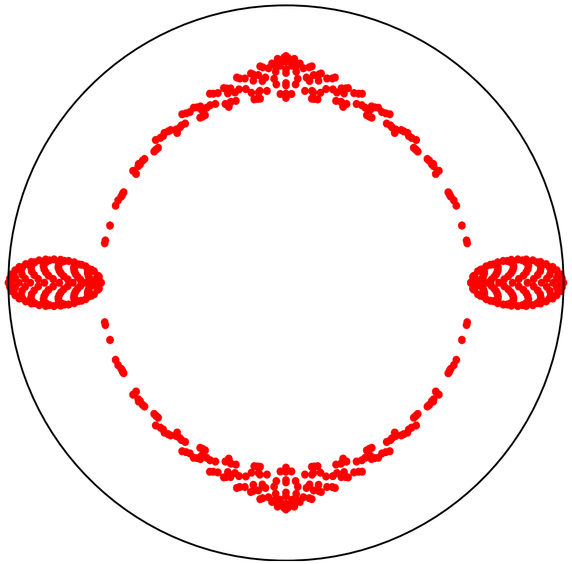
Theoretic Foundations of Grid-Coupling for Lattice-Boltzmann-Methods

Asymptotic Investigation of the LB Method - Part I

Martin Rheinländer



Depuis un demi-an beaucoup s'est changé,
dans la recherche je suis plongé.
Vraiment, ça progrèsse mieux,
merci la Vie, merci au Dieu !
Comme Christ est descendu portant la lumière,
la nouvelle méthode a brisé la barrière.
Peu à peu tout devient clair,
enfin, plus rien des mystères !

Doktoranden-Seminar
8th December 2003

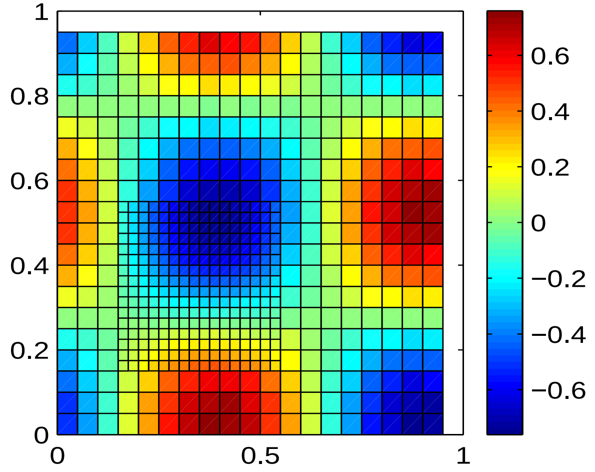
Project

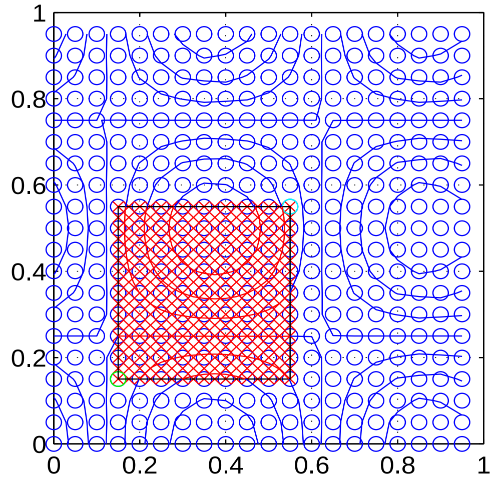
Task: Develop grid-coupling algorithms for the LB method

Motivation:
– A-priori grid refinement for flow simulation with LB
– Asymptotic Analysis: suitable tool to analyze numerical schemes like LB ?

Strategy:
– understand simple cases completely (rigorous)
– generalize to complicated problems (heuristic)

Tools: Asymptotic Analysis, Domain Decomposition





Grid coupling for the D2P4 model simulating the DAR equation

What am I doing ?

1) Fundamentals of Domain Decomposition for *Poisson* and *Stokes* equation

2) *Asymptotic analysis of the continous/discrete D1P3 model for* DAR *equation*

3) Asymptotic analysis of the continous/discrete D2P9 model for *Oseen* equation

4) Other LB models: D1P2, D2P4, D2P8

5) *Application of Equivalent Moment System: boundary and coupling conditions*

6) Strict Convergence for the continous D1P2 model
   $\rightarrow$ Discussion with *Prof. Unterreiter, Berlin*

7) Stability of LB algorithm $\leftrightarrow$ Spectrum of LB evolution matrix

8) Special analytic solutions as benchmarks

9) Matlab programming: testing uniform and coupled grids (D1P3, D2P4, D2P9)

Supervisor: *Prof. Junk, Saarbrücken*

The Boltzmann Equation

- Mesoscopic description of many particle systems:
  $\phi : [0,T) \times \Omega \times \mathbb{R}^3 \to \mathbb{R}_0^+$ particle density in *phase space*

- Evolution of $\phi(t,\mathbf{x},\mathbf{v})$: $\partial_t \phi + \mathbf{v} \cdot \nabla_{\mathbf{x}} \phi = Q(\phi,\phi)$ (*binary collisions*)

- macroscopic quantities: $\rho(t,\mathbf{x}) = \int_{\mathbb{R}^3} \phi \, d^3 v, \;\; \mathbf{u}(t,\mathbf{x}) = \ldots, \;\; T(t,\mathbf{x}) = \ldots$

- free stationary states (equilibrium) $\Leftrightarrow$ constant macroscopic quantities $\Leftrightarrow$
  time & space independent solution, *Maxwellians* $\mu(\rho,\mathbf{u},T)$: $Q(\mu,\mu) = 0$

Simplification of the Collision operator:

– System tries locally to relax towards equilibrium
– $Q(\phi,\phi) \to \frac{1}{\tau}(\mu^{\text{local}} - \phi)$

Fact: Mesoscopic Description $\xrightarrow{\text{Scaling}}$ Continuum Mechanics

The Idea of Lattice Boltzmann Methods

- Velocity space (Tangential Space of $\mathbf{x} \in \Omega$) $\rightarrow$ finite set of *discrete velocities*
  $\Rightarrow$ "Particles" move only in *discrete* directions with fixed speeds (*lattice*)

- **Ingredients of LB-type equation systems:**
  - Finite set of velocities $\mathcal{S}$
  - Weight function $\mathrm{w} : \mathcal{S} \rightarrow \mathbb{R}_0^+$
  - Structural equations = symmetry properties of the tensors T_n:

$$T_n := \sum_{\mathbf{s} \in \mathcal{S}} \mathrm{w}(\mathbf{s}) \underbrace{\mathbf{s} \otimes \ldots \otimes \mathbf{s}}_{n \text{ times}}$$

  - Density functions or *populations*: $\mathrm{p} : [0, T) \times \Omega \times \mathcal{S} \rightarrow \mathbb{R}$
  - Moments of p w.r.t. $\mathbf{s} \in \mathcal{S}$ (macroscopic = averaged quantities)
  - Counterpart of Maxwellians: equilibrium q depending on moments
  - Sytem of $\#\mathcal{S}$ coupled equations: $\partial_t \mathrm{p} + \mathbf{s} \cdot \nabla \mathrm{p} = \frac{1}{\tau}(\mathrm{q} - \mathrm{p})$

Remark: Different analysis despite of algebraic resemblence to Boltzmann

Question: What is the appropriate mathematical context / background?

Singular Perturbation

regular	=	☺ nice, good, predictable, normal	$\longrightarrow$	boring ☹
singular	=	☹ nasty, malign, malicious, uncontrolled	$\longrightarrow$	interesting ☺

Formal Definition $\rightarrow$ cf. *J.D. Murray, Asymptotic Analysis AMS 48*

Problems (P_ϵ) : $EQ_\epsilon(v,x)=0,\ AC_\epsilon$ and $(\mathrm{P}) : EQ(v,x)=0,\ AC$

u_ϵ: solution of (P_ϵ), u: solution of (P)

(P_ϵ) is a *regular perturbation* of (P) $:\Leftrightarrow$ u_ϵ *analytic* in ϵ $\wedge$ $u_\epsilon \stackrel{\text{uniform}}{\longrightarrow} u$

If $u_\epsilon \rightarrow u$ in weaker topology: (P_ϵ) *singular perturbation* of (P).

- Not always $(\mathrm{P}_0) = (\mathrm{P})$!!
- **Indicator:** ϵ multiplies highest derivative
- **Textbook Examples:**
  - *Boundary layer for convection dominated diffusion:*
    (P_ϵ) : $\epsilon\partial_x^2 u + \partial_x u = 0 \quad u(0)=a \quad u(1)=b \quad \longleftrightarrow \quad (\mathrm{P}) : \partial_x u = 0 \ u(0)=a$
  - *Slightly damped harmonic oscillator* $\leftrightarrow$ *frictionless harmonic oscillator*
    (for unbounded time interval)

Relaxation Formulation

Scalar conservation law:

$$\partial_t u \;+\; \partial_x\big(f(u)\big) \;=\; 0$$

1. Introduce flux as new variable: $v \;=\; f(u)$

2. $$\begin{aligned} \partial_t\, u \;+\; \partial_x v \;&=\; 0 \\ 0 \;&=\; f(u) \;-\; v \end{aligned} \qquad\qquad \begin{aligned} \partial_t\, u \;+\; \partial_x v \;&=\; 0 \\ \epsilon\,\big(\partial_t\, u \;+\; a\,\partial_x u\big) \;&=\; f(u) \;-\; v \end{aligned}$$

3. **Relaxation form:** $$\begin{aligned} \partial_t\, u \;+\; \partial_x v \;&=\; 0 \\ \partial_t\, u \;+\; a\,\partial_x u \;&=\; \tfrac{1}{\epsilon}\,\big(f(u) \;-\; v\big) \end{aligned}$$

Pros & Cons $\longrightarrow$ cf. *R. LeVeque ....*

- $+$ nonlinear flux terms shifted into source terms $\Rightarrow$ *linear* hyperbolic part
  $\Rightarrow$ simple structure of characteristics
- $+$ no nonlinear Riemann solver necessary
- $-$ larger system of equations
- $-$ stiff source terms

The D1P3 Model - Notation and Definitions

- Discrete velocities: $\mathrm{s} \in \{\mathrm{s}_0, \mathrm{s}_1, \mathrm{s}_2\} = \{0, -1, 1\} =: \mathcal{S}$
- Weights: $\mathrm{w} = \mathrm{w}(\mathrm{s}) \in \{\mathrm{w}_0, \mathrm{w}_1, \mathrm{w}_2\} = \{\frac{n-1}{n}, \frac{1}{2n}, \frac{1}{2n}\} \qquad n \geq 1$
- Populations: $\mathrm{p}_0,\ \mathrm{p}_1,\ \mathrm{p}_2\ \in \mathcal{F}([a,b] \times [0,T)) \qquad \mathrm{p}_k(t,x) \equiv \mathrm{p}(t,x,\mathrm{s}_k)$

  (Primary variables occuring in the LB equation!)

- Collision time: $\tau \in \mathcal{F}([a,b] \times [0,T))$ and collision frequency $\omega := \tau^{-1}$: $\tau > 0$
- External source: $k\ \in\ \mathcal{F}([a,b] \times [0,T))$

- The quantity of interest or the macroscopic quantity:

$$u(t,x) := \mathrm{p}_0(t,x) + \mathrm{p}_1(t,x) + \mathrm{p}_2(t,x) \quad u \in \mathcal{F}([a,b] \times [0,T))$$

(E.g. *density* $\vee$ *concentration* $\vee$ *velocity component* (for parallel shear flows))

The D1P3 Model - LB Equation

- Central equation: **Evolution Equation for the populations**

$$\begin{array}{lclcl}
\epsilon^2\,\partial_t \mathrm{p}_0 & & & = & \omega\big(\mathrm{q}_0(u) - \mathrm{p}_0\big) \;+\; \epsilon^2\,\mathrm{w}_0\,k \\
\epsilon^2\,\partial_t \mathrm{p}_1 & - & \epsilon\,\partial_x \mathrm{p}_1 & = & \omega\big(\mathrm{q}_1(u) - \mathrm{p}_1\big) \;+\; \epsilon^2\,\mathrm{w}_1\,k \\
\epsilon^2\,\partial_t \mathrm{p}_2 & + & \epsilon\,\partial_x \mathrm{p}_2 & = & \omega\big(\mathrm{q}_2(u) - \mathrm{p}_2\big) \;+\; \epsilon^2\,\mathrm{w}_2\,k
\end{array}$$

(Appropriate IC for p_1, p_2, $\mathrm{p}_3 \Rightarrow$ later!)

- **Possible kinetic B.C.:**

Periodic:	$\mathrm{p}_2(\cdot,a) =$	$\mathrm{p}_2(\cdot,b)$	$\mathrm{p}_1(\cdot,b) =$	$\mathrm{p}_1(\cdot,a)$
Bounce-Back Type 1:	$\mathrm{p}_2(\cdot,a) =$	$-\;\mathrm{p}_1(\cdot,a)$	$\mathrm{p}_1(\cdot,b) =$	$-\;\mathrm{p}_2(\cdot,b)$
Bounce-Back Type 2:	$\mathrm{p}_2(\cdot,a) =$	$\mathrm{p}_1(\cdot,a)$	$\mathrm{p}_1(\cdot,b) =$	$\mathrm{p}_2(\cdot,b)$

Try to show:

u is related to the solution $v \in \mathcal{F}([a,b] \times [0,T))$ of the following *Diffusion-Advection-Reaction (DAR)* limit-equation in conservation form:

$$\partial_t\,v \;+\; \partial_x\big(\mathsf{a}\,v \;-\; \nu\,\partial_x v\big) \;+\; c\,v \;=\; k \qquad \text{BC \& IC for } v$$

Given coefficients: Diffusivity ν, Advection a, Reactivity $c \in \mathcal{F}([a,b] \times [0,T))$

The D1P3 Model - Equilibrium

- Equilibrium couples LB equations: $\mathrm{q} = \mathrm{q}(u, \mathrm{s}) = \mathrm{q}(\mathrm{p}_0, \mathrm{p}_1, \mathrm{p}_2, \mathrm{s})$

- Equilibrium determines limit-equation in detail:

$$\begin{aligned} \mathrm{q}(u,\mathrm{s}) &= \mathrm{q}^D(u,\mathrm{s}) + \epsilon\, \mathrm{q}^A(u,\mathrm{s}) + \epsilon^2\, \mathrm{q}^R(u,\mathrm{s}) \\ &= \mathrm{w}\, u + \epsilon\; n\, \mathrm{w}\, \mathrm{s}\, a\, u - \epsilon^2\, \mathrm{w}\, \tau\, c\, u \end{aligned}$$

- Moments of discrete velocities w.r.t.the weights (structural equations):

$\sum \mathrm{w} = 1 \qquad \sum \mathrm{w}\, \mathrm{s} = 0 \qquad \sum \mathrm{w}\, \mathrm{s}^2 = \frac{1}{n}$ (Summation always over $\mathrm{s} \in \mathcal{S}$)

- Moments of discrete velocities w.r.t. the equilibrium:

$$\begin{array}{lll} \sum \mathrm{q}^D = u & \sum \mathrm{s}\, \mathrm{q}^D = 0 & \sum \mathrm{s}^2 \mathrm{q}^D = \frac{1}{n} u \\ \sum \mathrm{q}^A = 0 & \sum \mathrm{s}\, \mathrm{q}^A = a\, u & \sum \mathrm{s}^2 \mathrm{q}^A = 0 \\ \sum \mathrm{q}^R = -\tau\, c\, u & \sum \mathrm{s}\, \mathrm{q}^R = 0 & \sum \mathrm{s}^2 \mathrm{q}^R = -\frac{1}{n} \tau\, c\, u \end{array}$$

Formal Asymptotic Expansion: 0^{th} & 1^{st} Order

1. Regular asymptotic expansion: $\mathrm{p} = \mathrm{p}^{(0)} + \epsilon\, \mathrm{p}^{(1)} + \epsilon^2\, \mathrm{p}^{(2)} + \dots \quad (*)$ $\Rightarrow$
   Asymptotic expansion of u: $\quad u^{(l)}(t,x) = \sum \mathrm{p}^{(l)}(t,x,\mathrm{s}) \qquad l \geq 0$

2. Plug $(*)$ in subsequent LB-equation:

$$\epsilon^2\, \partial_t \mathrm{p} + \epsilon\, \mathrm{s}\, \partial_x \mathrm{p} = \omega\big(\mathrm{q}^D(u) + \epsilon\, \mathrm{q}^A(u) + \epsilon^2\, \mathrm{q}^R(u) - \mathrm{p}\big) + \epsilon^2\, \mathrm{w}\, k$$

3. Equate terms of equal power in ϵ:
   - 0^{th} order: $\mathrm{p}^{(0)} = \mathrm{q}^D(u^{(0)})$
   - 1^{st} order: $\mathrm{p}^{(1)} = \mathrm{q}^D(u^{(1)}) + \mathrm{q}^A(u^{(0)}) - \tau\, \mathrm{s}\, \partial_x \mathrm{p}^{(0)}$
     $= \mathrm{q}^D(u^{(1)}) + \mathrm{q}^A(u^{(0)}) - \tau\, \mathrm{s}\, \partial_x \mathrm{q}^D(u^{(0)})$

4. Moments needed to go on with 2^{nd} order:

$$\sum \mathrm{p}^{(1)} = u^{(1)} \qquad \sum \mathrm{s}\,\mathrm{p}^{(1)} = a\, u^{(0)} - \tfrac{\tau}{n}\partial_x\, u^{(0)} \qquad \sum \mathrm{s}^2\, \mathrm{p}^{(1)} = \tfrac{1}{n}\, u^{(1)}$$

Formal Asymptotic Expansion: 2^{nd} Order

$$\partial_t \mathrm{p}^{(0)} + \mathrm{s}\,\partial_x \mathrm{p}^{(1)} = \omega\left(\mathrm{q}^D(u^{(2)}) + \mathrm{q}^A(u^{(1)}) + \mathrm{q}^R(u^{(0)}) - \mathrm{p}^{(2)}\right) + \mathrm{w}\,k$$

Sum over $\mathrm{s} \in \mathcal{S}$ using moment relations $\Rightarrow$ evolution equation for $u^{(0)}$:

$$\partial_t u^{(0)} + \partial_x\left(a\,u^{(0)} - \tfrac{\tau}{n}\partial_x u^{(0)}\right) + c\,u^{(0)} = k \qquad (*)$$

Observations:

1. $u^{(0)}$ is an *exact* solution of the limit equation
2. Unfortunately, $u^{(0)}$ is not accesible. . .

But: Since $u = u^{(0)} + O(\epsilon)$, u is at least a 1^{st} order approximation! $\nu = \frac{\tau}{n}$

In order to obtain the 3^{rd} order, solve for $\mathrm{p}^{(2)}$,

$$\mathrm{p}^{(2)} = q^D(u^{(2)}) + q^A(u^{(1)}) + q^R(u^{(0)}) - \tau\partial_x \mathrm{p}^{(1)} - \tau\partial_t \mathrm{p}^{(0)} + \tau\,\mathrm{w}\,k$$

and compute the moments using $(*)$:

$$\sum \mathrm{p}^{(2)} = u^{(2)} \qquad \sum \mathrm{s}\,\mathrm{p}^{(2)} = a\,u^{(1)} - \tfrac{\tau}{n}\partial_x u^{(1)}$$

$$\sum \mathrm{s}^2\,\mathrm{p}^{(2)} = \tfrac{1}{n}u^{(2)} - \tfrac{n-1}{n}\tau\partial_x\left(a\,u^{(0)} - \tfrac{\tau}{n}\partial_x u^{(0)}\right)$$

Formal Asymptotic Expansion: 3^{rd} Order

$$\partial_t \mathrm{p}^{(1)} + \mathrm{s}\,\partial_x \mathrm{p}^{(2)} = \omega\left(\mathrm{q}^D(u^{(3)}) + \mathrm{q}^A(u^{(2)}) + \mathrm{q}^R(u^{(1)}) - \mathrm{p}^{(3)}\right)$$

Sum over $\mathrm{s} \in \mathcal{S}$ using the moment relations $\Rightarrow$ evolution equation for $u^{(1)}$:

$$\partial_t u^{(1)} + \partial_x\left(a\,u^{(1)} - \tfrac{\tau}{n}\partial_x u^{(1)}\right) + c\,u^{(1)} = 0$$

Observation: $u^{(1)}$ satisfies the *homogeneous* limit equation.

Assumptions:

i) BC for populations imply homogeneous BC for $u^{(1)}$

ii) IC for populations imply zero IC for $u^{(1)}$,i.e.: $u^{(1)}(0,\cdot) = 0$

Conclusion: Therefore $\forall\, t \geq 0$: $u^{(1)}(t,\cdot) \equiv 0 \quad \Rightarrow \quad u = u^{(0)} + O(\epsilon^2)$.
u approximates the solution of the limit equation up to terms of order $O(\epsilon^2)$!

Intention: Try to estimate leading order of error by computing $u^{(2)}$.

Formal Asymptotic Expansion: Higher Orders

- Derive the evolution equation for $u^{(l)}, l \geq 2$ recursively:
  - Suppose $\mathrm{p}^{(l+1)}$ and its moments to be known from the previous iteration
  - Sum $(2+l)^{th}$ order of LB equation over $\mathrm{s} \in \mathcal{S}$: $\partial_t\, u^{(l)} + \sum \mathrm{s}\, \mathrm{p}^{(l+1)} + c\, u^{(l)} = 0$

- **Definition:** *flux* of l^{th} order: $\hat{f}^{(l)} := a\, u^{(l)} - \frac{\tau}{n} \partial_x u^{(l)}$

$\sum \mathrm{s}\, \mathrm{p}^{(l+1)} \;=\; \hat{f}^{(l)} +$ terms depending on lower orders of u (source terms)

- Evolution equation of $u^{(2)}$:

$$\partial_t\, u^{(2)} + \partial_x\big(\, a\, u^{(2)} - \tfrac{\tau}{n}\, \partial_x\, u^{(2)}\,\big) + c\, u^{(2)} \;=\; \partial_x\big(\tau\, \partial_t \hat{f}^{(0)} - \tau\, \partial_x (\tau \tfrac{n-1}{n} \partial_x \hat{f}^{(0)})\,\big)$$

- **Remarks:**
  - Even with homogeneous IC and BC, $u^{(2)} \not\equiv 0$ in general due to source term.
  - Source term depends not on $u^{(1)}$ even if $\not\equiv 0$. (Seperates even/odd orders!)
  - $3^{rd}, 4^{th}$ derivatives of $u^{(0)}$ occuring in source term complicate estimation of $u^{(2)} \;\; \Leftarrow$ strong regularity requirements.

Representation of the Populations

Observation: The asymptotic expansions of the 3 populations $\mathrm{p}_1, \mathrm{p}_2, \mathrm{p}_3$ can be given only in terms of the asymptotic orders of u.

Assumption: For $j \in \mathbb{N}$: $u^{(2j+1)} \equiv 0 \quad \longrightarrow$ justification later!

$\Downarrow$

$$
\begin{aligned}
\mathrm{p}^{(0)} &= \mathrm{w} u^{(0)} \\
\mathrm{p}^{(1)} &= n\,\mathrm{w}\,\mathrm{s}\,\hat{f}^{(0)} \\
\mathrm{p}^{(2)} &= \mathrm{w}\,u^{(2)} - (n\,\mathrm{s}^2 - 1)\,\mathrm{w}\,\tau\,\partial_x \hat{f}^{(0)} \\
\mathrm{p}^{(3)} &= n\,\mathrm{w}\,\mathrm{s}\,\hat{f}^{(2)} + \mathrm{w}\,\mathrm{s}\,(n\mathrm{s}^2 - 1)\,\tau\,\partial_x(\tau\partial_x \hat{f}^{(0)}) - n\,\mathrm{w}\,\mathrm{s}\,\tau\,\partial_t \hat{f}^{(0)}
\end{aligned}
$$

$$
\mathrm{p}(t,x,\mathrm{s}) = \mathrm{p}^{(0)}(t,x,\mathrm{s}) + \epsilon\,\mathrm{p}^{(1)}(t,x,\mathrm{s}) + \epsilon^2\mathrm{p}^{(2)}(t,x,\mathrm{s}) + \epsilon^3\mathrm{p}^{(3)}(t,x,\mathrm{s}) + O(\epsilon^4)
$$

Observation: odd(even) asymptotic order $\longrightarrow$ odd(even) polynomials in s

Consequence: $\hat{f}^{(0)}$ and $\partial_x \hat{f}^{(0)}$ can be extracted up to terms of order $O(\epsilon^2)$.

Extracting "Hidden" Information

$$
\begin{aligned}
\mathrm{p}_2 + \mathrm{p}_1 + \mathrm{p}_0 &= \sum \mathrm{p} &&= u^{(0)} + \epsilon^2 u^{(2)} && + O(\epsilon^4) \\
\mathrm{p}_2 - \mathrm{p}_1 &= \sum \mathrm{p\,s} &&= \epsilon \hat{f}^{(0)} + \epsilon^3 \hat{f}^{(2)} - \epsilon^3 \partial_t \hat{f}^{(0)} && + O(\epsilon^4) \\
\mathrm{p}_2 + \mathrm{p}_1 &= \sum \mathrm{p\,s}^2 &&= \tfrac{1}{n} u^{(0)} + \tfrac{1}{n}\epsilon^2 u^{(2)} - \epsilon^2 \tau \tfrac{n-1}{n} \partial_x \hat{f}^{(0)} && + O(\epsilon^4)
\end{aligned}
$$

Definition: $f := \frac{1}{\epsilon}(\mathrm{p}_2 - \mathrm{p}_1), \qquad g := \frac{1}{\epsilon^2}\left(\sum \mathrm{ps}^2 - \frac{1}{n} \sum \mathrm{p} \right)$

Conclusions:

1. If the assumption holds, then:

$$
\begin{aligned}
f &= f^{(0)} + O(\epsilon^2) &&= a\, u^{(0)} - \tfrac{\tau}{n} \partial_x u^{(0)} + O(\epsilon^2) \\
g &= g^{(0)} + O(\epsilon^2) &&= -\tau \tfrac{n-1}{n} \partial_x \left(a\, u^{(0)} - \tfrac{\tau}{n} \partial_x u^{(0)} \right) + O(\epsilon^2)
\end{aligned}
$$

2. Solution of the LB equation $\Rightarrow$ approximate solution of the limit-equation $+$ approximation of its first and second derivatives.

The Equivalent Moment System (EMS)

Remarks:

– Definition of f, g motivated by the assumption, but *independent* of it

– Kinetic variables: $\mathrm{p}_1 \;\; \mathrm{p}_2 \;\; \mathrm{p}_3 \iff$ Physical variables (Moments): $u \;\; f \;\; g$

Idea: Express LB equation in terms of $u, f, g \;\; \rightarrow$ equivalent moment system:

Transformation:

$$\begin{aligned}
\partial_t \mathbf{p} \quad &+ \quad \tfrac{1}{\epsilon} S \partial_x \mathbf{p} &&= \tfrac{1}{\tau\epsilon^2}[Q_\epsilon \mathbf{p} - \mathbf{p}] + k\,\mathbf{w} \\
\partial_t M_\epsilon^{-1}\mathbf{m} \quad &+ \quad \tfrac{1}{\epsilon} S \partial_x M_\epsilon^{-1}\mathbf{m} &&= \tfrac{1}{\tau\epsilon^2}[Q_\epsilon M_\epsilon^{-1}\mathbf{m} - M_\epsilon^{-1}\mathbf{m}] + k\,\mathbf{w} \\
\partial_t \mathbf{m} \quad &+ \quad \tfrac{1}{\epsilon} M_\epsilon S M_\epsilon^{-1} \partial_x \mathbf{m} &&= \tfrac{1}{\tau\epsilon^2}[M_\epsilon Q_\epsilon M_\epsilon^{-1}\mathbf{m} - \mathbf{m}] + k\,M_\epsilon \mathbf{w}
\end{aligned}$$

$$\begin{aligned}
\partial_t u \; &+ \; \partial_x f + cu &&= k \\
\partial_t f \; &+ \; \tfrac{1}{n\epsilon^2}\partial_x u + \partial_x g &&= \tfrac{1}{\tau\epsilon^2}\left(au - f\right) \qquad && f = au - \tfrac{\tau}{n}\partial_x u - \epsilon^2\tau\,(\partial_t f + \partial_x g) \\
\partial_t g \; &+ \; \tfrac{n-1}{n\epsilon^2}\partial_x f &&= -\tfrac{1}{\tau\epsilon^2}\,g && g = -\tfrac{n-1}{n}\tau\,\partial_x f - \epsilon^2\tau\,\partial_t g
\end{aligned}$$

$$\mathbf{p} := (\mathrm{p}_0, \mathrm{p}_1, \mathrm{p}_2)^T, \;\; \mathbf{m} := (u, f, g)^T, \;\; \mathbf{w} := (\mathrm{w}_0, \mathrm{w}_1, \mathrm{w}_2)^T, \quad \mathbf{m} = M_\epsilon \mathbf{p}$$

Further Conclusions from the EMS

Observations:

1. Transformation matrix M_ϵ is orthogonal w.r.t. the scalar product generated by $\mathrm{Diag}(\mathbf{w})$, i.e.

$$M_\epsilon \, \mathrm{Diag}(\mathbf{w}) \, M_\epsilon^T = \mathrm{Diag}\big((1, \, \tfrac{1}{n\epsilon^2}, \, \tfrac{n-1}{n^2\epsilon^4})\big)$$

   Disadvantage: In contrast to LB equation: hyperbolic part NOT diagonal

2. EMS reveals resemblence to *relaxation systems*.

3. Trivial reduction to limit-equation NOT possible — *instead:*
   Infinite hierarchy of successively, formally solvable equations → Convergence ?

4. Equation for g not needed to obtain formally limit equation

Proposition:
Total decoupling of odd/even asymptotic orders of u, f, g
Proof: verification by induction using: only ϵ dependent coefficient is ϵ^2

Analysis of Kinetic Boundary Conditions

- **BC of Bounce-Back Type 1:** *left boundary*

  incoming $\mathrm{p}_2 = -$ outgoing $\mathrm{p}_1 \quad \Leftrightarrow \quad 0 \;=\; \mathrm{p}_2 + \mathrm{p}_1 \;=\; \epsilon^2 g + \frac{1}{n} u$

  $\Leftrightarrow \quad u^{(0)} = 0 \;\wedge\; u^{(1)} = 0 \;\wedge\; u^{(2)} = n\, g^{(0)} \;\wedge\; u^{(3)} = n\, g^{(1)} \;\wedge\; \ldots$

  homogeneous Dirichlet BC for $u^{(0)}$

- **BC of Bounce-Back Type 2:** *left boundary*

  incoming $\mathrm{p}_2 =$ outgoing $\mathrm{p}_1 \;\Leftrightarrow\; 0 \;=\; \mathrm{p}_2 - \mathrm{p}_1 \;=\; \epsilon\, f \;\Leftrightarrow\; f^{(l)} = 0 \;\forall\; l \in \mathbb{N}_0$

  $f^{(0)} = a\, u^{(0)} - \frac{\tau}{n} \partial_x u^{(0)} \;=\; 0$ Natural BC for $u^{(0)}$, since flux $= 0$ at boundary

  $a \neq 0$: *Robin* BC: , $a = 0$: *Neumann* BC for $u^{(0)}$

Observation: Odd/Even-decoupling not affected by BC

Proof of Assumption:
Kinetic BC $\Rightarrow$ homogeneous BC for $u^{(1)}$. $\Rightarrow \; u^{(1)} \equiv 0$ if initialized with 0.
Periodic BC: argue only with the evolution equations and IC.
Infer by induction: odd orders of u must vanish.

Grid Transformation of Populations

$$\mathbf{p} = M_\epsilon^{-1}\mathbf{m} \quad \Rightarrow \quad \mathrm{p} = \mathrm{w}\, u + \tfrac{1}{2}\mathrm{s}\,\epsilon f + \tfrac{1}{2}(3\mathrm{s}^2 - 2)\epsilon^2 g$$

$$\Longrightarrow \mathrm{p}^{(0)} = w\, u^{(0)} \quad \mathrm{p}^{(1)} = \tfrac{1}{2}\mathrm{s} f^{(0)} \quad \mathrm{p}^{(2)} = w\, u^{(2)} + \tfrac{1}{2}(3\mathrm{s}^2 - 2)\, g^{(0)}$$

1. Consider 2 LB systems: parameter $\epsilon_1 = \epsilon, \quad \epsilon_2 = \eta$
   but both approximating the same IBVP for the limit equation:

$$\begin{cases} \mathrm{p} = \mathrm{p}^{(0)} + \epsilon\, \mathrm{p}^{(1)} + \epsilon^2 \mathrm{p}^{(2)} + \dots & \rightarrow \quad u, \ f, \ g \\ \tilde{\mathrm{p}} = \mathrm{p}^{(0)} + \eta\, \mathrm{p}^{(1)} + \eta^2 \mathrm{p}^{(2)} + \dots & \rightarrow \quad \tilde{u}, \ \tilde{f}, \ \tilde{g} \end{cases}$$

$$\Longrightarrow \boxed{\tilde{\mathrm{p}} = \mathrm{p} + O(|\epsilon - \eta|)}$$

2. Recall:

$$\begin{aligned} u^{(0)} &= u + O(\epsilon^2) & f^{(0)} &= f + O(\epsilon^2) & g^{(0)} &= g + O(\epsilon^2) \\ u^{(0)} &= \tilde{u} + O(\eta^2) & f^{(0)} &= \tilde{f} + O(\eta^2) & g^{(0)} &= \tilde{g} + O(\eta^2) \end{aligned}$$

$$\Downarrow$$

$$\begin{aligned} \tilde{\mathrm{p}} &= \mathrm{p}^{(0)} + \eta \mathrm{p}^{(1)} + O(\eta^2) = w u^{(0)} + \tfrac{1}{2}\eta\, \mathrm{s} f^{(0)} + O(\eta^2) \\ &= w\left(u + O(\epsilon^2)\right) + \tfrac{1}{2}\eta\, \mathrm{s}\left(f + O(\epsilon^2)\right) + O(\eta^2) \end{aligned}$$

$$\Longrightarrow \boxed{\tilde{\mathrm{p}} = w\, u + \tfrac{1}{2}\eta\, \mathrm{s}\, f + O(\epsilon^2) + O(\eta^2)}$$

Asymptotic Consistency versus Finite Difference Consistency

- Two notions of **consistency**:
  - asymptotic consistency of order m:
    $$A_\epsilon u_\epsilon = 0 \ \wedge \ Av = 0 \ \Rightarrow |u_\epsilon - v| = O(\epsilon^m)$$
  - truncation error of order m:
    $$\mathrm{FDOp}_h(v) = O(h^m) \quad \text{if} \quad \mathrm{DiffOp}(v) = 0$$

- **Question:** Does LB provide the exact solution, if it is a 2^{nd} order polynomial?

  Background:
  FD methods based on Taylor series mostly do
  (One of the main debugging tools!)

  Example:
  Poisson Equation in 1D discretized with 3-point stencil:

$$\begin{aligned} D_h^+ D_h^- v &:= \tfrac{1}{2h^2}\left(v(x+h) - 2v(x) + v(x-h) \right) \\ &= \partial_x^2 v + \tfrac{1}{12}\partial_x^4 v h^2 + O(h^4) \end{aligned}$$

A Simple Analytic Example: Poiseuille Flow

- **Problem:**

$$\begin{cases} -\nu\, d_x^2 v(x) = k \\ v(-h) = 0 = v(h) \end{cases} \quad \Rightarrow \quad v(x) = \frac{k}{2\nu}\,(h^2 - x^2)$$

- **Intention:**

  Formulate and solve the associated LB problem
  Compare LB solution $u = \mathrm{p}_0 + \mathrm{p}_1 + \mathrm{p}_2$ with exact solution v

- **Stationary LB Equation:**

$$\begin{aligned} 0 &= \mathrm{p}_0 - \tfrac{n-1}{n}\, u - \tfrac{n-1}{n}\, \epsilon^2\, \tau\, k \\ \epsilon\, \tau\, \partial_x \mathrm{p}_1 &= \mathrm{p}_1 - \tfrac{1}{2n}\, u - \tfrac{1}{2n}\, \epsilon^2\, \tau\, k \\ -\ \epsilon\, \tau\, \partial_x \mathrm{p}_2 &= \mathrm{p}_2 - \tfrac{1}{2n}\, u - \tfrac{1}{2n}\, \epsilon^2\, \tau\, k \end{aligned}$$

Kinetic BC: $\mathrm{p}_2(-h) = -\mathrm{p}_1(-h) \ \wedge \ \mathrm{p}_1(h) = -\mathrm{p}_2(h)$

Try *ansatz* with quadratic polynomials reducing number of free parameter by symmetry arguments:

– u, p_0: symmetric w.r.t. 0
– $\mathrm{p}_1, \mathrm{p}_2$: equal amplitude, shifted in opposite directions by the same distance

Solution of the Example Problem

- **Ansatz** with *non-negative* unknowns: $a\ b\ c\ w\ z\ q\ r$

$$\begin{array}{rcccc} u(x) &=& a\,(w-x)\,(w+x) &=& aw^2 - ax^2 \\ \mathrm{p}_0(x) &=& b\,(z-x)\,(z+x) &=& bz^2 - bx^2 \\ \mathrm{p}_1(x) &=& c\,(q-x)\,(r+x) &=& -cx^2 + c(q-r)x + cqr \\ \mathrm{p}_2(x) &=& c\,(r-x)\,(q+x) &=& -cx^2 + c(r-q)x + cqr \end{array}$$

- **Calculation:**
  - kinetic BC: $r\,q = h^2$
  - LBE for p_0: x^2-term: $b = \frac{n-1}{n}\,a$ constant-term: $a(z^2 - w^2) = \epsilon^2\,\tau\,k\ \ (*)$
  - LBE for p_1: x^2-term: $c = \frac{1}{2n}\,a$ x-term: $2\epsilon\tau = r - q$
    constant-term: $a(w^2 - h^2) = 2a\epsilon^2\tau^2 - \epsilon^2\tau k\ \ (**)$
  - Def. of u: constant-term: $(n-1)z^2 + h^2 = nw^2\ \ (***)$

$$(*) + (**) \quad \Rightarrow \quad z = \sqrt{h^2 + 2\epsilon^2\tau}$$

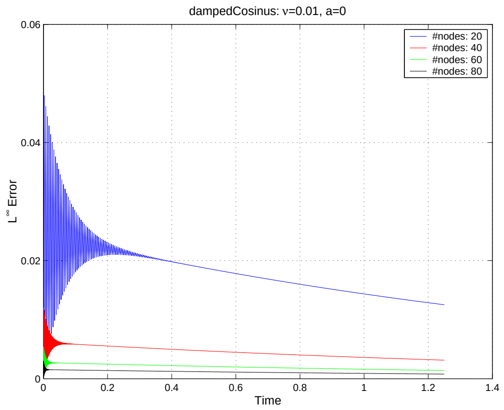
use in $(***)$: $\Rightarrow\ w = \sqrt{h^2 + 2\frac{n-1}{n}\epsilon^2\tau^2}$ utilizing $(*)$: $\Rightarrow\ a = \frac{1}{2}\,\frac{n}{\tau}\,k$

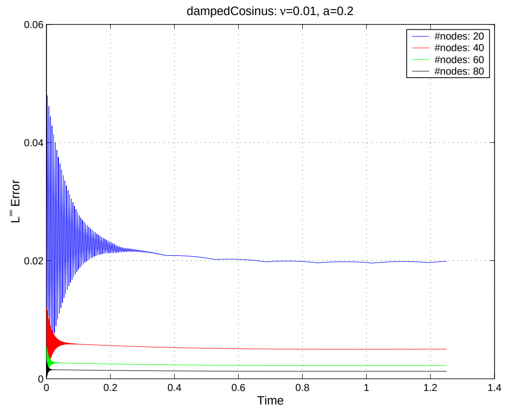
Result: $$u = \frac{k}{2\nu}\left(h^2 - x^2 + 2\,\frac{n-1}{n}\,\epsilon^2\,\tau^2\right) = v + 2\frac{k(n-1)}{2\nu n}\,\epsilon^2\,\tau^2$$

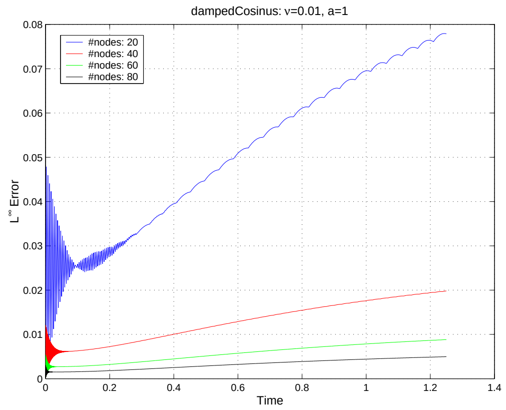
Convergence Tests: D1P2 Model $\nu = 0.01$

Configuration: $\mathbb{T}^1 \cong [0,1]$ with periodic BC — Damped Travelling Cosinus

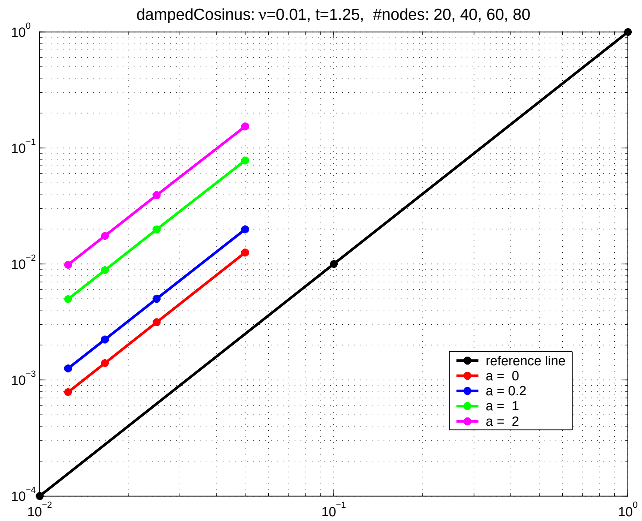
$a \in \{0, 0.2, 1, (2)\}$ #(Grid Nodes) $\in \{20, 40, 60, 80\}$ — uniform grid





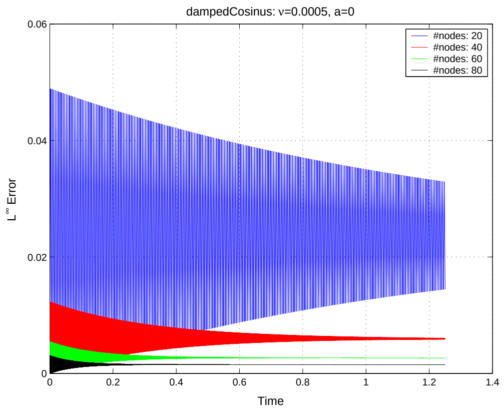


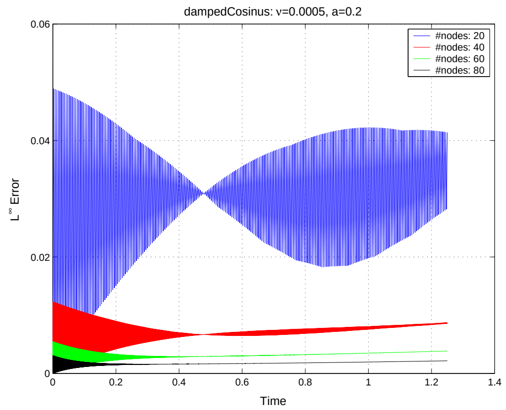
- Logarithmic convergence diagram for final iteration
- Predicted convergence order of 2 clearly visible
- Increase of error for faster advection

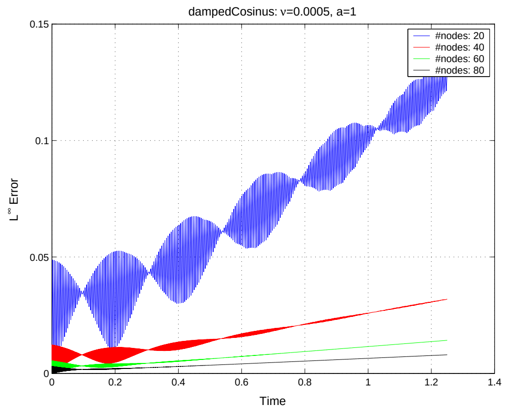


Convergence Tests: D2P1 Model $\nu = 0.0005$

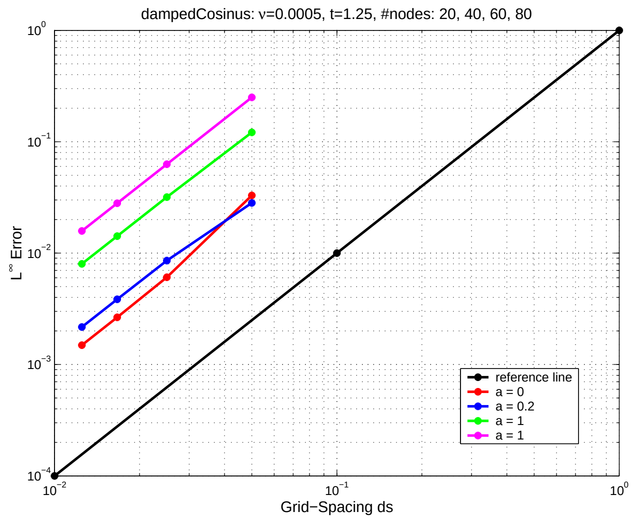
Configuration: $\mathbb{T}^1 \cong [0,1]$ with periodic BC — Damped Travelling Cosinus
$a \in \{0, 0.2, 1, (2)\}$ $\#$(Grid Nodes) $\in \{20, 40, 60, 80\}$ — uniform grid







- Small diffusivity ν, low grid resolution $\Rightarrow$ highly oscillating *initial layer*
- Slight deviation from predicted convergence order in logarithmic diagram (red/blue line) probably due to strong initial layer on coarsest grid



Open Problems

- **Asymptotics:**

  Till now: Study of the *regular asymptotic behavior* of LB system

  $\Rightarrow$ How can the singular behavior be resolved, e.g. *initial layers* ?

- **Strict Convergence Results:**

  Till now: Attempt to prove convergence of the continous D1P2.model with Fourier series $\Rightarrow$ More general techniques, energy estimates ?

- Analysis of boundary and coupling conditions for D2P9-model leads to contradictive equations in the 2^{nd} order

- Classic discrete LB schemes $\leftrightarrows$ Discretizations consistent to the continous LB equations (Finite Volume Methods)

Appendix

- *DAR*-equilibrium-matrix defined by the relation $\mathbf{q} = Q_\epsilon \mathbf{p}$:

$$Q_\epsilon = \begin{pmatrix} \frac{n-1}{n} - \frac{n-1}{n}\epsilon^2 \tau c & 0 & 0 \\ 0 & \frac{1}{2n} - \frac{1}{2}\epsilon \, a - \frac{1}{2n}\epsilon^2 \tau c & 0 \\ 0 & 0 & \frac{1}{2n} + \frac{1}{2}\epsilon \, a - \frac{1}{2n}\epsilon^2 \tau c \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

- Moment transformation matrix defined by the relation $\mathbf{m} = M_\epsilon \mathbf{p}$:

$$M_\epsilon = \begin{pmatrix} 1 & 1 & 1 \\ 0 & -\frac{1}{\epsilon} & \frac{1}{\epsilon} \\ -\frac{1}{n\epsilon^2} & \frac{n-1}{n\epsilon^2} & \frac{n-1}{n\epsilon^2} \end{pmatrix} \qquad M_\epsilon^{-1} = \begin{pmatrix} \frac{n-1}{n} & 0 & -\epsilon^2 \\ \frac{1}{2n} & -\frac{1}{2}\epsilon & \frac{1}{2}\epsilon^2 \\ \frac{1}{2n} & \frac{1}{2}\epsilon & \frac{1}{2}\epsilon^2 \end{pmatrix}$$

- Transformed velocity-matrix and transformed equilibrium-matrix:

$$M_\epsilon S M_\epsilon^{-1} = \begin{pmatrix} 0 & \epsilon & 0 \\ \frac{1}{\epsilon n} & 0 & \epsilon \\ 0 & \frac{n-1}{\epsilon n} & 0 \end{pmatrix} \qquad M_\epsilon Q_\epsilon M_\epsilon^{-1} = \begin{pmatrix} 1 - \epsilon^2 \tau c & 0 & 0 \\ a & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$