Asymptotic analysis of lattice Boltzmann methods

Stability and multiscale expansions

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Introduction

Problem:

- consistency analysis → relatively simple
- stability analysis → complicated, tricky

Background-question: Can formal asymptotic expansions help to formulate hypotheses about the stability behavior of a numerical scheme?

Here: Case study of a model problem.

Additional motivation: complete understanding of an exemplary lattice Boltzmann algorithm with all inherent features like:

- convergence, time-scales, initial layers, boundary layers, stability, consistency, spectrum of evolution operator, etc.

Outline:

1st part: Stability analysis based on diagonalization of evolution matrix → attempt to be mathematically rigorous

2nd part: (involving more intuition) presents twoscale expansions as possible & desirable tool to analyze stability → comparison and short discussion with stability analysis
Introduction

Velocity set: $s_1 = -1 \quad s_2 = 1$

Population functions: $F_1, F_2$

Update rule: $F_k(t + \Delta t, x + s_k \Delta x) = F_k(t, x) + \left[ J F(t, x) \right]_k$

BGK collision operator: $J = \omega (E_q - I)$

Equilibrium: $E_q F = E(U)$

Mass moment: $U = F_1 + F_2$

### Scaling

**hyperbolic**

$\Delta x = h, \Delta t = h$

$E_k(U) = \frac{1}{2} (1 + s_k a) U$

$\partial_t u + a \partial_x u = 0$

**parabolic**

$\Delta x = h, \Delta t = h^2$

$E_k(U) = \frac{1}{2} (1 + hs_k a) U$

$\partial_t u + a \partial_x u - \left( \frac{1}{\omega} - \frac{1}{2} \right) \partial_x^2 u = 0$

Abbreviations: $\forall$ means 'for All', $\exists$ means 'it Exists'.

The model algorithm

<table>
<thead>
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**Scaling**

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Stability

Matrix formulation of the algorithm

Iteration = evolution step
• collision (nodal operation)
• transport (left/right shift)

1) \( \tilde{F}(t,x) = (I + J)F(t,x) \)

\[
\begin{bmatrix}
\tilde{F}_1(t,x) \\
\tilde{F}_2(t,x)
\end{bmatrix} = \begin{pmatrix}
\alpha & \beta \\
\gamma & \delta
\end{pmatrix} \begin{bmatrix}
F_1(t,x) \\
F_2(t,x)
\end{bmatrix}
\]

\[
C = \begin{bmatrix}
\alpha & \ldots & \beta \\
\ldots & \alpha & \ldots & \beta \\
\ldots & \ldots & \alpha & \ldots & \beta \\
\gamma & \ldots & \delta & \ldots \\
\ldots & \gamma & \ldots & \delta \\
\ldots & \ldots & \gamma & \ldots & \delta
\end{bmatrix}
\]

2) \( F_k(t + h,x) = \tilde{F}_k(t,x - s_k h) \)

\( \tilde{F}_1 \) hops to the left as \( s_1 = -1 \)
\( \tilde{F}_2 \) hops to the right as \( s_2 = 1 \)

\[
T = \begin{bmatrix}
1 & & & & \\
& 1 & & & \\
& & 1 & & \\
& & & 1 & \\
& & & & 1
\end{bmatrix}
\]
Stability

Characteristic polynomial of the evolution matrix

Block-structure of evolution matrix:

\[
E := \begin{pmatrix} L & 0 \\ 0 & R \end{pmatrix} \begin{pmatrix} \alpha I & \beta I \\ \gamma I & \delta I \end{pmatrix}
\]

transport collision

Spectrum of shift matrices \( L, R \) (transport matrix): unit roots \( w, w^2, ..., w^N \)

\[ w := e^{\frac{2\pi i}{N}} \]

Eigenvectors \( \implies \) discrete Fourier transform yields diagonalized transport matrix, which respects special structure of collision matrix.

\( \implies \) Characteristic polynomial decomposes into product of quadratic polynomials:

\[
\lambda \mapsto \prod_{m=0}^{N-1} \left[ (\alpha w^m - \lambda)(\delta w^{-m} - \lambda) - \beta \gamma \right]
\]

\[
\chi(\lambda; \frac{2\pi m}{N})
\]

\[
\chi(\lambda; \varphi) := \lambda^2 + [(\omega - 2)\cos \varphi + i \omega a \sin \varphi] \lambda + (1 - \omega)
\]
Stability

Spectrum of the evolution matrix & spectral portraits

Eigenvalues of evolution operator associated to arbitrary grid are contained in:

\[ \mathcal{S}(\omega, a) := \left\{ \lambda \in \mathbb{C} \mid \exists \phi \in [0, 2\pi) \text{ with } \chi(\lambda; \phi) = 0 \right\} \]

\[ \text{spec}(E) \subset \mathcal{S}(\omega, a) \quad \text{samples spectral limit set uniformly w.r.t. } \phi \]

\[ \omega = 0.6 \quad \text{under-relaxation} \quad 0 < \omega < 1 \]

\[ \omega = 1.6 \quad \text{over-relaxation} \quad 1 < \omega < 2 \]
Observation: \(\forall \omega \in [0,2]: \mathcal{S}(\omega,a) \subseteq \overline{D_1}(0) \iff |a| \leq 1\)

\(\forall a \in [-1,1]: \mathcal{S}(\omega,a) \subseteq \overline{D_1}(0) \iff \omega \in [0,2]\) \quad \text{stable}

\(\mathcal{S}(\omega,a) \not\subseteq \overline{D_1}(0) \iff \omega \notin [0,2] \text{ or } a \notin [-1,1]\) \quad \text{unstable}
Stability

CFL condition:

\[
|a| \leq \frac{\Delta x}{\Delta t} = \begin{cases} 
\frac{\Delta x}{h} = 1 & \text{hyperbolic scaling} \\
\frac{\Delta x}{h^2} = \frac{1}{h} & \text{parabolic scaling}
\end{cases} \quad \Leftrightarrow \quad |ah| \leq 1
\]

**Theorem:** The lattice-Boltzmann algorithm (as defined previously) respects the CFL-condition, i.e. \( \rho(E) \leq 1 \) for \( 0 \leq \omega \leq 2, \ -1 \leq a \leq 1 \).

**Sketch of the proof:** Estimate the zeros of \( \chi(\lambda;\varphi) \) depending on \( a, \omega \)

\[
\lambda(\varphi) = -\frac{1}{2} \left[ (\omega - 2) \cos \varphi + i \omega a \sin \varphi \right] \pm \sqrt{\frac{1}{4} \left[ (\omega - 2) \cos \varphi + i \omega a \sin \varphi \right]^2 - (1 - \omega)}
\]

Better idea: consider first special cases like \( \omega = 1 \) or \( \varphi = 0, \ \varphi = \pi \)

Discuss then the general case using the *theorem of Rouché* (\( \rightarrow \) complex analysis).

**N.B.:** The CFL-condition does not hold if the *periodic* boundary conditions are replaced by *bounce-back* like boundary conditions.
Stability

Norm stability

Differential equation \[ Df = r \]  
FD-discretization \[ D_h F_h = R_h \]

The numeric scheme is \textbf{stable} w.r.t. \( \| \cdot \|_h \) if:

\[ \exists K > 0 : \forall \text{ grids} : \| D_h^{-1} \|_h < K \]

Especially this means for an \textit{explicit} scheme like the \textit{lattice-Boltzmann algorithm}:

\[ \exists K > 0 : \forall \text{ grids} : \forall n \in \mathbb{N}_0, n\Delta t \leq T_{\text{max}} : \| E^n \| < K \]

\textbf{Observation:} The condition \( \text{spec}(E) \subseteq \overline{D_1}(0) \Leftrightarrow \rho(E) \leq 1 \) is only necessary for stability but not sufficient. However \( E \) is diagonalizable (no nontrivial Jordan blocks):

\[ \Rightarrow \forall \text{ grids} : \exists K_h > 0 : \forall n \in \mathbb{N} : \| E^n \|_h < K_h \]
**Fact:** \[ \|A\|_2^2 = \sup_{\|x\|_2 = 1} \|Ax\|_2^2 = \sup_{\|x\|_2 = 1} \langle Ax, Ax \rangle = \sup_{\|x\|_2 = 1} \langle AA^*x, x \rangle = \rho(AA^*) \]

\[ \Rightarrow \text{ invariance w.r.t. unitary transformations (e.g. discrete Fourier trafo)} \]

**Theorem:** The evolution matrix of the LB algorithm (previously defined) satisfies the stability condition w.r.t. the L2-norm, if \( 0 \leq \omega \leq 2, \ -1 \leq a \leq 1 \).

**Proof:** Discrete Fourier trafo (+permutation of indices) of evolution matrix \( \to \) block-diagonal matrix with 2x2 blocks:

\[
M(\varphi) := \begin{pmatrix} \alpha e^{i\varphi} & \beta e^{i\varphi} \\ \gamma e^{-i\varphi} & \delta e^{-i\varphi} \end{pmatrix} \quad \varphi \in \frac{2\pi}{N} \{0, 1, \ldots, N - 1\} \quad \Rightarrow \quad \|E^n\|_2 \leq \max_{\varphi \in [0, 2\pi]} \|M^n(\varphi)\|_2
\]

Define family of continuous functions: \( f_n : [0, 2\pi] \to \mathbb{R}, \quad f_n(\varphi) := \|M^n(\varphi)\|_2, \quad n \in \mathbb{N} \)

Each \( M(\varphi) \) is diagonalizable and \( \rho(M(\varphi)) \leq 1 \) \( \Rightarrow \exists C_\varphi > 0 : \sup_{n \in \mathbb{N}} \|M^n(\varphi)\|_2 < C_\varphi \)

\( \Rightarrow (f_n)_{n \in \mathbb{N}} \) pointwise bounded. *Principle of uniform boundedness:* \( (f_n)_{n \in \mathbb{N}} \) locally bounded

Due to compactness of \([0, 2\pi] : (f_n)_{n \in \mathbb{N}} \) globally bounded. \( \blacksquare \)

**Short course (L2):** All expansions hold in the 2-norm at least.

**Remark:** *Diffusive scaling* \( \to \) stability result in maximum-norm (uses positivity of evolution matrix)
Motivation: linear $\leftrightarrow$ quadratic time scale

Observation: advection $\rightarrow$ linear time scale

deformation (flattening) $\rightarrow$ quadratic time scale

Linear time: $t_1(G_j) = n_j h_j$

Quadratic time: $t_2(G_j) = n_j h_j^2$

Coarse grid: 30 nodes \( h_1 = \frac{1}{30} \)

Fine grid: 60 nodes \( h_2 = \frac{1}{60} \) \quad \{ \omega = 1.7, \ a = 0.5 \)
Motivation: linear ↔ cubic time scale

Observation: advection → linear time scale
distortion (undulations) → cubic time scale

Coarse grid: 60 nodes
Fine grid: 120 nodes

\[
\begin{align*}
\omega &= 2.0, \quad a = 0.5 \\
\end{align*}
\]

linear time: \( t_1(G_j) = n_j h_j \)
cubic time: \( t_3(G_j) = n_j h_j^3 \)

Coarse grid: 60 nodes \( h_1 = \frac{1}{60} \)
Fine grid: 120 nodes \( h_2 = \frac{1}{120} \)
Multiscale expansion

Regular versus twoscale expansion – the idea

Approximate \textit{grid function} of LB-algorithm by \textit{regular expansion}:

\[
F(t, x) = f^{[\alpha]}(t, x) = f^{(0)}(t, x) + h f^{(1)}(t, x) + \ldots + h^\alpha f^{(\alpha)}(t, x)
\]

\(\begin{aligned}
&\text{grid function} \\
&x = x_i = ih \\
&t = t_n = nh
\end{aligned}\)

\(\begin{aligned}
&\text{prediction function} \\
&0'\text{th asymptotic order function} \\
&1'\text{st asymptotic order function}
\end{aligned}\)

Requirement

\[
f^{[\alpha]}_k(t + h, x + s_k h) = f^{[\alpha]}(t, x) + \left[J f^{[\alpha]}(t, x)\right]_k + O(h^{\alpha+1})
\]

apply Taylor expansion

residual

determines order functions uniquely \(\rightarrow\) \textit{consistency analysis}, e.g. \(u^{(0)} = f_1^{(0)} + f_2^{(0)}\)

must satisfy: \(\partial_t u^{(0)} + a\partial_x u^{(0)} = 0\)

\(\rightarrow\) details: short course L2 (M. Junk)

\textbf{Shortcomings:} appearence of secular terms \(\rightarrow\) regular expansion only valid for time intervals of length \(O(1)\) \(\rightarrow\) not capturing long time behavior over \(O(\frac{1}{h})\) intervals.

\textbf{Twoscale ansatz:} 2 time variables to take into account observed effects.

\[
F(t, x) = f^{[\alpha]}(t, h t, x) = f^{(0)}(t, h t, x) + h f^{(1)}(t, h t, x) + \ldots + h^\alpha f^{(\alpha)}(t, h t, x)
\]

\[
F(t, x) = f^{[\alpha]}(t, h^2 t, x) = f^{(0)}(t, h^2 t, x) + h f^{(1)}(t, h^2 t, x) + \ldots + h^\alpha f^{(\alpha)}(t, h^2 t, x)
\]
Why do we expect a multiscale expansion to tell something about stability?

Instabilities may become noticeable near the boundary of the stability domain as background phenomena occurring in slower time scales.

1 is always eigenvalue of evolution operator independently of \( \omega, a \).

associated eigenvector = constant vector (= projection of smooth function onto grid)

Eigenvalues around 1 can be expanded w.r.t. \( h \)

\[
|\lambda| = 1 + h^\ell c_\ell + h^{\ell+1} c_{\ell+1} + \ldots, \quad c_\ell \neq 0
\]

Indicator for instability: \( 1 < < |\lambda|^n \approx (1 + h^\ell c_\ell)^n, \quad h \sim \frac{1}{N} \)

\( \Rightarrow \quad n \approx N^\ell \quad \text{recall} \quad N \gg 1 \quad \Rightarrow \quad \left(1 + \frac{c_\ell}{N^\ell}\right)^{N^\ell} \approx \exp(c_\ell) \)

Impact of instability on eigenvalues around 1 becomes only visible in a slow time scale if \( \ell > 1 \)
Multiscale expansion

The outcome – evolution equations

**Procedure** to derive determining equations for order functions similar to regular case.

**Strategy:** minimize the residual $\leftrightarrow$ maximize order of residual $\rightarrow$ details: short course L2 (M. Junk)

**Result** for the leading (0'th) order:

i) Evolution in the *fast time* variable described by *advection equation*:

$$\partial_{t_1} u^{(0)}(t_1, t_2, x) + a \partial_x u^{(0)}(t_1, t_2, x) = 0$$

ii) Evolution in the *slow time* variable:

**General case** $\omega \neq 2$: *diffusion equation*

$$\partial_{t_2} u^{(0)}(t_1, t_2, x) - \mu \partial_x^2 u^{(0)}(t_1, t_2, x) = 0$$

**Special case** $\omega = 2$: *dispersive equation*

$$\partial_{t_2} u^{(0)}(t_1, t_3, x) - \tilde{\lambda} \partial_x^3 u^{(0)}(t_1, t_3, x) = 0$$

Coefficients:

- $\mu = \left(\frac{1}{\omega} - \frac{1}{2}\right)(1-a^2)$
- $\tilde{\lambda} = -\frac{1}{6}a(1-a^2)$

**What do we learn?**

1) possibility to get a precise *quantitative* prediction of grid function.

2) *quantitative* understanding of the observed effects $\rightarrow$ see later

Typical effect of PDE evolution operator on initial condition: damping, flattening $\rightarrow$ undulating, oscillating

**Implications** concerning *stability*: $\mu < 0 \Rightarrow$ *backward diffusion equation*

- ill-posed IVP $\rightarrow$ instabilities expected $\leftrightarrow$ stable behavior for $\mu \geq 0$

- dispersive equation indifferent w.r.t. sign of $\tilde{\lambda}$ $\Rightarrow$ no hypothesis!
Deceptive cases:

1) violation of CFL condition with unstable explicit relaxation: \( \omega = 2.05, \ a = 1.01 \)

2) violation of CFL condition with limit value for \( \omega \)
\( \omega = 2.00, \ a = 1.05 \)

Hypothesis about stability based on multiscale expansion should fail if:

1) Near 1, only eigenvalues pertaining to 'non-smooth' eigenvectors move out of closed unit disk as \( \omega, a \) leave domain of stability.

2) Eigenvalues do not cross boundary of unit disk inside vicinity of 1.
Multiscale expansion & Conclusion

**Test: approximation by twoscale ansatz**

Another aspect of two scale expansion:

**Prediction** of the (numeric) mass moment:

\[ F_1(nh, jh) + F_2(nh, jh) = U(nh, jh) \iff u^{(0)}(nh, nh^2, jh) \]

**Nasty example:** arbitrarily smooth but not analytic (\( n \)th derivative cannot be bounded by \( C^n \))

**Observation:** good approximation over time intervals of increasing length:

\[ O\left(\frac{1}{h}\right) = O(N) \quad \text{and even} \quad O\left(\frac{1}{h^2}\right) = O(N^2) \]

<table>
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<th>time interval</th>
<th>error</th>
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<td>( O(1) )</td>
<td>( O(h^4) )</td>
</tr>
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Conclusion

With exception of the corners the boundary of the actual stability domain is accurately described. Corners seem like „magic doors“ to falsely pretended stability domains.

High order prediction of mass moment.

Some instabilities cannot be captured due to implicit smoothness assumption of prediction function (e.g. Taylor expansion).

Final judgement needs more case studies.
Above all: →clarify ideas & notions being still vague e.g. classification of instabilities → topic of future work
improve consistency by systematic analysis & test stability experimentally

- guidance to modify bad scheme:
  try to shift break down of regular expansion into higher order

- good scheme: behaves regularly ⇒ well describable by regular expansion