Asymptotic analysis of lattice Boltzmann methods

Stability and multiscale expansions

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Problem:

- **consistency analysis** $\longrightarrow$ **relatively simple**
- **stability analysis** $\longrightarrow$ **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.

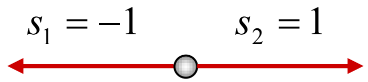
Additional motivation: *complete understanding of an exemplary lattice Boltzmann algorithm with all inherent features like:*

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
$\rightarrow$ attempt to be mathematically rigorous

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

Velocity set:



Population functions: $\mathsf{F}_1, \mathsf{F}_2$

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

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

Equilibrium: $E_q \mathsf{F} = \mathrm{E}(U)$ Mass moment: $U = \mathsf{F}_1 + \mathsf{F}_2$

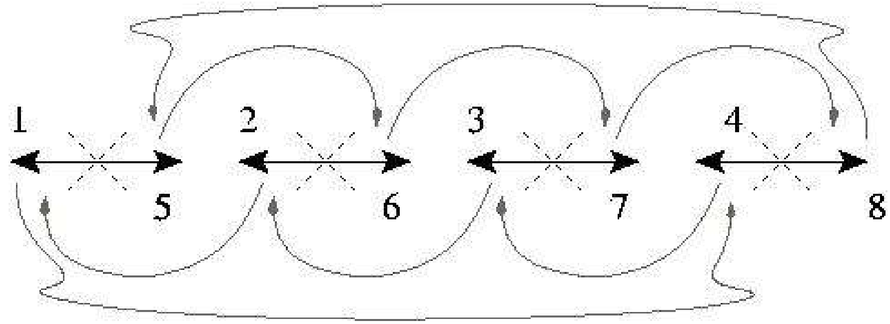
Scaling

hyperbolic	*parabolic*
$\Delta x = h,\ \Delta t = h$	$\Delta x = h,\ \Delta t = h^2$
$\mathsf{E}_k(U) = \frac{1}{2}(1 + s_k a)U$	$\mathsf{E}_k(U) = \frac{1}{2}(1 + h s_k a)U$
$\partial_t u + a \partial_x u = 0$	$\partial_t u + a\partial_x u - (\frac{1}{\omega} - \frac{1}{2})\partial_x^2 u = 0$

Abbreviations: $\forall$ means *‚for **A**ll‘*, $\exists$ means *‚it **E**xists‘.*

Iteration = evolution step

- collision (nodal operation)
- transport (left/right shift)



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

$$\begin{pmatrix} \tilde{\mathsf{F}}_1(t,x) \\ \tilde{\mathsf{F}}_2(t,x) \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \begin{pmatrix} \mathsf{F}_1(t,x) \\ \mathsf{F}_2(t,x) \end{pmatrix}$$

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

$\tilde{\mathsf{F}}_1$ hops to the left as $s_1 = -1$

$\tilde{\mathsf{F}}_2$ hops to the right as $s_2 = 1$

$$\boldsymbol{C} = \left(\begin{array}{cccc|cccc} \alpha & . & . & . & \beta & . & . & . \\ . & \alpha & . & . & . & \beta & . & . \\ . & . & \alpha & . & . & . & \beta & . \\ . & . & . & \alpha & . & . & . & \beta \\ \hline \gamma & . & . & . & \delta & . & . & . \\ . & \gamma & . & . & . & \delta & . & . \\ . & . & \gamma & . & . & . & \delta & . \\ . & . & . & \gamma & . & . & . & \delta \end{array}\right)$$

$$\boldsymbol{T} = \left(\begin{array}{cccc|cccc} . & 1 & . & . & . & . & . & . \\ . & . & 1 & . & . & . & . & . \\ . & . & . & 1 & . & . & . & . \\ 1 & . & . & . & . & . & . & . \\ \hline . & . & . & . & . & . & . & 1 \\ . & . & . & . & 1 & . & . & . \\ . & . & . & . & . & 1 & . & . \\ . & . & . & . & . & . & 1 & . \end{array}\right)$$

Block-structure of evolution matrix:

$$E := \underbrace{\begin{pmatrix} L & 0 \\ 0 & R \end{pmatrix}}_{\text{transport}} \underbrace{\begin{pmatrix} \alpha I & \beta I \\ \gamma I & \delta I \end{pmatrix}}_{\text{collision}}$$

Spectrum of shift matrices L, R (transport matrix): *unit roots* $w, w^2, \ldots, w^N \quad w := \mathrm{e}^{\frac{2\pi \mathrm{i}}{N}}$

Eigenvectors $\Longrightarrow$ *discrete Fourier transform* yields diagonalized transport matrix,

which respects special structure of collision matrix.

$\Longrightarrow$ Characteristic polynomial decomposes into product of quadratic polynomials:.

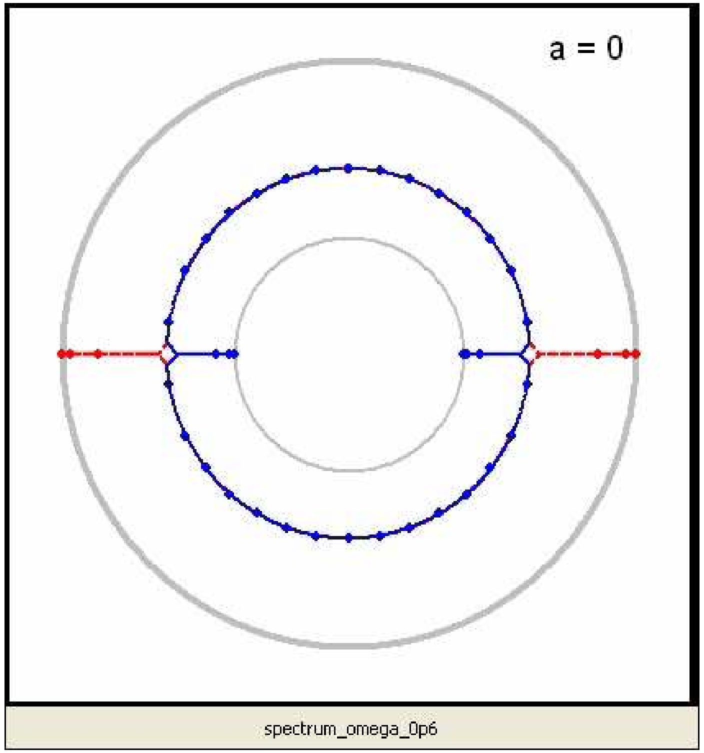
$$\lambda \mapsto \prod_{m=0}^{N-1} \Big[\underbrace{(\alpha w^m - \lambda)(\delta \overline{w}^m - \lambda) - \beta\gamma}_{\chi(\lambda; \frac{2\pi m}{N})} \Big]$$

$$\chi(\lambda;\varphi) := \lambda^2 + [(\omega - 2)\cos\varphi + \mathrm{i}\,\omega\, a \sin\varphi]\lambda + (1-\omega)$$

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

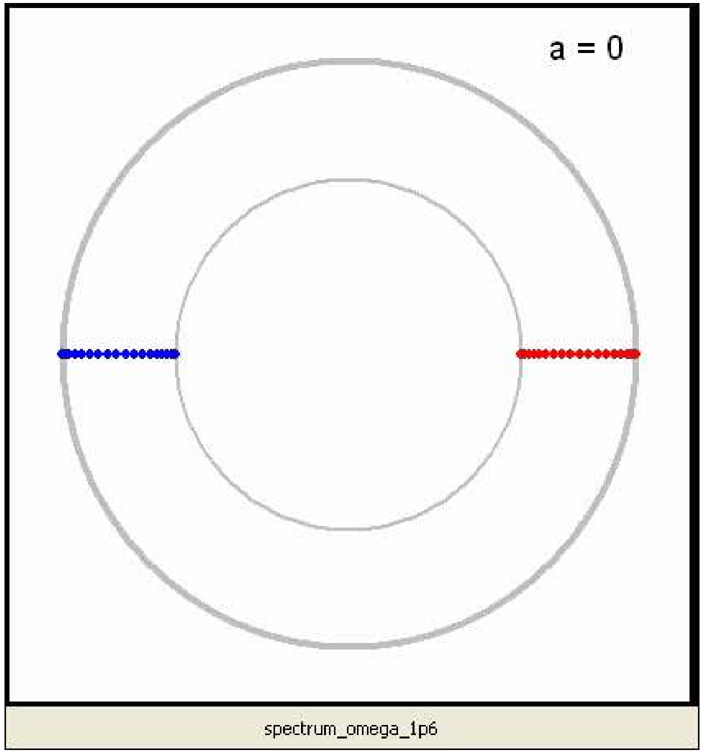
$$\mathscr{S}(\omega,a) := \left\{\lambda \in \mathbb{C} \,\middle|\, \exists\varphi \in [0,2\pi) \text{ with } \chi(\lambda;\varphi) = 0\right\}$$

$\mathrm{spec}\,(E) \subset \mathscr{S}\,(\omega, a)$ samples *spectral limit set* uniformly w.r.t. φ



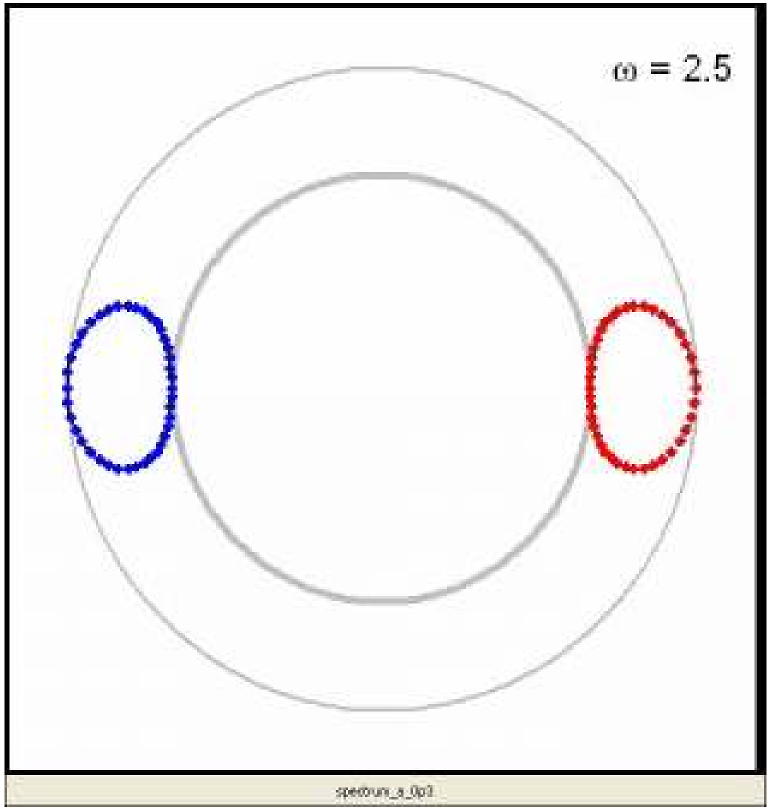
$\omega = 0.6$

under-relaxation $0 < \omega < 1$

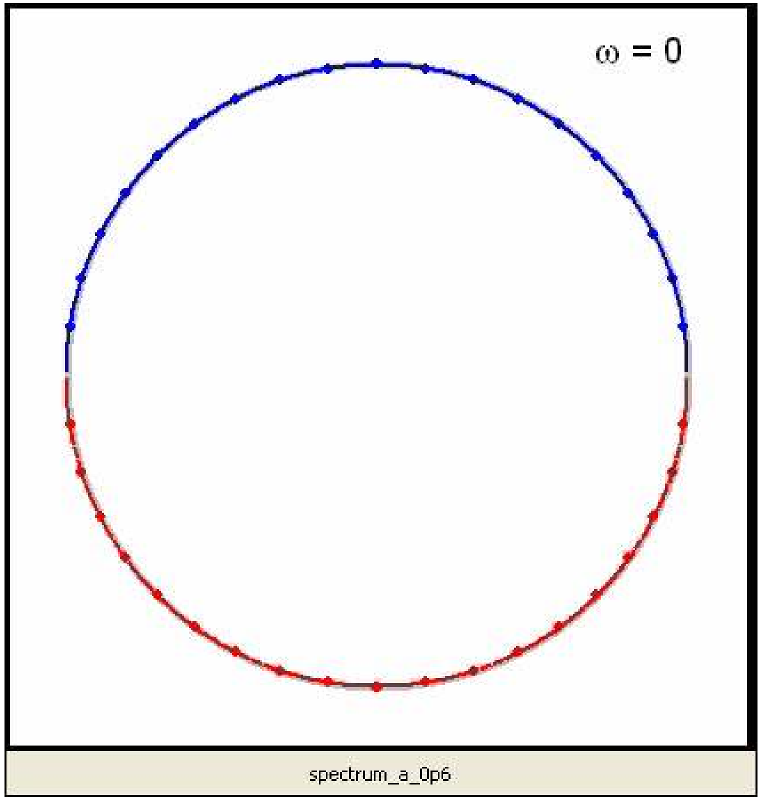


$\omega = 1.6$

over-relaxation $1 < \omega < 2$



$a = 0.3$



$a = 0.6$

Observation: $\forall\, \omega \in [0,2]:\ \mathscr{S}(\omega,a) \subset \overline{D}_1(0) \Leftrightarrow |a| \leq 1$

$\forall\, a \in [-1,1]:\ \mathscr{S}(\omega,a) \subset \overline{D}_1(0) \Leftrightarrow \omega \in [0,2]$ } **stable**

$\mathscr{S}(\omega,a) \not\subset \overline{D}_1(0) \Leftrightarrow \omega \notin [0,2]$ or $a \notin [-1,1]$ } **unstable**

CFL condition: $|a| \leq \dfrac{\Delta x}{\Delta t} = \begin{cases} \frac{h}{h} = 1 & \text{hyperbolic scaling} \\ \frac{h}{h^2} = \frac{1}{h} & \text{parabolic scaling} \quad \Leftrightarrow \quad |ah| \leq 1 \end{cases}$

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, ω

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

Better idea: consider first special cases like $\omega = 1$ or $\varphi = 0, \; \varphi = \pi.$

Discuss then the general case using the *theorem of Rouché* (→ complex analysis).■

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

Differential equation $Df = r$

FD-discretization $D_h F_h = R_h$

The numeric scheme is **stable** w.r.t. $\|\cdot\|_h$ if:

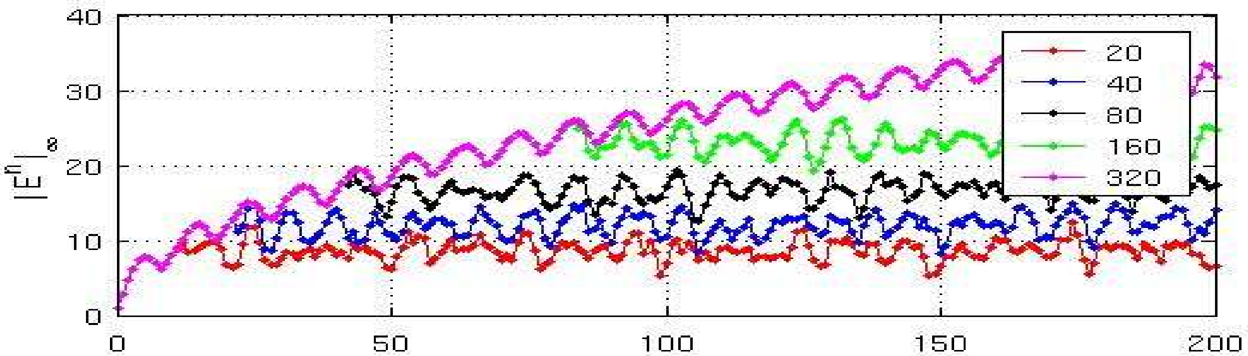
$$\exists K > 0 : \forall \text{grids} : \quad \|D_h^{-1}\|_h < K$$

Especially this means for an *explicit* scheme like the *lattice-Boltzmann algorithm*:

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

Observation: The condition $\text{spec}(E) \subset \overline{D}_1(0) \Leftrightarrow \rho(E) \le 1$ is only necessary for stability but not sufficient. However E is diagonalizable (no nontrivial Jordan blocks):

$$\Rightarrow \ \forall \text{grids} : \exists K_h > 0 : \forall n \in \mathbb{N} : \quad \|E^n\|_h < K_h$$



Fact: $\|A\|_2^2 = \sup_{\|x\|_2=1} \|Ax\|_2^2 = \sup_{\|x\|_2=1} \langle Ax, Ax \rangle = \sup_{\|x\|_2=1} \langle AA^* x, x \rangle = \rho(AA^*)$

$\Longrightarrow$ invariance w.r.t. unitary transformations (e.g. discreteFourier trafo)

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

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

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

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

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

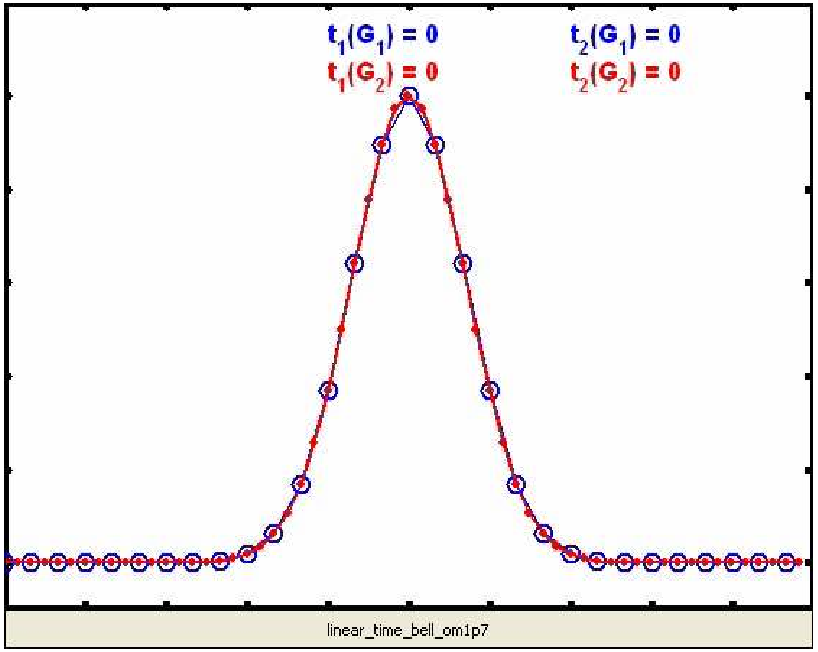
$\Rightarrow$ $(f_n)_{n\in\mathbb{N}}$ *pointwise* bounded. *Principle of uniform boundedness:* $(f_n)_{n\in\mathbb{N}}$ *locally* bounded

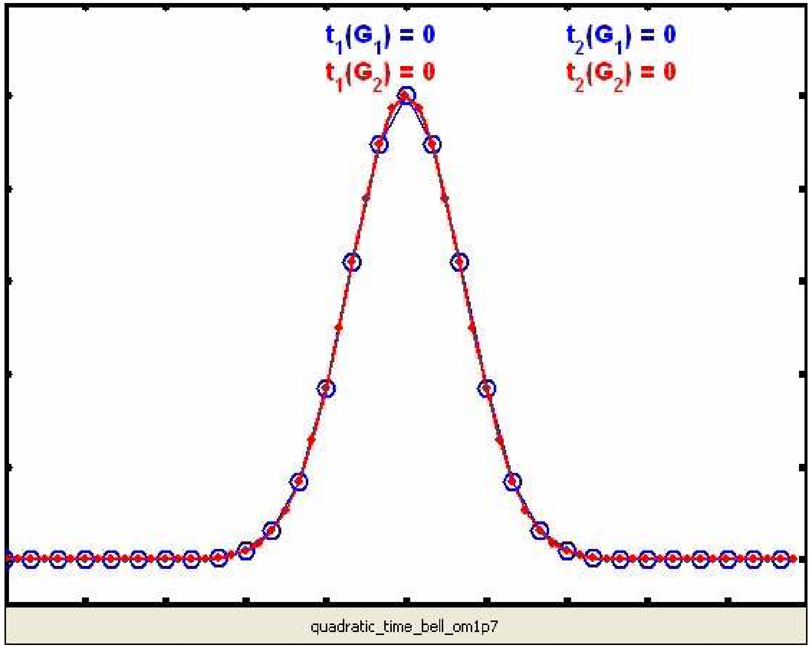
Due to compactness of $[0,2\pi]$: $(f_n)_{n\in\mathbb{N}}$ *globally* bounded. ■

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

Remark: *Diffusive scaling* $\rightarrow$ stability result in *maximum-norm (uses positivity of evolution matrix)*

Motivation: linear ↔ quadratic time scale





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

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

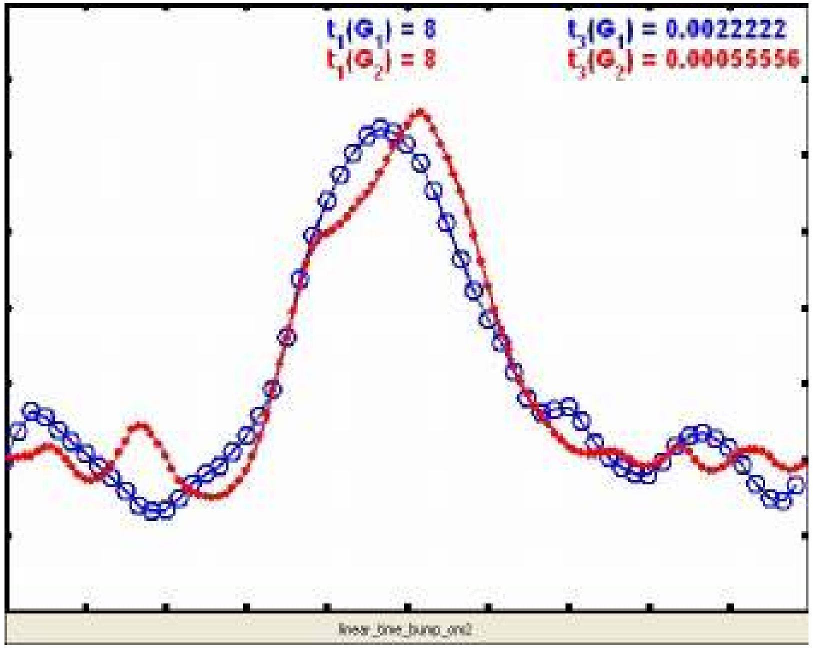
Coarse grid: 30 nodes $h_1 = \frac{1}{30}$

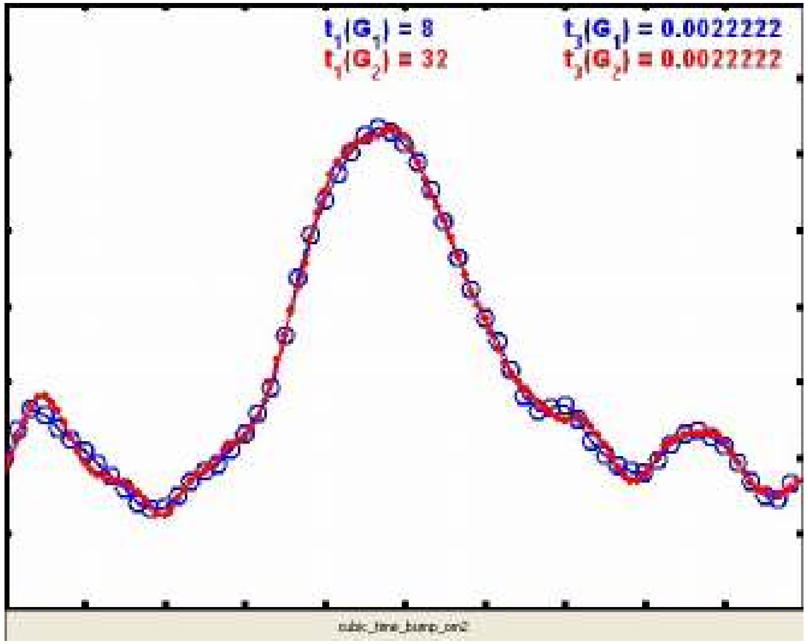
Fine grid: 60 nodes $h_2 = \frac{1}{60}$

$\omega = 1.7, \quad a = 0.5$

Observation: advection → *linear* time scale
deformation (flattening) → *quadratic* time scale

Motivation: linear↔cubic time scale





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 $h_2 = \frac{1}{120}$

$\omega = 2.0, \quad a = 0.5$

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

Approximate *grid function* of LB-algorithm by *regular expansion*:

$$\underbrace{\mathsf{F}(t,x)}_{\text{grid function}} = \underbrace{\mathsf{f}^{[\alpha]}(t,x)}_{\text{prediction function}} = \underbrace{\mathsf{f}^{(0)}(t,x)}_{\text{0'th asymptotic order function}} + h\,\underbrace{\mathsf{f}^{(1)}(t,x)}_{\text{1'st asymptotic order function}} + \ldots + h^{\alpha}\,\mathsf{f}^{(\alpha)}(t,x)$$

grid function: $x = x_i = ih$, $t = t_n = nh$

!

Requirement $$\underbrace{\mathsf{f}_k^{[\alpha]}(t+h, x+s_k h)}_{\text{apply Taylor expansion}} = \mathsf{f}_k^{[\alpha]}(t,x) + \left[J\,\mathsf{f}^{[\alpha]}(t,x)\right]_k + \underbrace{O(h^{\alpha+1})}_{\text{residual}}$$

determines order functions uniquely → *consistency analysis*, e.g. $u^{(0)} = \mathsf{f}_1^{(0)} + \mathsf{f}_2^{(0)}$

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

→ details: short course L2 (M. Junk)

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

Twoscale ansatz: 2 time variables to take into account observed effects.

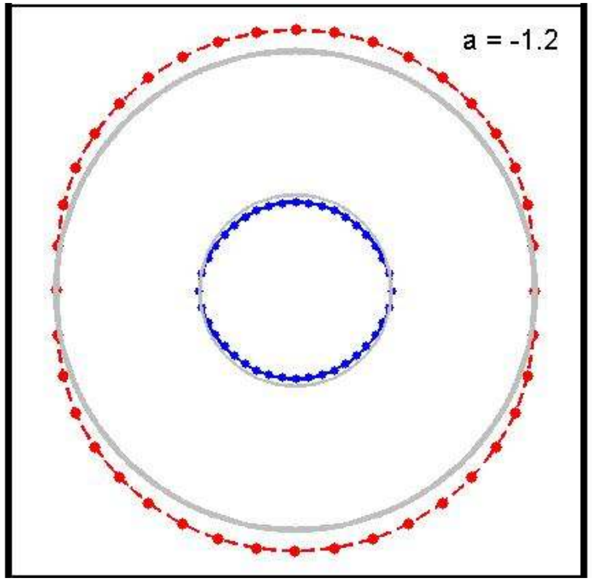
$$\mathsf{F}(t,x) = \mathsf{f}^{[\alpha]}(t,ht,x) = \mathsf{f}^{(0)}(t,ht,x) + h\,\mathsf{f}^{(1)}(t,ht,x) + \ldots + h^{\alpha}\,\mathsf{f}^{(\alpha)}(t,ht,x)$$

$$\mathsf{F}(t,x) = \mathsf{f}^{[\alpha]}(t,h^2t,x) = \mathsf{f}^{(0)}(t,h^2t,x) + h\,\mathsf{f}^{(1)}(t,h^2t,x) + \ldots + h^{\alpha}\,\mathsf{f}^{(\alpha)}(t,h^2t,x)$$

- 2nd time variable – formally independent but coupled if compared with grid function.
- Order functions are *not uniquely* determined → further assumptions & restrictions.
- *Easy to compute* if regular expansion is available!

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 occuring in slower time scales.

1 is always eigenvalue of evolution operator independently of ω, a.
associated eigenvector = constant vector (= projection of *smooth* function onto grid)



Eigenvalues around 1 can be expanded w.r.t. h

$$|\lambda| = 1 + h^{\ell} c_{\ell} + h^{\ell+1} c_{\ell+1} + \ldots , \qquad c_{\ell} \neq 0$$

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

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

Impact of instability on eigenvalues around 1 becomes only visible in a slow time scale if $\ell > 1$

Procedure to derive determining equations for order functions *similar* to regular case.
Strategy: minimize the residual ↔ maximize order of residual → **details: short course L2 (M. Junk)**

Result for the leading (0'th) order:

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

$$\partial_{t_1} u^{(0)}(t_1, t_k, x) + a\partial_x u^{(0)}(t_1, t_k, x) = 0 \qquad k = 2,3$$

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***

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

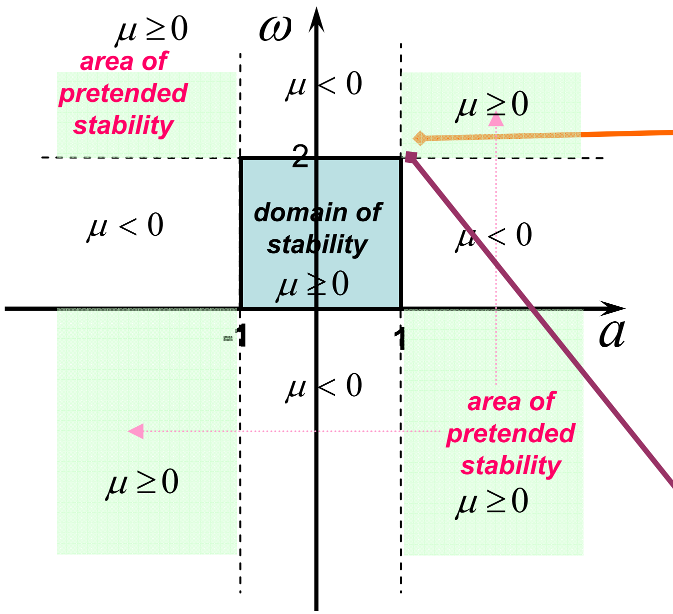
Coefficients: $\mu = \left(\frac{1}{\omega} - \frac{1}{2}\right)\left(1 - a^2\right)$ $\qquad \tilde{\lambda} = -\frac{1}{6} a \left(1 - a^2\right)$

What do we learn? 1) possibility to get a precise *quantitative* prediction of grid function.
2) *quantitative* understanding of the observed effects └→ *see later*

Typical effect of PDE evolution operator on initial condition: damping, flattening --- undulating, oscillating

Implications concerning *stability*: $\mu < 0 \;\Rightarrow$ *backward diffusion equation*
ill-posed IVP → instabilities expected ↔ stable behavior for $\mu \geq 0$
dispersive equation *indifferent* w.r.t. sign of $\tilde{\lambda}$ $\Rightarrow$ no hypothesis!

Comparison and limits of stability prediction



sign of diffusivity coefficient $\mu = \left(\frac{1}{\omega} - \frac{1}{2}\right)\left(1 - a^2\right)$

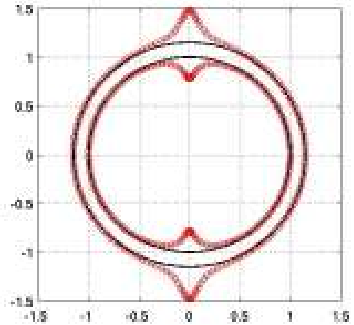
Hypothesis about stability based on multiscale expansion should fail if:

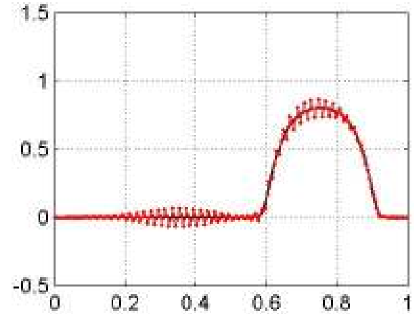
1) Near 1, only eigenvalues pertaining to ‚non-smooth' eigenvectors move out of closed unit disk as ω, a leave domain of stability.

2) Eigenvalues do not cross boundary of unit disk inside vicinity of 1.

Deceptive cases:

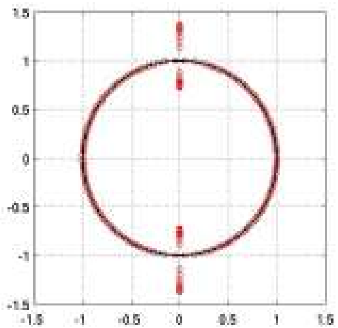
1) violation of CFL condition with unstable explicit relaxation: $\omega = 2.05, \quad a = 1.01$

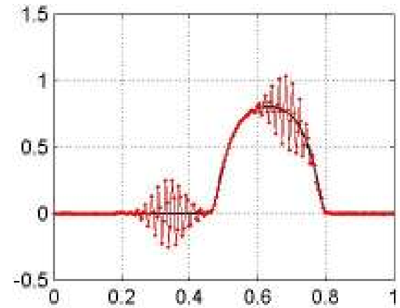




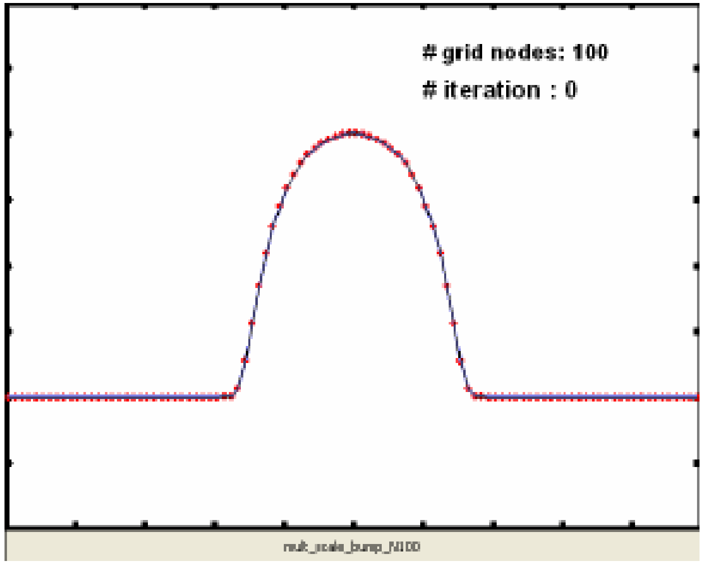
2) violation of CFL condition with limit value for ω

$\omega = 2.00, \quad a = 1.05$

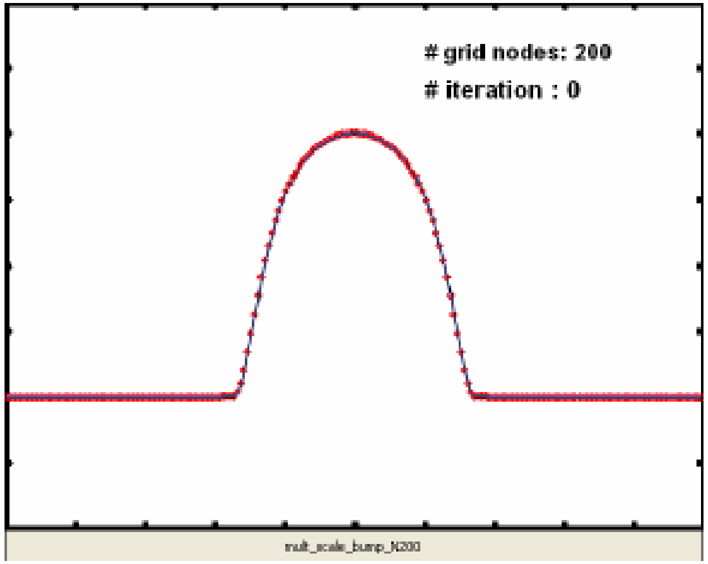




Test: approximation by twoscale ansatz



Snapshots $\omega = 2 \quad a = 0.8$



Another aspect of two scale expansion:

Prediction of the (numeric) mass moment:

$$\mathsf{F}_1(nh, jh) + \mathsf{F}_2(nh, jh) = U(nh, jh) \quad \leftrightarrow \quad u^{(0)}(nh, nh^2, jh)$$

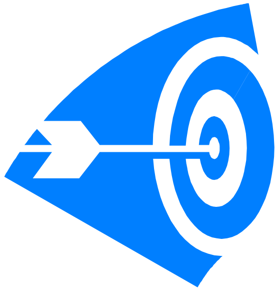
Nasty example: arbitrarily smooth *but* not analytic (n'th derivative cannot be bounded by C^n)

Observation: good approximation over time intervals of increasing length:

$O\left(\frac{1}{h}\right) = O(N)$ and even $O\left(\frac{1}{h^2}\right) = O\left(N^2\right)$

time interval	error
$O(1)$	$O(h^4)$
$O(\frac{1}{h})$	$O(h^3)$
$O(\frac{1}{h^2})$	$O(h^2)$

Conclusion

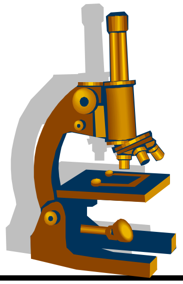


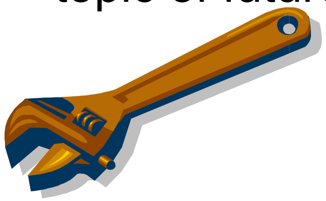
With exception of the corners the boundary of the actual stability domain is accurately described. Corners seem like „magic doors“ to falsely pretended stability domains.

High order prediction of mass moment.

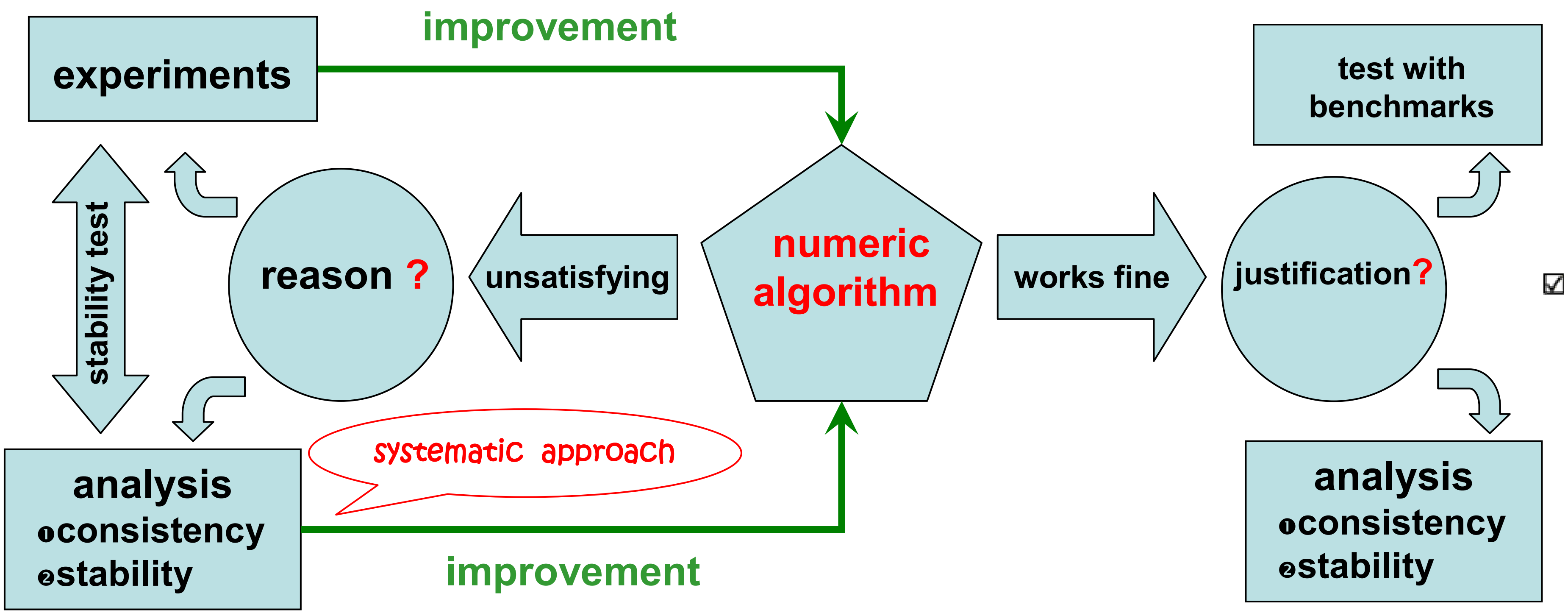
Some instabilities cannot be captured due to implicit smoothness assumption of prediction function (e.g. Taylor expansion).

Final judgement needs more case studies.
Above all: →clarify ideas & notions being still vague
e.g. classification of instabilities → topic of future work





Relevance of analysis -- the cycle of development .



- *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* $\Longrightarrow$ *well describable by regular expansion*