Automatic Smooth Initialization for LBM

Martin Rheinländer

Arbeitsgruppe Numerik
FB Mathematik & Statistik
Universität Konstanz

Joint work with

Michael Junk (Konstanz) & **Pieter Van Leemput** (Leuven)

Correspondence: populations $\leftrightarrow$ moments

$$\mathsf{F} = (\mathsf{F}_1, \ldots, \mathsf{F}_K) \qquad \mathsf{M} = (\overbrace{\mathsf{M}_1, \ldots, \mathsf{M}_C}^{\text{conserved moments}}, \ldots, \mathsf{M}_K)$$

$$\mathsf{F} = M^{-1}\mathsf{M} \qquad \mathsf{M} = M\mathsf{F}$$

Physical ICs $\longrightarrow$ (subset of) conserved moments for $t = 0$

Standard initialization (equilibrium) $\longrightarrow$ oscillating initial layers ☹

Correspondence: populations $\leftrightarrow$ moments

$$\mathsf{F} = (\mathsf{F}_1, \ldots, \mathsf{F}_K) \qquad \mathsf{M} = (\overbrace{\mathsf{M}_1, \ldots, \mathsf{M}_C}^{\text{conserved moments}}, \ldots, \mathsf{M}_K)$$

$$\mathsf{F} = M^{-1}\mathsf{M} \qquad \mathsf{M} = M\mathsf{F}$$

Physical ICs $\longrightarrow$ (subset of) conserved moments for $t = 0$

Standard initialization (equilibrium) $\longrightarrow$ oscillating initial layers ☹

$\Rightarrow$ Preprocess $\mathsf{F} = (\mathsf{F}_1, \ldots, \mathsf{F}_K)$ before starting LB simulation

CR initialization scheme (*Mei et al., Van Leemput et al.*):

pick some $\mathsf{G}(0)$, (e.g. equilibrium determined by $\mathsf{M}_1(0), \ldots, \mathsf{M}_C(0)$)

repeat

$\tilde{\mathsf{F}} := \mathrm{LBM}(\mathsf{G}(n))$	(regular LB time step)
$\tilde{\mathsf{M}} := M\tilde{\mathsf{G}}$	(traform to moments)
$\mathsf{M}(n+1) \leftarrow \tilde{\mathsf{M}}$	(constraint: reset known moments)
$\mathsf{G}(n+1) = M^{-1}\mathsf{M}(n+1)$	(convert moments to populations)

until ($\|\mathsf{M}(n+1) - \mathsf{M}(n)\| < TOL$)

initialize LB simulation by setting $\mathsf{F}(0) = \mathsf{G}(\infty)$

D1Q2 algorithm solving IVP: $\begin{cases} \partial_t \rho + a\partial_x \rho = & 0 \\ \rho(0,\cdot) & = \rho_0 \end{cases}$

$$\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \mathsf{F}_{-1} \\ \mathsf{F}_{+1} \end{pmatrix} = \begin{pmatrix} R \\ \Phi \end{pmatrix}$$

R: mass moment (conserved)
Φ: flux moment

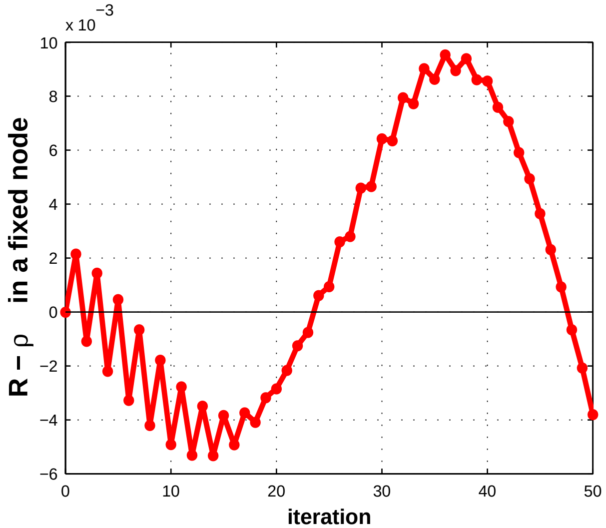
Initialization of moments: $\begin{cases} R(0) = \rho_0 & \Leftarrow \quad R \approx \rho \\ \Phi(0) = ? \end{cases}$

D1Q2 algorithm solving IVP: $\begin{cases} \partial_t \rho + a\partial_x \rho = & 0 \\ \rho(0,\cdot) & = \rho_0 \end{cases}$

$$\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \mathsf{F}_{-1} \\ \mathsf{F}_{+1} \end{pmatrix} = \begin{pmatrix} R \\ \Phi \end{pmatrix} \begin{matrix} \text{mass moment (conserved)} \\ \text{flux moment} \end{matrix}$$

Initialization of moments: $\begin{cases} R(0) = \rho_0 & \Leftarrow \quad R \approx \rho \\ \Phi(0) = ? & \end{cases}$

Error $R - \rho$ plotted versus iteration



Init. by equilibrium

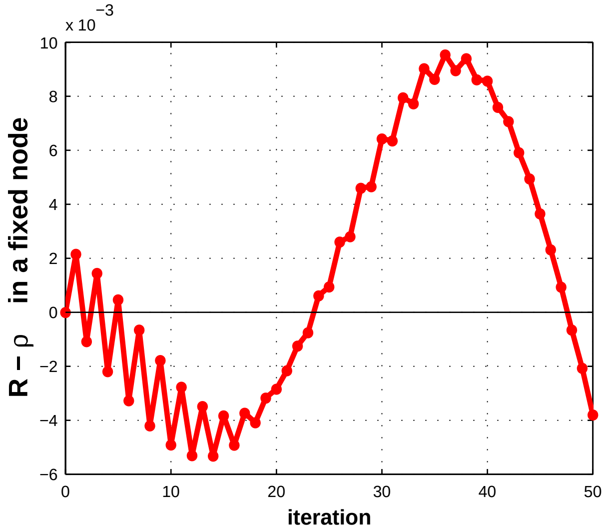
$$\begin{pmatrix} \mathsf{F}_{-1}(0) \\ \mathsf{F}_{+1}(0) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1-a \\ 1+a \end{pmatrix} \rho_0$$

D1Q2 algorithm solving IVP: $\begin{cases} \partial_t \rho + a \partial_x \rho = & 0 \\ \rho(0,\cdot) & = \rho_0 \end{cases}$

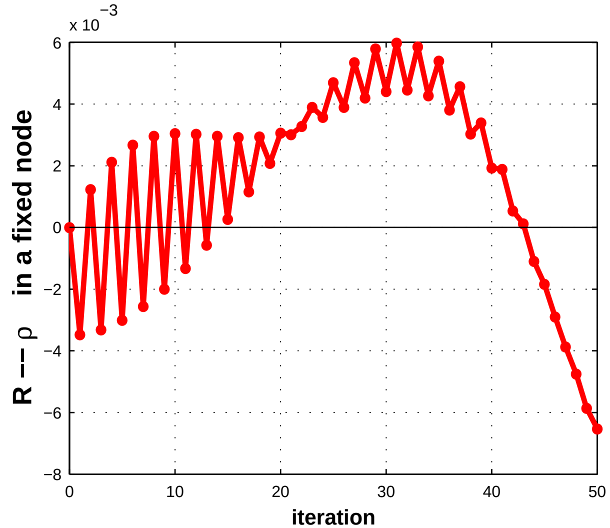
$$\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \mathsf{F}_{-1} \\ \mathsf{F}_{+1} \end{pmatrix} = \begin{pmatrix} R \\ \Phi \end{pmatrix} \quad \begin{matrix} \text{mass moment (conserved)} \\ \text{flux moment} \end{matrix}$$

Initialization of moments: $\begin{cases} R(0) = \rho_0 & \Leftarrow \quad R \approx \rho \\ \Phi(0) = ? \end{cases}$

Error $R - \rho$ plotted versus iteration



Init. by equilibrium
$\begin{pmatrix} \mathsf{F}_{-1}(0) \\ \mathsf{F}_{+1}(0) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1-a \\ 1+a \end{pmatrix} \rho_0$



Initialization by constrained runs scheme

Observation: Oscillations (initial layer) persist!

What does the CRS yield? $\rightarrow$ fixed point iteration for $\mathsf{F}(0)$:

$$\overbrace{\mathsf{G}(n+1)}^{\mathsf{G}(\infty)=\mathsf{F}(0)} = M^{-1}\Big[\Pi\, M\, \underbrace{E\ \overbrace{\mathsf{G}(n)}^{\mathsf{G}(\infty)=\mathsf{F}(0)}}_{\text{LB step}} + \binom{\rho_0}{0}\Big], \qquad \Pi\binom{x}{y} := \binom{0}{y}$$

What does the CRS yield? $\to$ fixed point iteration for $\mathsf{F}(0)$:

$$\overbrace{\mathsf{G}(n+1)}^{\mathsf{G}(\infty)=\mathsf{F}(0)} = M^{-1}\Big[\Pi\, M\, \underbrace{E\ \overbrace{\mathsf{G}(n)}^{\mathsf{G}(\infty)=\mathsf{F}(0)}}_{\text{LB step}} + \binom{\rho_0}{0}\Big], \qquad \Pi\binom{x}{y} := \binom{0}{y}$$

Resulting regular expansion for $\mathsf{F}(0)$ w.r.t. grid spacing h:

$$\mathsf{F}(0) = \tfrac{1}{2}(1 + a\mathsf{s})\rho_0 \ - \ \tfrac{1}{2\omega} h \partial_x \rho_0 \mathsf{s} \ + \ \mathrm{O}(h^2)$$

What does the CRS yield? $\rightarrow$ fixed point iteration for $\mathsf{F}(0)$:

$$\overbrace{\mathsf{G}(n+1)}^{\mathsf{G}(\infty)=\mathsf{F}(0)} = M^{-1}\Big[\Pi\, M \underbrace{E\ \overbrace{\mathsf{G}(n)}^{\mathsf{G}(\infty)=\mathsf{F}(0)}}_{\text{LB step}} + \binom{\rho_0}{0}\Big], \qquad \Pi\binom{x}{y} := \binom{0}{y}$$

Resulting regular expansion for $\mathsf{F}(0)$ w.r.t. grid spacing h:

$$\mathsf{F}(0) = \tfrac{1}{2}(1 + a\mathsf{s})\rho_0 \ - \ \tfrac{1}{2\omega} h \partial_x \rho_0 \mathsf{s} \ + \ \mathrm{O}(h^2)$$

What does the LBA require to evolve smoothly? (regular expansion of LBA)

$$\mathsf{F}(0) = \tfrac{1}{2}(1 + a\mathsf{s})\rho_0 \ - \ \tfrac{1}{2\omega} h (1 - a^2) \partial_x \rho_0 \mathsf{s} \ + \ \mathrm{O}(h^2)$$

What does the CRS yield? $\rightarrow$ fixed point iteration for $\mathsf{F}(0)$:

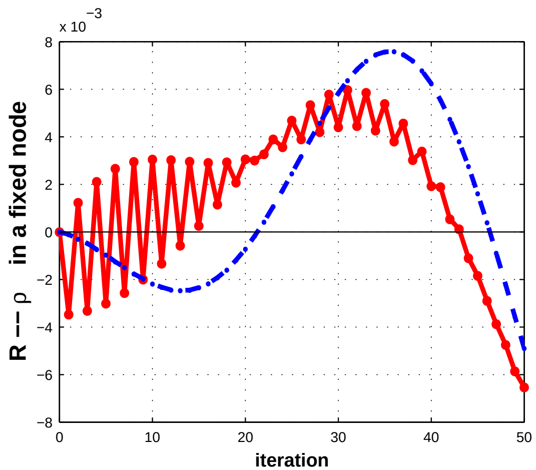
$$\overbrace{\mathsf{G}(n+1)}^{\mathsf{G}(\infty)=\mathsf{F}(0)} = M^{-1}\Big[\Pi\, M\, \underbrace{E\;\overbrace{\mathsf{G}(n)}^{\mathsf{G}(\infty)=\mathsf{F}(0)}}_{\text{LB step}} + \binom{\rho_0}{0}\Big], \qquad \Pi\binom{x}{y} := \binom{0}{y}$$

Resulting regular expansion for $\mathsf{F}(0)$ w.r.t. grid spacing h:

$$\mathsf{F}(0) = \tfrac{1}{2}(1 + a\mathsf{s})\rho_0 \;-\; \tfrac{1}{2\omega} h \partial_x \rho_0 \mathsf{s} \;+\; \mathrm{O}(h^2)$$

What does the LBA require to evolve smoothly? (regular expansion of LBA)

$$\mathsf{F}(0) = \tfrac{1}{2}(1 + a\mathsf{s})\rho_0 \;-\; \tfrac{1}{2\omega} h (1 - a^2) \partial_x \rho_0 \mathsf{s} \;+\; \mathrm{O}(h^2)$$



Comparison of error $R - \rho$

CRS versus analytic init.

What does the CRS yield? $\rightarrow$ fixed point iteration for $\mathsf{F}(0)$:

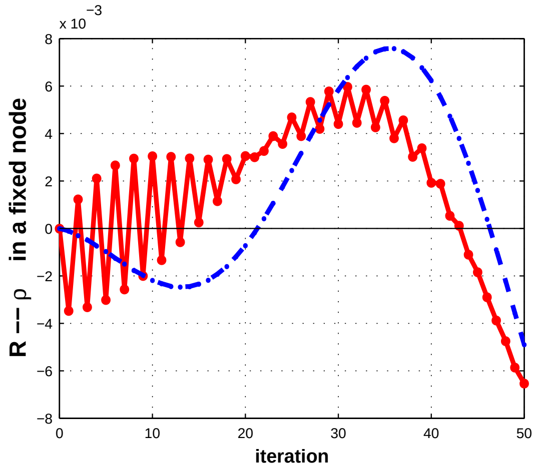
$$\overbrace{\mathsf{G}(n+1)}^{\mathsf{G}(\infty)=\mathsf{F}(0)} = M^{-1}\Big[\Pi\, M\, \underbrace{E\ \overbrace{\mathsf{G}(n)}^{\mathsf{G}(\infty)=\mathsf{F}(0)}}_{\text{LB step}} + \binom{\rho_0}{0}\Big], \qquad \Pi\binom{x}{y} := \binom{0}{y}$$

Resulting regular expansion for $\mathsf{F}(0)$ w.r.t. grid spacing h:

$$\mathsf{F}(0) = \tfrac{1}{2}(1 + a\mathsf{s})\rho_0 \; - \; \tfrac{1}{2\omega} h \partial_x \rho_0 \mathsf{s} \; + \; \mathrm{O}(h^2)$$

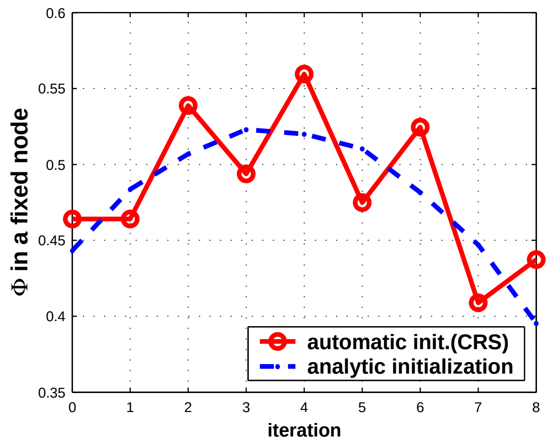
What does the LBA require to evolve smoothly? (regular expansion of LBA)

$$\mathsf{F}(0) = \tfrac{1}{2}(1 + a\mathsf{s})\rho_0 \; - \; \tfrac{1}{2\omega} h (1 - a^2) \partial_x \rho_0 \mathsf{s} \; + \; \mathrm{O}(h^2)$$



Comparison of error $R - \rho$

CRS versus analytic init.



Similar oscillations in Φ

Effect of CRS: $\Phi(0) = \Phi(\Delta t)$

What does the CRS yield? $\rightarrow$ fixed point iteration for $\mathsf{F}(0)$:

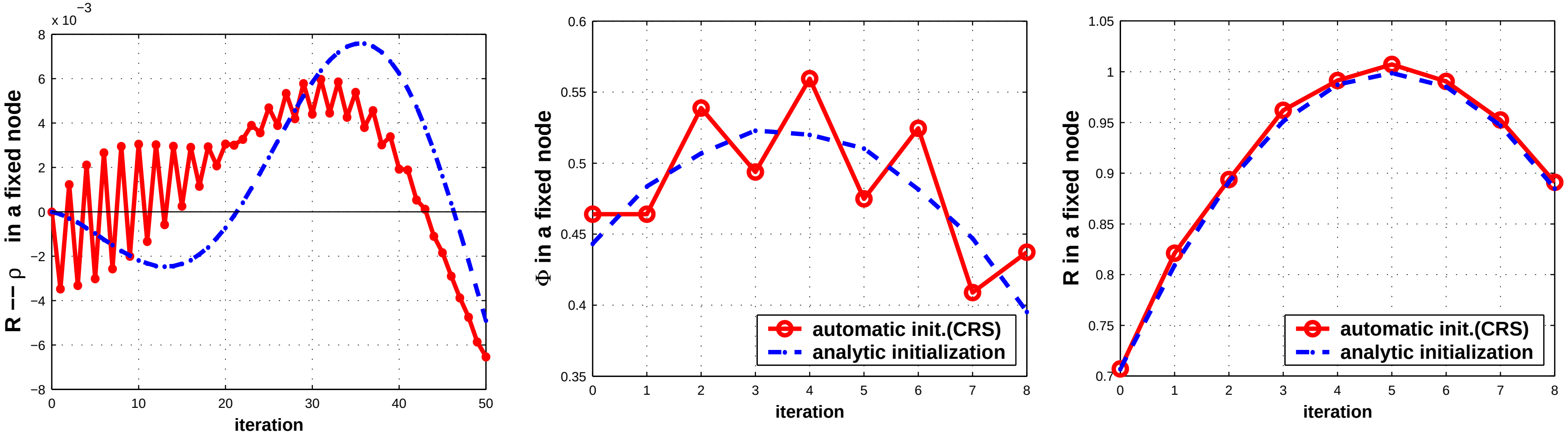
$$\overbrace{\mathsf{G}(n+1)}^{\mathsf{G}(\infty)=\mathsf{F}(0)} = M^{-1}\Big[\Pi\, M\, \underbrace{E\ \overbrace{\mathsf{G}(n)}^{\mathsf{G}(\infty)=\mathsf{F}(0)}}_{\text{LB step}} + \binom{\rho_0}{0}\Big], \qquad \Pi\binom{x}{y} := \binom{0}{y}$$

Resulting regular expansion for $\mathsf{F}(0)$ w.r.t. grid spacing h:

$$\mathsf{F}(0) = \tfrac{1}{2}(1 + a\mathsf{s})\rho_0 \;-\; \tfrac{1}{2\omega} h\partial_x\rho_0\mathsf{s} \;+\; \mathrm{O}(h^2)$$

What does the LBA require to evolve smoothly? (regular expansion of LBA)

$$\mathsf{F}(0) = \tfrac{1}{2}(1 + a\mathsf{s})\rho_0 \;-\; \tfrac{1}{2\omega} h(1-a^2)\partial_x\rho_0\mathsf{s} \;+\; \mathrm{O}(h^2)$$



Comparison of error $R - \rho$ — CRS versus analytic init.

Similar oscillations in Φ — Effect of CRS: $\Phi(0) = \Phi(\Delta t)$

Oscillations not visible in R

moving cosine, 20 nodes, monitor node 3, $\omega = 1.99$, $a = 0.51$

Hypothesis I:

> *Optimal initialization* corresponds to *regular expansion*.

Optimal $\stackrel{?}{=}$ minimized error, maximal 'smoothness'

Hypothesis I:

Optimal initialization corresponds to *regular expansion*.

Optimal $\stackrel{?}{=}$ minimized error, maximal 'smoothness'

$$\mathsf{F}(0) = \mathsf{f}^{(0)}(0) + h\mathsf{f}^{(1)}(0) + h^2\mathsf{f}^{(2)}(0) + \ldots$$

where in case of the model LBA
$$\begin{cases} \mathsf{f}^{(0)}(0) = \frac{1}{2}(1 + a\mathsf{s})\,\rho_0 \\ \mathsf{f}^{(1)}(0) = -\frac{1}{2\omega}(1 - a^2)\mathsf{s}\,\partial_x \rho_0 \\ \mathsf{f}^{(2)}(0) = -\frac{1}{\omega}(\frac{1}{\omega} - \frac{1}{2})(1 - a^2)a\mathsf{s}\,\partial_x^2 \rho_0 \end{cases}$$

Difficulty: Generally $\mathsf{f}^{(1)}(0), \mathsf{f}^{(2)}(0), \ldots$ complicated to ascertain!

Request for initializer (sort of iterative scheme fitting into LB framework) building up regular expansion automatically

Hypothesis I:

Optimal initialization corresponds to *regular expansion*.

Optimal $\stackrel{?}{=}$ minimized error, maximal 'smoothness'

$$\mathsf{F}(0) = \mathsf{f}^{(0)}(0) + h\mathsf{f}^{(1)}(0) + h^2\mathsf{f}^{(2)}(0) + \ldots$$

where in case of the model LBA $\begin{cases} \mathsf{f}^{(0)}(0) = \frac{1}{2}(1 + a\mathsf{s})\,\rho_0 \\ \mathsf{f}^{(1)}(0) = -\frac{1}{2\omega}(1 - a^2)\mathsf{s}\,\partial_x\rho_0 \\ \mathsf{f}^{(2)}(0) = -\frac{1}{\omega}(\frac{1}{\omega} - \frac{1}{2})(1 - a^2)a\mathsf{s}\,\partial_x^2\rho_0 \end{cases}$

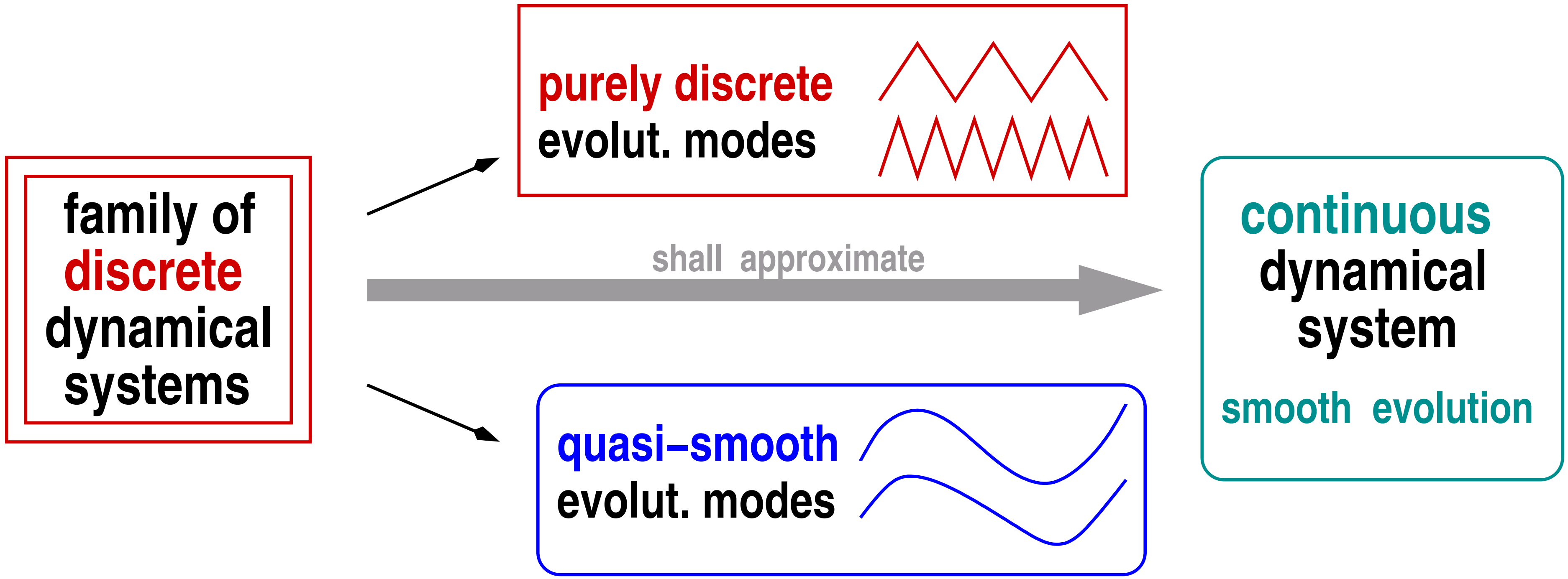
Difficulty: Generally $\mathsf{f}^{(1)}(0), \mathsf{f}^{(2)}(0), \ldots$ complicated to ascertain!

Request for initializer (sort of iterative scheme fitting into LB framework) building up regular expansion automatically

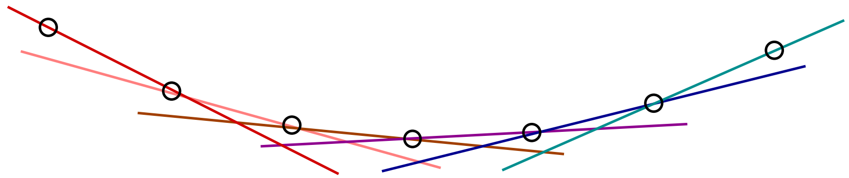
Hypothesis II:

$\longrightarrow$ practical characterization of regular expansion

Optimal initialization $\Leftrightarrow$ *'smooth'* initial behavior.


family of
discrete
dynamical
systems
purely discrete
evolut. modes
shall approximate
quasi–smooth
evolut. modes
continuous
dynamical
system
smooth evolution

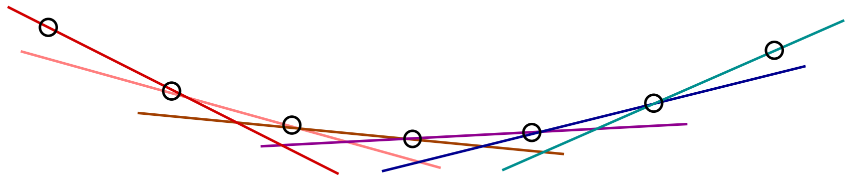
‘Discrete’ smoothness:



A sequence of grid functions approximates a smooth function:

$\Leftrightarrow$ Value in each node is approximated by inter-/extrapolating the values of surrounding nodes.

‘Discrete’ smoothness:



A sequence of grid functions approximates a smooth function:

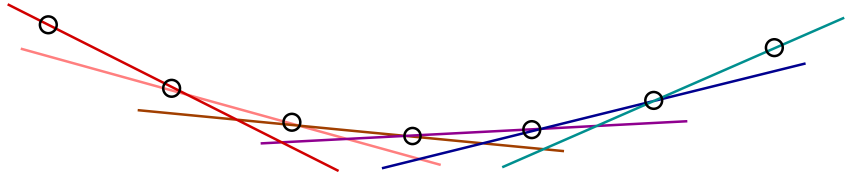
$\Leftrightarrow$ Value in each node is approximated by inter-/extrapolating the values of surrounding nodes.

Application to initialization problem

$$\begin{pmatrix} \mathsf{F}_{-1} \\ \mathsf{F}_{+1} \end{pmatrix} \quad \leftrightarrow \quad \begin{pmatrix} R \\ \Phi \end{pmatrix} \quad \begin{matrix} \text{prescribed by macroscopic IC} \\ \text{unspecified \& freely disposable} \end{matrix}$$

Initialization of Φ shall enforce its smooth evolution.

‘Discrete’ smoothness:



A sequence of grid functions approximates a smooth function:

$\Leftrightarrow$ Value in each node is approximated by inter-/extrapolating the values of surrounding nodes.

Application to initialization problem

$$\begin{pmatrix} \mathsf{F}_{-1} \\ \mathsf{F}_{+1} \end{pmatrix} \quad \leftrightarrow \quad \begin{pmatrix} R \\ \Phi \end{pmatrix} \begin{matrix} \text{prescribed by macroscopic IC} \\ \text{unspecified \& freely disposable} \end{matrix}$$

Initialization of Φ shall enforce its smooth evolution.

Choose $\Phi(0)$ such that

$$\Phi(0) \overset{!}{=} \underbrace{\mathcal{I}\Big(0;\ \Phi(\Delta t), ..., \Phi(n\Delta t)\Big)}_{\substack{\text{unique interpolation polynomial} \\ \deg\mathcal{P} = n-1}}$$

Linear extrapolation: $\begin{cases} R(0) = \rho_0 \\ \Phi(0) = 2\Phi(\Delta t) - \Phi(2\Delta t) \end{cases}$

$$\Leftrightarrow \quad \boxed{\mathsf{F}(0) \overset{!}{=} M^{-1}\Big[\Pi\, M\, \big(2E - E^2\big)\mathsf{F}(0) \;+\; \big(\begin{smallmatrix}\rho_0 \\ 0\end{smallmatrix}\big)\Big]}$$

Consistency result: $\quad \mathsf{F}(0) = \mathsf{f}^{(0)}(0) + h\mathsf{f}^{(1)}(0) + \mathrm{O}(h^2)$

Linear extrapolation: $\left\{ \begin{array}{l} R(0) = \rho_0 \\ \Phi(0) = 2\Phi(\Delta t) - \Phi(2\Delta t) \end{array} \right.$

$$\Leftrightarrow \quad \boxed{\mathsf{F}(0) \stackrel{!}{=} M^{-1}\Big[\Pi\, M\, \big(2E - E^2\big)\mathsf{F}(0) \;+\; \big(\begin{smallmatrix}\rho_0\\0\end{smallmatrix}\big)\Big]}$$

Consistency result: $\mathsf{F}(0) = \mathsf{f}^{(0)}(0) + h\mathsf{f}^{(1)}(0) + \mathrm{O}(h^2)$

Quadratic extrapolation: $\left\{ \begin{array}{l} R(0) = \rho_0 \\ \Phi(0) = 3\Phi(\Delta t) - 3\Phi(2\Delta t) + \Phi(3\Delta t) \end{array} \right.$

$$\Leftrightarrow \quad \boxed{\mathsf{F}(0) \stackrel{!}{=} M^{-1}\Big[\Pi\, M\, \big(3E - 3E^2 + E^3\big)\mathsf{F}(0) \;+\; \big(\begin{smallmatrix}\rho_0\\0\end{smallmatrix}\big)\Big]}$$

Consistency result: $\mathsf{F}(0) = \mathsf{f}^{(0)}(0) + h\mathsf{f}^{(1)}(0) + h^3\mathsf{f}^{(2)}(0) + \mathrm{O}(h^3)$

Linear extrapolation: $\begin{cases} R(0) = \rho_0 \\ \Phi(0) = 2\Phi(\Delta t) - \Phi(2\Delta t) \end{cases}$

$$\Leftrightarrow \quad \boxed{\mathsf{F}(0) \overset{!}{=} M^{-1}\Big[\Pi\, M\, \big(2E - E^2\big)\mathsf{F}(0) \; + \; \binom{\rho_0}{0}\Big]}$$

Consistency result: $\mathsf{F}(0) = \mathsf{f}^{(0)}(0) + h\mathsf{f}^{(1)}(0) + \mathrm{O}(h^2)$

Quadratic extrapolation: $\begin{cases} R(0) = \rho_0 \\ \Phi(0) = 3\Phi(\Delta t) - 3\Phi(2\Delta t) + \Phi(3\Delta t) \end{cases}$

$$\Leftrightarrow \quad \boxed{\mathsf{F}(0) \overset{!}{=} M^{-1}\Big[\Pi\, M\, \big(3E - 3E^2 + E^3\big)\mathsf{F}(0) \; + \; \binom{\rho_0}{0}\Big]}$$

Consistency result: $\mathsf{F}(0) = \mathsf{f}^{(0)}(0) + h\mathsf{f}^{(1)}(0) + h^3\mathsf{f}^{(2)}(0) + \mathrm{O}(h^3)$

Remark: Nearest neighbor (constant) extrapolation

$\longrightarrow$ condition of original CRS: $\mathsf{F}(0) = \mathsf{f}^{(0)}(0) + \mathrm{O}(h)$

ICs for $\mathsf{F}(0)$ are of type: $x = Ax + b \quad \Leftrightarrow \quad (I - A)x = b$ $(*)$

$$A := \underbrace{M^{-1}\Pi M}_{=:\tilde{\Pi}}\,\mathcal{I}_k(E) \qquad \text{with e.g.} \quad \begin{cases} \mathcal{I}_1(z) := 2z - z^2 \\ \mathcal{I}_2(z) := 3z - 3z^2 + z^3 \\ \mathcal{I}_3(z) := 4z - 6z^2 + 4z^3 - z^4 \end{cases}$$

Remarks: *Unique solvability* of $(*)$ $\longrightarrow$ theoretic issue to be investigated.

Solvability provided $\longrightarrow$ solution of $(*)$ by whatever method one likes.

Preferably: iterative methods $\longrightarrow$ avoid setting up matrices $\longrightarrow$ easily integrable within the LB framework

ICs for $\mathsf{F}(0)$ are of type: $x = Ax + b \quad \Leftrightarrow \quad (I - A)x = b$ $(*)$

$$A := \underbrace{M^{-1}\Pi M}_{=:\tilde{\Pi}} \mathcal{I}_k(E) \qquad \text{with e.g.} \quad \begin{cases} \mathcal{I}_1(z) := 2z - z^2 \\ \mathcal{I}_2(z) := 3z - 3z^2 + z^3 \\ \mathcal{I}_3(z) := 4z - 6z^2 + 4z^3 - z^4 \end{cases}$$

Remarks: *Unique solvability* of $(*)$ $\longrightarrow$ theoretic issue to be investigated.

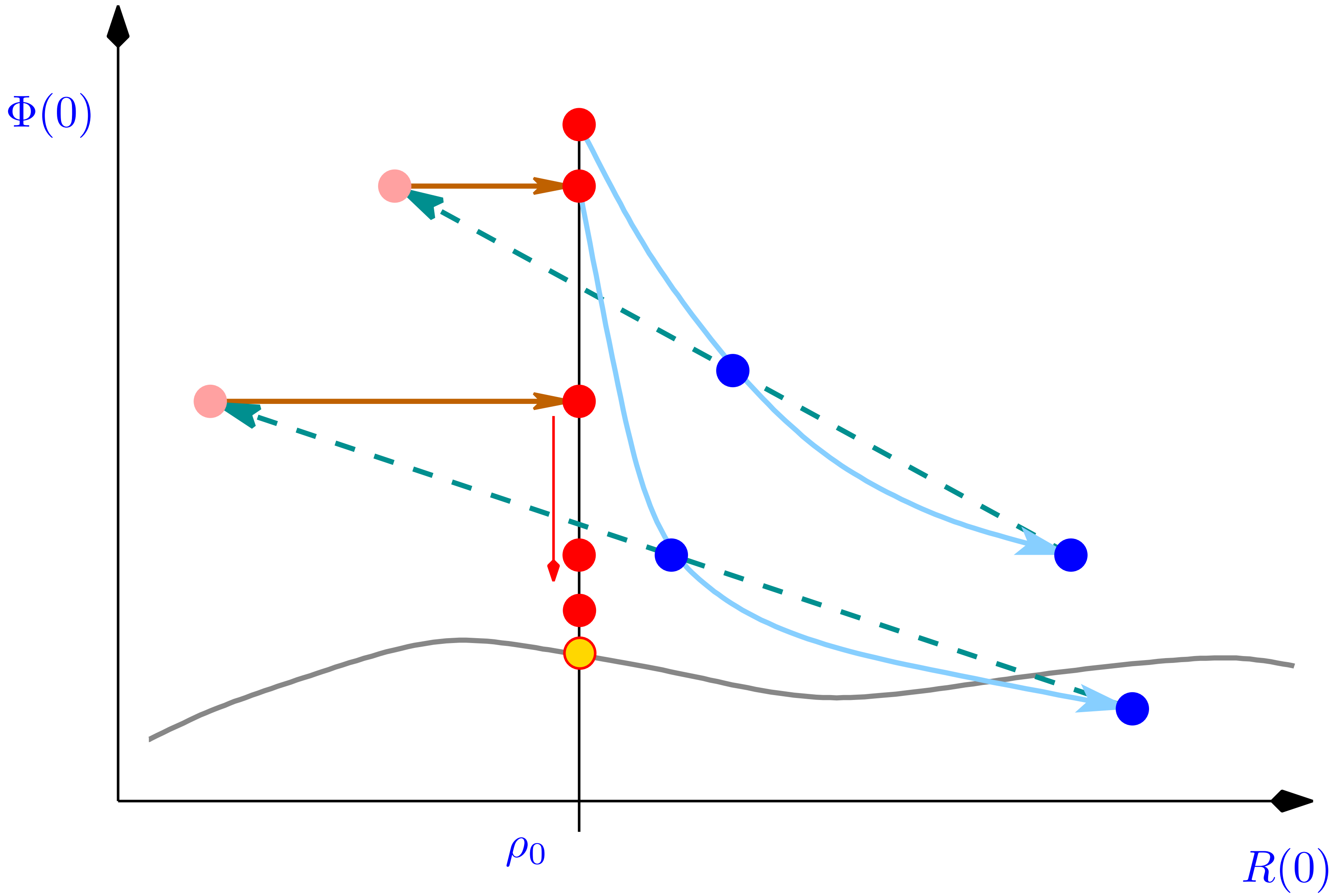
Solvability provided $\longrightarrow$ solution of $(*)$ by whatever method one likes.

Preferably: iterative methods $\longrightarrow$ avoid setting up matrices $\longrightarrow$ easily integrable within the LB framework

Proceeding analogously to original CR $\longrightarrow$ direct iterative solution:

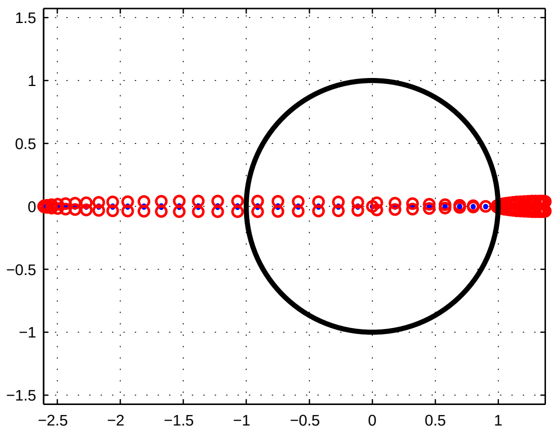
$$\boxed{x_{n+1} = Ax_n + b} \qquad \Rightarrow \qquad x_n = A^n x_0 + \sum_{k=0}^{n-1} A^k b$$

For arbitrary b, x_0: $\quad \underset{x=Ax+b}{x_n \xrightarrow{n\to\infty} x} \qquad \Leftrightarrow \qquad \varrho(A) < 1$

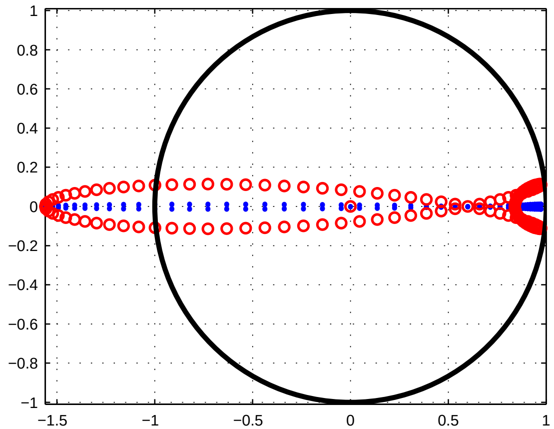

$\Phi(0)$
ρ_0
$R(0)$

Spectral plots of A with *linear* extrapolation ($\circ\ a = 0.95,\quad \bullet\ a = 0.1$)

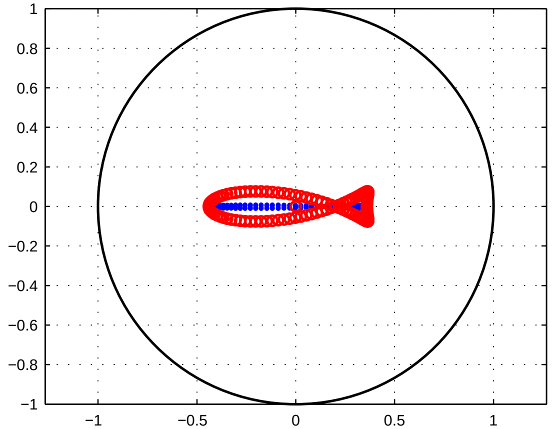
Numerical test for D1Q2 model algorithm: $\mathbf{spec}(A) \subset \overline{D_1(0)}$ **for** $\omega \in [0.586,\ 1.414]$



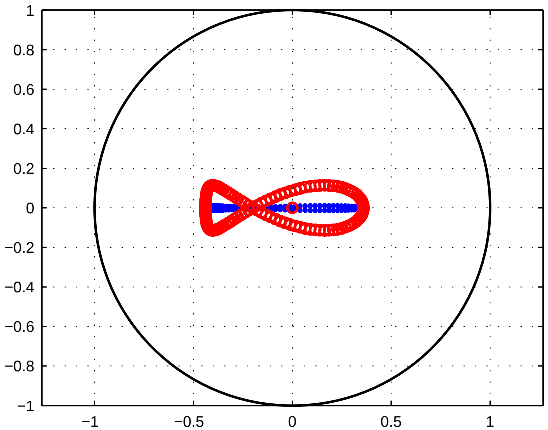
ω = 0.1



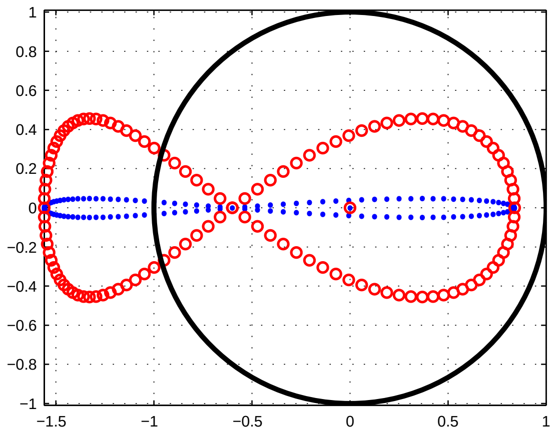
ω = 0.4



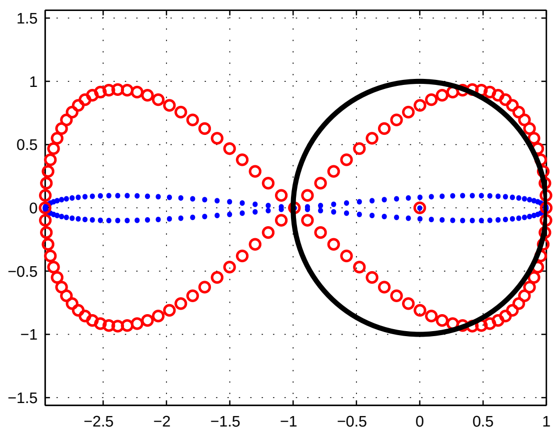
ω = 0.8



ω = 1.2

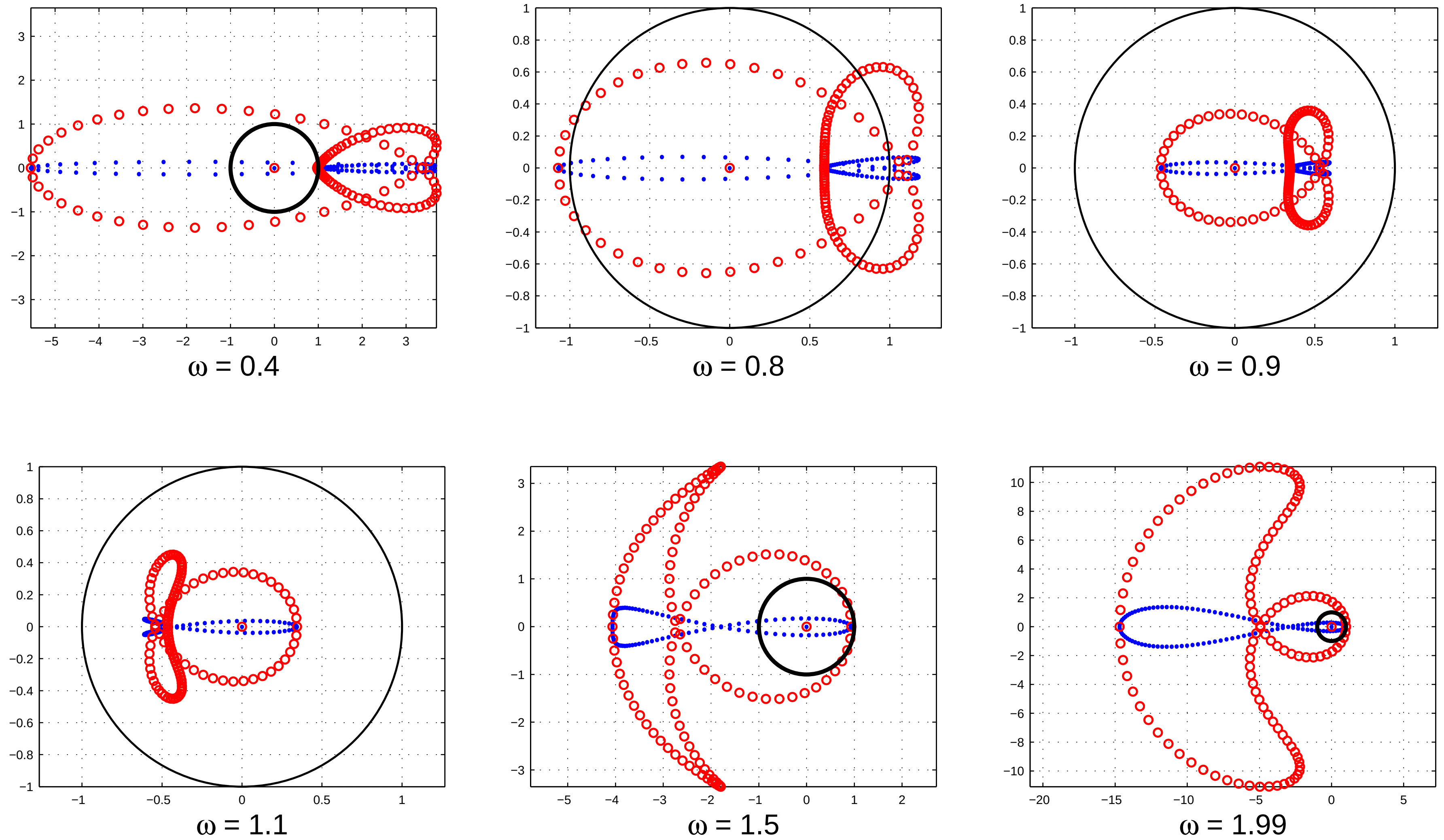


ω = 1.6



ω = 1.99

Spectral plots of A with *cubic* extrapolation (o $a = 0.95$, • $a = 0.1$)



Improvement: Assume $\operatorname{spec}(A) \subset \{z \in \mathbb{C} |\ \operatorname{Re}(z) < 1\}$

$$\Rightarrow \quad \underbrace{x = Ax + b}_{(\star\star)}$$ can be solved *iteratively*. (Well-suited for LBM!)

Use technique of *relaxation* motivated by:

- Assumption $\Rightarrow \quad \operatorname{spec}(A - I) \subset \{z \in \mathbb{C} |\ \operatorname{Re}(z) < 0\} \quad \Rightarrow \quad \lim_{\lambda \to \infty} \mathrm{e}^{\lambda(A-I)} = 0$
- Consider ODE: $\frac{\mathrm{d}}{\mathrm{d}\lambda} x(\lambda) = (A - I)x(\lambda) + b$

  $$x(\lambda) = \mathrm{e}^{\lambda(A-I)} x_0 + (A - I)^{-1} b \quad \xrightarrow{\lambda \to \infty} \quad (I - A)^{-1} b$$ (solution of $(\star\star)$)

- Discretize, e.g., by explicit Euler $\longrightarrow$ iterate until *stationarity* is reached.

Improvement: Assume $\text{spec}(A) \subset \{z \in \mathbb{C} | \operatorname{Re}(z) < 1\}$

$$\Rightarrow \quad \underbrace{x = Ax + b}_{(\star\star)} \quad \text{can be solved } \textit{iteratively}.$$

(Well-suited for LBM!)

Use technique of *relaxation* motivated by:

- Assumption $\Rightarrow$ $\text{spec}(A - I) \subset \{z \in \mathbb{C} | \operatorname{Re}(z) < 0\} \quad \Rightarrow \quad \lim_{\lambda \to \infty} \mathrm{e}^{\lambda(A-I)} = 0$
- Consider ODE: $\frac{\mathrm{d}}{\mathrm{d}\lambda} x(\lambda) = (A - I)x(\lambda) + b$

$$x(\lambda) = \mathrm{e}^{\lambda(A-I)} x_0 + (A - I)^{-1} b \quad \xrightarrow{\lambda \to \infty} \quad (I - A)^{-1} b$$

(solution of $(\star\star)$)

- Discretize, e.g., by explicit Euler $\longrightarrow$ iterate until *stationarity* is reached.

Stabilized iteration: choose $\Delta\lambda$ such that

$$\text{spec}\big(\Delta\lambda(A - I)\big) \subset D_1(-1) \quad \Leftrightarrow \quad \varrho\big(I + \Delta\lambda(A - I)\big) < 1$$

$$\boxed{x_{n+1} = x_n + \Delta\lambda(A - I)x_n + \Delta\lambda b}$$

convergence $\longrightarrow$ Neumann series

What has been presented?

- CR initialization scheme may be *ineffective*

- Regular expansion $\leftrightarrow$ $\left\{ \begin{array}{c} \text{optimal} \\ \text{smooth} \end{array} \right\}$ initialization

- IC for $\mathsf{F}(0)$: $\longrightarrow$ regular expansion for $t = 0$ up to k^{th} order

$$(*) \quad \boxed{\mathsf{F}(0) = M^{-1}\Pi M\,\mathcal{I}_k(E)\,\mathsf{F}(0) \;+\; M^{-1}\tilde{\mathsf{M}}(0)} \qquad \tilde{\mathsf{M}}(0) = \begin{pmatrix} \mathsf{M}_1(0) \\ \vdots \\ \mathsf{M}_b(0) \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$(*)$ is valid independent of specific evolution operator E/LBM

- How to solve $(*)$, especially in LB framework?

Tests (model problem) for $k \leq 3$: $\left\{ \begin{array}{lll} \text{direct iteration} & |1-\omega| & \text{if small enough} \\ \text{relaxed iteration} & \omega \geq 1 & \end{array} \right.$