Analysis and Synthesis of Lattice-Boltzmann Methods

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http://www.math.uni-konstanz.de/numerik/

Contents

- Boundary Conditions
- Layer Analysis
- Convergence
- Summary

LBM setup and benchmark problem

Initial Condition: $f_i(0, \boldsymbol{j}) = f_i^{eq}(\hat{\rho} = 1, \hat{\boldsymbol{u}} = 0)$

Impulsive inflow: $U_{in} = y(1-y), \qquad V_{in} = 0$

Consistency: 0^{th} order accuracy

Numerical pressure and velocity at a monitor point in the wake:



Initial Condition:
$$f_i(0, \boldsymbol{j}) = f_i^{eq}(\hat{\rho} = 1, \hat{\boldsymbol{u}} = 0)$$



Numerical pressure and velocity at a monitor point in the wake:



Boundary condition at rigid walls

<u>Plane wall</u>: bounce back at $\frac{1}{2}$ link Consistency: Velocity: 2^{nd} order,

<u>Curved wall</u>: POP_1 or BFLPressure: 1^{st} order



• N. Thürey et. al.(TH):

$$f_i(n+1, j) = f_i^{eq}(n, j) + f_{i^*}^{eq}(n, j) - f_{i^*}(n, j)$$

Analysis $\implies S[\boldsymbol{u}]\boldsymbol{n} = 0$

• Neumann condition(NBC):

$$f_i(n+1, \boldsymbol{j}_0) = f_{i^*}^c(n, \boldsymbol{j}_0 + h\boldsymbol{c}_i) + 2c_s^2 f_i^* \hat{\boldsymbol{u}}(n, \boldsymbol{j}) \cdot \boldsymbol{c}_i$$

Analysis $\Longrightarrow \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{n}}(t, \boldsymbol{x}) = 0$



Outflow conditions

• Zero normal Stress condition(ZNS):

$$f_3(n+1, \mathbf{j}) = F_3^{eq}(1, \hat{\mathbf{u}}(n, \mathbf{j})) - ((2\nu A - \mathbf{I})(\mathbf{f} - \mathbf{f}^{eq}))_3,$$

$$f_i(n+1, \mathbf{j}) = F_i^{eq}(1, \hat{\mathbf{u}}(n, \mathbf{j})) - \frac{f_i^*}{f_3^*} (2\nu A(\mathbf{f} - \mathbf{f}^{eq}))_3, \quad i = 6, 7$$

Analysis
$$\implies (-pI + 2\nu S[u])n = 0$$

PSfrag replacements



Unsteady flow with Re = 100



Solid line: L/H = 5, dashed line: L/H = 3, dotted line: L/H = 2.

Dash-dotted line: reference values.

Pressure and velocity along the central line





Boundary layers at outflow PSfrag replacements

Analysis is necessary!

Overview

- LB-algorithms produce unwanted numerical effects.
- To understand better disturbing phenomena like initial and boundary layers
 → study model problems.
- Analytically tractable, exhibit similar features despite their simplicity.

- So far: mainly using regular expansions for the analysis of numerical algorithms/ parameter-depending ODEs/PDEs.
- Here: demonstration by two examples, how to apply irregular expansions.
- Concluding remarks about asymptotic expansions and convergence.

Analysis of an Initial Layer



Aller Anfang ist nicht nur schwer, sondern verläuft auch selten glatt. v

The D1P2 Leattice-Boltzmann Equation (Model Problem)

• Velocity space: $x \xrightarrow{1} 0 \xrightarrow{2} 0$ Population functions: $f_1, f_2 : [0, T] \times [0, L] \rightarrow \mathbb{R}$

v

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• Mass moment: $u = f_1 + f_2$, 1^{st} moment (flux): $\phi = \epsilon^{-1}(f_2 - f_1)$

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- LB equation with diffusive scaling:

v

$$\partial_t f_1 - \epsilon^{-1} \partial_x f_1 = -\epsilon^{-2} \omega \left[f_1 - \frac{1}{2} u \right] = -\epsilon^{-2} \frac{\omega}{2} \left[f_1 - f_2 \right]$$
$$\partial_t f_2 + \epsilon^{-1} \partial_x f_2 = -\epsilon^{-2} \omega \left[f_2 - \frac{1}{2} u \right] = -\epsilon^{-2} \frac{\omega}{2} \left[f_2 - f_1 \right]$$

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$$\partial_t \mathbf{f}_2 + \boldsymbol{\epsilon}^{-1} \partial_x \mathbf{f}_2 = -\boldsymbol{\epsilon}^{-2} \omega \left[\mathbf{f}_2 - \frac{1}{2} u \right] = -\boldsymbol{\epsilon}^{-2} \frac{\omega}{2} \left[\mathbf{f}_2 - \mathbf{f}_1 \right]$$

• Linear transformation $f_1, f_2 \leftrightarrow u, \phi$ leads to equivalent moment system:

$$\partial_t u + \partial_x \phi = 0 \qquad \partial_x \partial_t \phi = -\partial_t^2 u \partial_t \phi + \epsilon^{-2} \partial_x u = -\epsilon^{-2} \omega \phi \qquad \partial_x \phi = -\epsilon^2 \tau \partial_x \partial_t \phi - \tau \partial_x^2 u$$

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• Closed scalar equation in u: $\epsilon^2 \tau \partial_t^2 u + \partial_t u - \tau \partial_x^2 u = 0$

- Velocity space: $x \xrightarrow{1} \longrightarrow 2$ Population functions: $f_1, f_2 : [0, T] \times [0, L] \rightarrow \mathbb{R}$
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- Boundary conditions: $f_2(t,0) = -f_1(t,0) \Leftrightarrow u(t,0) = 0$

- Velocity space: $x \stackrel{1}{\longleftarrow} \stackrel{0}{\longrightarrow} Population functions: f_1, f_2 : [0, T] \times [0, L] \rightarrow \mathbb{R}$
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- Boundary conditions: $f_2(t,0) = -f_1(t,0) \Leftrightarrow u(t,0) = 0$
- Initial conditions: $f_1(0,\cdot), f_2(0,\cdot) \Leftrightarrow u(0,\cdot), \partial_t u(0,\cdot) = -\partial_x \phi(0,\cdot)$

•	Reformulated LB equation	$\stackrel{\epsilon\downarrow 0}{\leadsto}$	Target equation
EQ:	$\epsilon^2 \tau \partial_t^2 u + \partial_t u - \tau \partial_x^2 u = 0$) (EQ:	$\partial_t v - \tau \partial_x^2 v = 0$
BC:	$u(\cdot, 0) = 0 \wedge u(\cdot, L) = 0$	\rightarrow BC :	$v(\cdot,0) = 0 \ \land \ v(\cdot,L) = 0$
IC:	$u(0,\cdot) = g \wedge \partial_t u(0,\cdot) = h$	$h \int \mathbf{IC}$:	$v(0,\cdot) = g$

- Reformulated LB equation EQ: $\epsilon^2 \tau \partial_t^2 u + \partial_t u - \tau \partial_x^2 u = 0$ BC: $u(\cdot, 0) = 0 \land u(\cdot, L) = 0$ IC: $u(0, \cdot) = g \land \partial_t u(0, \cdot) = h$ $\begin{cases}
 \mathsf{EQ:} & \partial_t v - \tau \partial_x^2 v = 0 \\
 \mathsf{BC:} & v(\cdot, 0) = 0 \land v(\cdot, L) = 0 \\
 \mathsf{IC:} & v(0, \cdot) = g
 \end{cases}$
- Theorem:

$$\begin{array}{cccc} u & \xrightarrow{\boldsymbol{\epsilon} \to 0} & v & \text{ in } \mathcal{C}_b\big([0,\infty), \mathcal{L}^2(0,L)\big) \\ \partial_t u & \xrightarrow{\boldsymbol{\epsilon} \to 0} & \partial_t v & \text{ in } \mathcal{C}_b\big([\boldsymbol{\theta},\infty), \mathcal{L}^2(0,L)\big) & \text{ with } \boldsymbol{\theta} > 0 \end{array}$$

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• Compatible initialization: $h \stackrel{!}{=} \partial_t v(0, \cdot) = \tau \partial_x^2 v(0, \cdot) = \tau \partial_x^2 g \qquad \Rightarrow \theta = 0$

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- Compatible initialization: $h \stackrel{!}{=} \partial_t v(0, \cdot) = \tau \partial_x^2 v(0, \cdot) = \tau \partial_x^2 g \qquad \Rightarrow \theta = 0$
- Fourier ansatz: $u(t,x) = \sum_{n} \sigma_{\epsilon,n}(t) s_n(x)$, $v(t,x) = \sum_{n} \sigma_n(t) s_n(x)$

The Fourier coefficient functions

$$\begin{array}{ccc} & \mathsf{Perturbed problem} & \stackrel{\epsilon \downarrow 0}{\sim} & \mathsf{Limit problem} \\ \mathsf{EQ:} & \epsilon^2 \tau \ddot{\sigma}_{\epsilon} + \dot{\sigma}_{\epsilon} + \lambda \sigma_{\epsilon} = 0 \\ \mathsf{IC:} & \sigma_{\epsilon}(0) = \alpha \ \land \ \dot{\sigma}_{\epsilon}(0) = \beta \end{array} \right\} & \begin{cases} \mathsf{EQ:} & \dot{\sigma} + \lambda \sigma = 0 \\ \mathsf{IC:} & \sigma(0) = \alpha \\ \mathsf{IC:} & \sigma(0) = \alpha \end{cases}$$

• Fourier coefficients = time evolution of single-mode solution of original PDE



- Regular expansion: $\sigma_{\epsilon}(t) = \varsigma^{(0)}(t) + \epsilon^2 \varsigma^{(2)}(t) + \dots$
- Two-scale expansion: $\sigma_{\epsilon}(t) = \sigma^{(0)}(t/\epsilon^2, t) + \epsilon^2 \sigma^{(2)}(t/\epsilon^2, t) + \dots$

Regular Expansion

$$\sigma_{\epsilon}(t) = \varsigma^{(0)}(t) + \epsilon^2 \varsigma^{(2)}(t) + \epsilon^4 \varsigma^{(4)}(t) \dots$$

• ODEs determining the asymptotic order functions:

$$\begin{aligned} \epsilon^{0} &: & \dot{\varsigma}^{(0)} + \lambda \varsigma^{(0)} = & 0 & \varsigma^{(0)}(0) = \alpha & \dot{\varsigma}^{(0)}(0) = \beta \\ \epsilon^{2} &: & \dot{\varsigma}^{(2)} + \lambda \varsigma^{(2)} = -\tau \ddot{\varsigma}^{(0)} & \varsigma^{(2)}(0) = 0 & \dot{\varsigma}^{(2)}(0) = 0 \\ \epsilon^{4} &: & \vdots \end{aligned}$$

Regular Expansion

$$\sigma_{\epsilon}(t) = \varsigma^{(0)}(t) + \epsilon^2 \varsigma^{(2)}(t) + \epsilon^4 \varsigma^{(4)}(t) \dots$$

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• ill-posed IVPs \Rightarrow failure of regular expansion!

Regular Expansion

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- ill-posed IVPs \Rightarrow failure of regular expansion!
- Way-out: $\beta \to \beta_{\epsilon} = \beta^{(0)} + \epsilon^2 \beta^{(2)} + \dots$ with: $\beta^{(0)} = \dot{\varsigma}^{(0)}(0) \wedge \beta^{(2)} = \dot{\varsigma}^{(2)}(0) \wedge \dots$
- $\zeta^{(2k)}(0) = \alpha \delta_{0k}$ given $\Rightarrow \dot{\zeta}^{(0)}(0), \dot{\zeta}^{(2)}(0), \dots$ a priori computable: $\dot{\zeta}^{(0)}(0) = -\alpha \lambda \Rightarrow \ddot{\zeta}^{(0)}(0) = \alpha \lambda^2 \Rightarrow \dot{\zeta}^{(2)}(0) = -\tau \alpha \lambda^2 \dots$
- What about arbitrary β ? \rightarrow Two-scale expansion.



Generally: $\phi^{(2k+2)} \leftarrow \dot{\phi}^{(2k)}(0), \ \dot{\zeta}^{(2k)}(0), \ \ddot{\phi}^{(2k)} \leftarrow \phi^{(2k)}(0), \ \ddot{\zeta}^{(2k-2)}$



Generally: $\phi^{(2k+2)} \leftarrow \dot{\phi}^{(2k)}(0), \ \dot{\zeta}^{(2k)}(0), \ \ddot{\phi}^{(2k)} \leftarrow \phi^{(2k)}(0), \ \ddot{\zeta}^{(2k-2)}(0), \ \dot{\zeta}^{(2k-2)}(0), \ \dot{\zeta}^{(2k-2)}(0$



• Hierarchic ODE-system defining the asymptotic order functions:

Generally: $\phi^{(2k+2)} \leftarrow \dot{\phi}^{(2k)}(0), \ \dot{\zeta}^{(2k)}(0), \ \ddot{\phi}^{(2k)} \leftarrow \phi^{(2k)}(0), \ \ddot{\zeta}^{(2k-2)}$



 $\epsilon = 0.17, \ \tau = 0.3, \ \lambda = 4\tau\pi^2$, Caution: Differentiating the expansion for σ_{ϵ} does not directly yield the expansion for $\frac{\mathrm{d}}{\mathrm{d}t}\sigma_{\epsilon}$ 32

0.025

0.035

0.03

0.04

0.045

Verification of the Two-Scale Expansion $\leftrightarrow \sigma^{(0)} + \epsilon^2 \sigma^{(2)}$ 2) σ_{ϵ} 0.9 -2 0.8 0.7 0.6 -6 0.5 0.4 PSfrag replacements Sfrag replacements_{0.3} $\sigma_{\epsilon}^{pressure_{0.2}}$ $pressure _{x}^{v}$ -10 $\frac{\mathrm{d}}{\mathrm{d}t}\sigma_{\epsilon}$ 0.02 0.04 0.06 0.08 0.1 0.02 0.06 0 0.04 0.08 0.1 0.12 -2.5-3.5 0.7 PSfrag replacements Sfrag replacements pressure x $pressure_{x}^{\check{u}_{0.6}}$

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0.002

0

0.004

0.006

0.008

0.01



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periodic BC, $\theta = 3$, $\omega = (\theta \nu + 0.5)^{-1}$, red=20, blue=40, green=80 nodes
cross-section of u_x in x-dir.





o: Bouzidi, *: Bounce-back

C'est surtout grâce aux conditions de bord, qu'un schéma numérique est précis et fort. Finalement, elles décident de son sort. (Si l'on va l'utiliser ou rejeter.) 5-point stencil discretizing the 2nd derivative $\frac{d^2}{dx^2}$ • Poisson PSfrag replacements $u(0) = u_0$, $u(L) = u_L$ and u''(x) = f(x) for $x \in (0, L)$ • Discretization in the bulk: $u_{pressure}$ $\frac{1}{h^2} \underbrace{\left[a, b, \frac{*}{c}, b, a\right]_h u(x)}_{au(x-2h)+bu(x-h)+cu(x)+bu(x+h)+au(x+2h)} = u''(x) + O(h^4)$



• Modified stencil in x_1 (and anlogously in x_{N-1}) by extrapolation:

nearest-neighbor
$$v_{-1} = v_0 \implies h^{-2}[b+a, \overset{*}{c}, b, a]v_1 = f(h)$$

linear $v_{-1} = 2v_0 - v_1 \implies h^{-2}[b+2a, c\overset{*}{-}a, b, a]v_1 = f(h)$

$$a = -\frac{1}{12}, \ b = \frac{16}{12}, \ c = -\frac{30}{12}$$

A little Experiment

Periodic Boundary Conditions

• EQ: $\partial^2 u_P = -\frac{4\pi^2}{L^2} \sin(2\pi x/L)$ BC: $u_P(0) = u_P(L)$ **Dirichlet Boundary Conditions**

EQ:
$$\partial^2 u_D = -\frac{4\pi^2}{L^2} \sin(2\pi x/L)$$

BC: $u_D(0) = 0 \land u_D(L) = 0$

- Solution: $u_P(x) = u_D(x) = u(x) = \sin(2\pi x/L)$
- Numeric solution using the 5-point stencil



Conclusion: The figures suggest, that in the case of periodic boundary conditions the error can be described by smooth functions. In contrast to v_P the numeric solution of the nearest neighbor extrapolation scheme v_D reveals a strongly grid-dependent behavior (the unscaled error develops steeper and steeper jumps). Furthermore the convergence order may be significantly impaired by the boundary conditions.

Additional condition: $\sum_i v_{P,i} = 0$ to get expected solution.

• Ansatz: $u^{[n]} := (\hat{u}^{(0)} + s^{(0)}) + h(\hat{u}^{(1)} + s^{(1)}) + \ldots + h^n(\hat{u}^{(n)} + s^{(n)})$

with $\begin{cases} \text{ smooth, grid-independent functions } u^{(0)}, u^{(1)}, \dots \text{ restricted onto the grid} \\ (\text{pure}) \text{ grid functions } s^{(0)}, s^{(1)}, \dots \end{cases}$

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with $\left\{ \begin{array}{l} {\rm smooth,\ grid-independent\ functions\ } u^{(0)}, u^{(1)}, \ldots {\rm\ restricted\ onto\ the\ grid\ (pure)\ grid\ functions\ } s^{(0)}, s^{(1)}, \ldots \end{array} \right.$

• Residual:
$$r^{[n]} := \hat{D}u^{[n]} - \varsigma = \begin{cases} u_0^{[n]} & - u_0 \\ \frac{1}{h^2}[a+b, \overset{*}{c}, b, a]u_1^{[n]} & - f(h) \\ \frac{1}{h^2}[a, b, \overset{*}{c}, b, a] u_i^{[n]} & - f(ih) & i \in \{2, ..., N-2\} \\ \frac{1}{h^2}[a, b, \overset{*}{c}, a+b]u_{N-1}^{[n]} & - f(Nh-h) \\ u_N^{[n]} & - u_L \end{cases}$$

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• Perform Taylor expansion of $u^{(k)}$ up to the order n-k.

• Ansatz: $u^{[n]} := (\hat{u}^{(0)} + s^{(0)}) + h(\hat{u}^{(1)} + s^{(1)}) + \ldots + h^n(\hat{u}^{(n)} + s^{(n)})$

with $\left\{ \begin{array}{l} {\rm smooth,\ grid-independent\ functions\ } u^{(0)}, u^{(1)}, \ldots {\rm\ restricted\ onto\ the\ grid\ (pure)\ grid\ functions\ } s^{(0)}, s^{(1)}, \ldots \end{array} \right.$

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$$r^{[n]} := \hat{D}u^{[n]} - \varsigma = \begin{cases} u_0^{[n]} & - u_0 \\ \frac{1}{h^2}[a+b, \overset{*}{c}, b, a]u_1^{[n]} & - f(h) \\ \frac{1}{h^2}[a, b, \overset{*}{c}, b, a] u_i^{[n]} & - f(ih) & i \in \{2, ..., N-2\} \\ \frac{1}{h^2}[a, b, \overset{*}{c}, a+b]u_{N-1}^{[n]} & - f(Nh-h) \\ u_N^{[n]} & - u_L \end{cases}$$

- Perform Taylor expansion of $u^{(k)}$ up to the order n-k.
- Requirement: $r^{[n]} = O(h^n) \Rightarrow$ Defining equations for unknown $u^{(0)}, s^{(0)}, ...$

• Ansatz: $u^{[n]} := (\hat{u}^{(0)} + s^{(0)}) + h(\hat{u}^{(1)} + s^{(1)}) + \ldots + h^n(\hat{u}^{(n)} + s^{(n)})$

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• BVPs demanded for
$$u^{(0)}, u^{(4)}$$
:
$$\begin{cases} u^{(0)}(0) = u_0 \wedge u^{(0)}(L) = u_L \wedge \partial^2 u = f \\ u^{(4)}(0) = 0 & \wedge u^{(4)}(L) = 0 & \wedge \partial^2 u = -\frac{1}{90} \partial^6 u^{(0)} \end{cases}$$

• Equations demanded for $s^{(1)}$:

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- However: Damping property yields boundedness of $s^{(1)}$.
- Convergence is established in spite of negative consistency order!

Validation I



Validation II



random polynomial: $u(x) = -6.667x^7 + 5.89x^6 + 2.48x^5 - 3.46x^4 + 2.69x^3 + 9.71x^2 - 3.45x - 7.32$

Approach to Convergence by Asymptotics



u pressure

Part 3: A few words about convergence & Retrospect

Asymptotic Expansions and Convergence

• Setting: $\epsilon \in (0,1]$: $A_{\epsilon}z = 0$, $z = z_{\epsilon} \in \mathbb{Z}_{\epsilon}$



Part 3: A few words about convergence & Retrospect

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pressure

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$$||x_{\epsilon} - z_{\epsilon}|| = ||(A_{\epsilon}^{-1} \circ A_{\epsilon})x_{\epsilon} - (A_{\epsilon}^{-1} \circ A_{\epsilon})z_{\epsilon}||$$

= $\operatorname{Lip}_{A_{\epsilon}^{-1}}||A_{\epsilon}x_{\epsilon} - \overbrace{A_{\epsilon}z_{\epsilon}}^{=0}|| = \operatorname{Lip}_{A_{\epsilon}^{-1}}||r_{\epsilon}|| \xrightarrow{\epsilon \to 0}{!} 0$

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- Examples of application: convergence proofs for the D1P2- and D1P3-model with different linear equilibria and periodic boundary conditions:
 - LB-equation: \mathcal{L}^2 -stability based on an energy estimate
 - LB-algorithm: ℓ^{∞} -stability using structure & positivity of evolution operator

Brief Retrospect

- Relevance of irregular expansions for
 - "continuous" problems,
 - discrete problems.
- Enables us to obtain complete understanding.



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- bounce back rule on specific bounded domains $(\frac{1}{2} \text{ link})$

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- requires smooth (Navier-)Stokes solutions
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- boundary layers reduce order of expansion $(\frac{1}{2}$ links help a little)

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- advantage of MRT: indication to set unused $\lambda \, {\rm 's}$ to 1

Convergence

• periodic domain, smooth start or compatible initialization

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• bounded domain $(\frac{1}{2} \text{ link})$, pressure and stress initialization

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• understand lattice Boltzmann algorithms

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