On recovering the second-order convergence of LBM with reaction-type source terms

Grzegorz Gruszczyński[a,b], Michał Dzikowski[b], Łukasz Łaniewski-Wołłk[c]

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[a]Warsaw University of Technology, Faculty of Power and Aeronautical Engineering
[b]University of Warsaw, Interdisciplinary Centre for Mathematical and Computational Modelling
[c]School of Mechanical and Mining Engineering, The University of Queensland, St Lucia, Australia

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Introduction

Goal

Simulate an Advection-Diffusion-Reaction Equation (ADRE) with an **implicit** source term.

$$\frac{\partial}{\partial t}\phi + \nabla \cdot (\mathbf{u}\phi) = \nabla \cdot (M\nabla\phi) + Q(\phi, \mathbf{x}, t) \tag{1}$$

The ADRE can be simulated by a discrete Boltzmann equation,

$$\frac{\partial}{\partial t} h_i + \sum_j e_i^j \frac{\partial}{\partial x_j} h_i = \frac{1}{\tau}\left(h_i^{\mathrm{eq}}(\phi, \mathbf{u}) - h_i\right) + q_i(\phi, \mathbf{x}, t), \tag{2}$$

where $\phi = \sum_i h_i = \sum_i h_i^{\mathrm{eq}}(\phi, \mathbf{u})$, and $Q = \sum q_i$.

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where $\phi = \sum_i h_i = \sum_i h_i^{eq}(\phi, \mathbf{u})$, and $Q = \sum q_i$.

The i-th characteristic of DBE is given by:
$\mathbf{x}(s) = \mathbf{x} + s\,\mathbf{e}_i$, and $t(s) = t + s$.

$$\underbrace{\int_0^1 \left(\frac{\partial}{\partial t} h_i + e_i^j \frac{\partial}{\partial x_j} h_i\right) ds}_{I_1} = \underbrace{\int_0^1 \left(\frac{1}{\tau}\left(h_i^{eq} - h_i\right) + q_i\right) ds}_{I_2}. \tag{3}$$

Notice: The space and time integration is not treated independently in the construction of a LBM scheme.

The first integral can be evaluated directly, as it is a material derivative of h_i,

$$I_1 = \int_0^1 \left(\frac{\partial}{\partial t} h_i + e_i^j \frac{\partial}{\partial x_j} h_i \right) ds = h_i(\hat{\mathbf{x}}, \hat{t}\,) - h_i(\mathbf{x}, t). \tag{4}$$

where $\hat{\mathbf{x}} = \mathbf{x} + \mathbf{e}_i$, $\hat{t} = t + 1$, $\hat{\phi} = \phi(\hat{\mathbf{x}}, \hat{t})$, etc.

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where $\hat{\mathbf{x}} = \mathbf{x} + \mathbf{e}_i$, $\hat{t} = t + 1$, $\hat{\phi} = \phi(\hat{\mathbf{x}}, \hat{t})$, etc.

The second integral can be approximated by the trapezoidal rule,

$$\begin{aligned} I_2 &= \int_0^1 \left(\frac{1}{\tau} \left(h_i^{\mathrm{eq}} - h_i \right) + q_i \right) ds \\ &\simeq \frac{1}{2} \left[\frac{1}{\tau} \left(h_i^{\mathrm{eq}}(\hat{\phi}, \hat{\mathbf{u}}) - h_i(\hat{\mathbf{x}}, \hat{t}) \right) + q_i(\hat{\phi}, \hat{\mathbf{x}}, \hat{t}) \right] + & (5) \\ &+ \frac{1}{2} \left[\frac{1}{\tau} \left(h_i^{\mathrm{eq}}(\phi, \mathbf{u}) - h_i(\mathrm{x}, t) \right) + q_i(\phi, \mathbf{x}, t) \right]. & (6) \end{aligned}$$

Redefinition of variables

Collecting the future variables dependent on $\hat{\mathbf{x}}$ and $\hat{t}$ collected on the left hand side gives,

$$\left[1+\frac{1}{2\tau}\right] h_i(\hat{\mathbf{x}},\hat{t}\,) - \frac{1}{2\tau} h_i^{\mathrm{eq}}(\hat{\phi},\hat{\mathbf{u}}) - \frac{1}{2} q_i(\hat{\phi},\hat{\mathbf{x}},\hat{t}\,) =$$
$$\left[1-\frac{1}{2\tau}\right] h_i(\mathbf{x},t\,) + \frac{1}{2\tau} h_i^{\mathrm{eq}}(\phi,\mathbf{u}) + \frac{1}{2} q_i(\phi,\mathbf{x},t).$$

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$$\left[1-\frac{1}{2\tau}\right]h_i(\mathbf{x},t\,)+\frac{1}{2\tau}h_i^{\mathrm{eq}}(\phi,\mathbf{u})+\frac{1}{2}q_i(\phi,\mathbf{x},t).$$

The new density (denoted with a tilde) is defined as,

$$\tilde{h}_i(\bullet)=\left[1+\frac{1}{2\tau}\right]h_i(\bullet)-\frac{1}{2\tau}h_i^{eq}(\bullet)-\frac{1}{2}q_i(\bullet)$$
$$\implies h_i(\bullet)=\frac{1}{1+\frac{1}{2\tau}}\left(\tilde{h}_i(\bullet)+\frac{1}{2\tau}h_i^{eq}(\bullet)+\frac{1}{2}q_i(\bullet)\right),$$

where $\bullet$ is a placeholder for variables in either t or $\hat{t}$.

The Discrete Boltzmann equation

Collecting the future variables dependent on $\hat{\mathbf{x}}$ and $\hat{t}$ collected on the left hand side gives,

$$\left[1+\frac{1}{2\tau}\right] h_i(\hat{\mathbf{x}},\hat{t}\,) - \frac{1}{2\tau} h_i^{\mathrm{eq}}(\hat{\phi},\hat{\mathbf{u}}) - \frac{1}{2} q_i(\hat{\phi},\hat{\mathbf{x}},\hat{t}\,) =$$
$$\left[1-\frac{1}{2\tau}\right] h_i(\mathbf{x},t\,) + \frac{1}{2\tau} h_i^{\mathrm{eq}}(\phi,\mathbf{u}) + \frac{1}{2} q_i(\phi,\mathbf{x},t). \tag{7}$$

The new density (denoted with a tilde) is defined as,

$$\tilde{h}_i(\bullet) = \left[1+\frac{1}{2\tau}\right] h_i(\bullet) - \frac{1}{2\tau} h_i^{eq}(\bullet) - \frac{1}{2} q_i(\bullet) \Leftrightarrow \tag{8}$$

$$\Leftrightarrow h_i(\bullet) = \frac{1}{1+\frac{1}{2\tau}} \left(\tilde{h}_i(\bullet) + \frac{1}{2\tau} h_i^{eq}(\bullet) + \frac{1}{2} q_i(\bullet)\right), \tag{9}$$

where $\bullet$ is a placeholder for variables in either t or $\hat{t}$.

Next, we substitute LHS of eq. (7) with LHS of eq. (8)
and $h_i(\mathbf{x},t\,)$ from RHS of eq. (7) with RHS of eq. (9).

After integrating with trapezoidal rule and redefinition of variables an explicit evolution scheme, is obtained,

$$\tilde{h}_i(\mathbf{x}+\mathbf{e}_i, t+1) = \tilde{h}_i^\star(\mathbf{x}, t) = (1-\omega)\tilde{h}_i(\mathrm{x}, t) + \omega h_i^{\mathrm{eq}}(\phi, \mathbf{u}) + \left(1-\frac{\omega}{2}\right) q_i(\phi, \mathbf{x}, t). \tag{10}$$

Notice the implicit dependence on the scalar field, ϕ.

What is the relation between $\tilde{\phi} = \sum_i \tilde{h}_i$ and $\phi = \sum_i h_i$?

Calculation of the scalar field

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What is the relation between $\tilde{\phi} = \sum_i \tilde{h}_i$ and $\phi = \sum_i h_i$?

$$\begin{aligned}\tilde{\phi} = \sum_i \tilde{h}_i &= \left(1 + \frac{1}{2\tau}\right)\sum_i h_i(\mathbf{x}, t) - \frac{1}{2\tau}\sum_i h_i^{\mathrm{eq}}(\phi, \mathbf{u}) - \frac{1}{2}\sum_i q_i(\phi, \mathbf{x}, t) \\ &= \phi - \frac{1}{2}Q(\phi, \mathbf{x}, t).\end{aligned} \tag{11}$$

This is still an implicit equation, however, given the function $Q = Q(\phi)$ we can attempt to solve it for.

Scaling of LBM

The ADRE can be expressed in a non-dimensional form as:

$$\frac{\partial}{\partial t}\phi + \mathbf{PeFo}\nabla \cdot (\mathrm{u}\phi) = \mathbf{Fo}\Delta\phi + \mathbf{DaFo}P(\phi). \tag{12}$$

For each LBM grid, there are corresponding values of M, λ, and U that preserve the similarity numbers $\mathbf{Fo} = \frac{MT}{L^2}$, $\mathbf{Da} = \frac{\lambda L^2}{M}$ and $\mathbf{Pe} = \frac{UL}{M}$.

We can construct a series of lattices using a scaling factor $\varepsilon_k \to 0$

	characteristic		simulation parameters		
scaling	length	time	M	U	λ
acoustic	$L_k = \varepsilon_k^{-1} L_0$	$T_k = \varepsilon_k^{-1} T_0$	$M_k = \varepsilon_k^{-1} M_0$	$U_k = U_0$	$\lambda_k = \varepsilon_k \lambda_0$
diffusive	$L_k = \varepsilon_k^{-1} L_0$	$T_k = \varepsilon_k^{-2} T_0$	$M_k = M_0$	$U_k = \varepsilon_k U_0$	$\lambda_k = \varepsilon_k^2 \lambda_0$

Convergence Study

Convergence of LBM to ADRE

Consider a simple ADRE with linear source term,

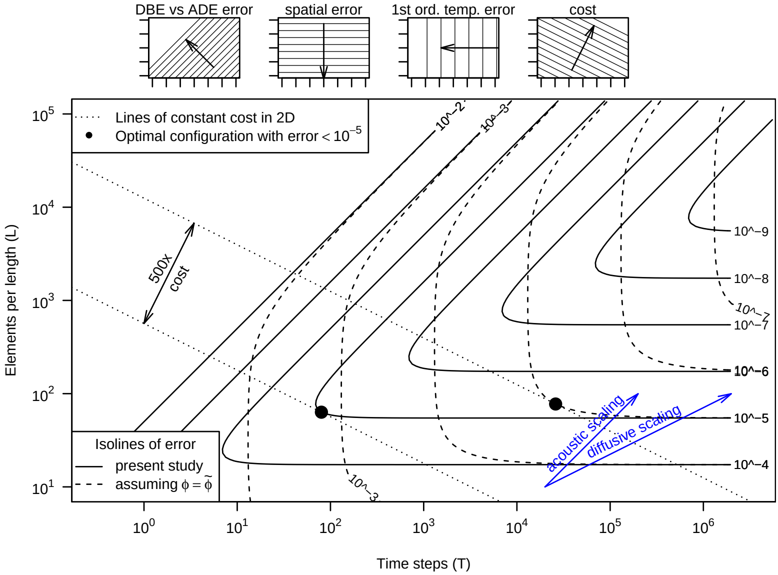
$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) = \nabla \cdot (M \nabla \phi) + \underbrace{\lambda(\gamma(\mathbf{x}) - \phi)}_{Q=Q(\phi)}. \tag{13}$$

The analytical solution will be a transition between the initial condition ($\phi\,|_{t=0} = Pe^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$ and $\gamma = Ge^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$) and the steady state,

$$\phi_{\text{analytical}}(\mathrm{x}, t) = \left(e^{-at}P + (1 - e^{-at})a^{-1}\lambda G\right) e^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}, \tag{14}$$

where $a = \lambda + \mathrm{i}\,(\mathbf{u} \cdot \mathbf{k}) + M\,(\mathbf{k} \cdot \mathbf{k})$.

Error landscape



Consider the Allen-Cahn solidification equation,

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathrm{u}\phi) = \nabla \cdot (M \nabla \phi) + \underbrace{\lambda \phi \left(1 - \phi^2\right)}_{Q = Q(\phi)}.$$

To calculate the intensity of the source term we need to find $\phi = \phi(\tilde{\phi})$ to plug in to $Q = Q(\phi)$.

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To calculate the intensity of the source term we need to find $\phi = \phi(\tilde{\phi})$ to plug in to $Q = Q(\phi)$.

The implicit relation between ϕ and $\tilde{\phi}$ is,

$$\tilde{\phi} = \sum_i \tilde{h}_i = \phi - \frac{1}{2}Q(\phi) = \phi - \frac{1}{2}\lambda\phi\left(1-\phi^2\right) = \phi\left(1 - \frac{\lambda}{2}\left(1-\phi^2\right)\right).$$

Practical example: Convergence study

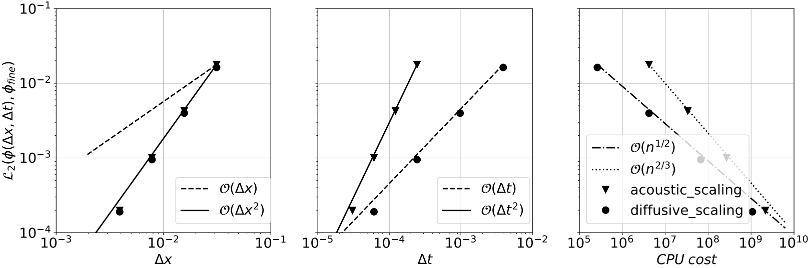
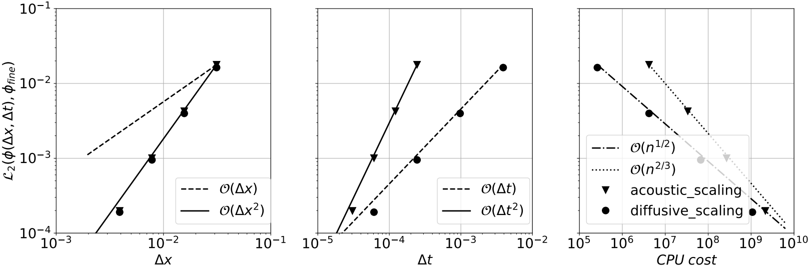


Figure 1: Results for **Da** $= 1000$, **Pe** $= 500$, **Fo** $= 0.001$



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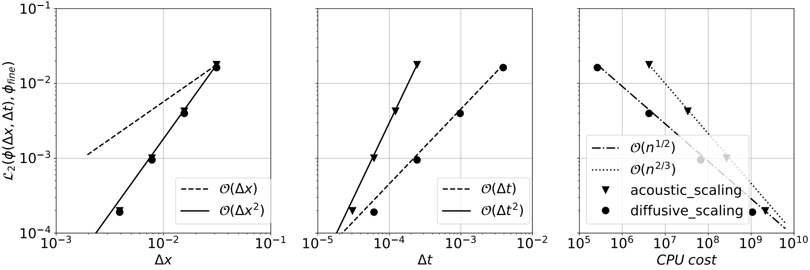
Remarks:

- Can we progress along iso-lines of error to obtain the same convergence plot with lower computational cost?



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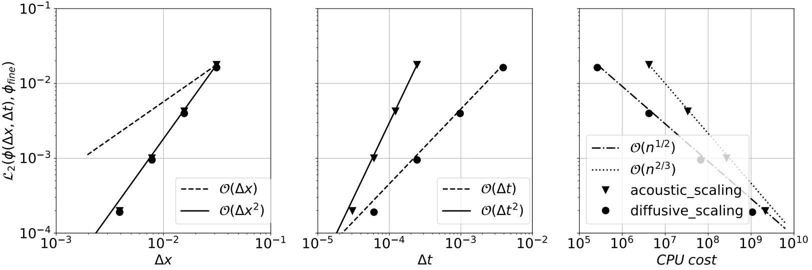

Figure 1: Results for $\mathbf{Da} = 1000$, $\mathbf{Pe} = 500$, $\mathbf{Fo} = 0.001$

Remarks:

- Can we progress along iso-lines of error to obtain the same convergence plot with lower computational cost?
- Why only acoustic scaling provided 2-nd order convergence with respect to time step?
- Which scaling is computationally cheaper?

Conclusions

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- To find the value of the source term $Q = Q(\phi)$, one have to solve $\tilde{\phi} = \sum_i \tilde{h}_i = \phi - \frac{1}{2}Q(\phi) \implies \phi = ...$
- The acoustic scaling can be viewed as finer integration of DBE along characteristic.
- The diffusive scaling compares solutions from different characteristics.
- The 45 degree slope of isoline of error is origins from the fact that LBM converges to DBE, which is not necessary the macroscopic PDE (like ADRE) one wanted to solve.
- It is easier to do a good simulation, than to find ”CPU cheapest” simulation parameters.
- Is there any other scaling (path) across error landscape ;-) ?

Questions?

?

ggruszczynski@gmail.com

Manuscript [1]: `https://arxiv.org/abs/2107.03962`
TCLB solver [2, 3]: `https://github.com/CFD-GO/TCLB`

References

- Grzegorz Gruszczyński, Michał Dzikowski, and Łukasz Łaniewski Wołłk. *On recovering the second-order convergence of the lattice Boltzmann method with reaction-type source terms*. 2021. arXiv: 2107.03962 [physics.flu-dyn].
- Ł. Łaniewski-Wołłk and J. Rokicki. "Adjoint Lattice Boltzmann for topology optimization on multi-GPU architecture". *Computers and Mathematics with Applications* 71 (2016), pp. 833–848. DOI: 10.1016/j.camwa.2015.12.043.

References II

- Łukasz Łaniewski-Wołłk et al. *CFD-GO/TCLB: Version 6.5.* Version v6.5.0. 2020. DOI: 10.5281/zenodo.4074541. URL: https://github.com/CFD-GO/TCLB.
- Baochang Shi and Zhaoli Guo. "Lattice Boltzmann model for nonlinear convection-diffusion equations". *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics* 79.1 (2009). ISSN: 15393755. DOI: 10.1103/PhysRevE.79.016701.
- Baochang Shi et al. "A new scheme for source term in LBGK model for convection-diffusion equation". *Computers and Mathematics with Applications* 55.7 (2008), pp. 1568–1575. ISSN: 08981221. DOI: 10.1016/j.camwa.2007.08.016.

(Supplementary material)
Comparison of approaches to the source term integration

Another approach

Contrary to the previously proposed scheme, Shi et al. [5, 4] utilized $\phi = \overline{\phi} = \sum_i \overline{h}_i$ where $\overline{h}$ is a shifted variable, analogous to $\tilde{h}_i$, but without the contribution of q_i.

$$\overline{h}_i^{\star}(\mathbf{x}, t) = (1-\omega)\overline{h}_i(\mathbf{x}, t) + \omega h_i^{\mathrm{eq}}(\phi, \mathbf{u}) + q_i(\phi, \mathbf{x}, t) + \frac{1}{2}\left(\frac{\partial}{\partial t} + \mathbf{e}_i \cdot \nabla\right) q_i. \tag{15}$$

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If a forward FD is used the result is equivalent to that obtained through the trapezoidal rule (with appropriate redefinition of variables),

$$\begin{aligned} q_i(\phi, \mathbf{x}, t) + \frac{1}{2}\left(\frac{\partial}{\partial t} + \mathbf{e}_i \cdot \nabla\right) q_i(\phi, \mathbf{x}, t) &= q_i(\phi, \mathbf{x}, t) + \frac{1}{2}\left(q_i(\hat{\phi}, \hat{\mathbf{x}}, \hat{t}\,) - q_i(\phi, \mathbf{x}, t)\right) \\ &= \frac{1}{2}\left(q_i(\hat{\phi}, \hat{\mathbf{x}}, \hat{t}\,) + q_i(\phi, \mathbf{x}, t)\right). \end{aligned}$$

(Supplementary material)
Equivalent forms
of collision operator
in the moments' space

Moments of the distribution

The raw moments can be expressed as $\boldsymbol{\Upsilon} = \mathbb{M}\mathsf{h}$.

The moments of the discrete equilibrium are defined as, $\boldsymbol{\Upsilon}^{\mathsf{eq}}(\phi, \mathsf{u}) = \phi\,\boldsymbol{\Gamma}(\mathsf{u})$, where,

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The moments of the discrete equilibrium are defined as, $\boldsymbol{\Upsilon}^{\text{eq}}(\phi, \mathbf{u}) = \phi\,\boldsymbol{\Gamma}(\mathbf{u})$, where,

$$\boldsymbol{\Gamma}(\mathbf{u}) = \begin{bmatrix} 1 \\ u_x \\ u_y \\ c_s^2 + u_x^2 \\ c_s^2 + u_y^2 \\ u_x u_y \\ u_y(c_s^2 + u_x^2) \\ u_x(c_s^2 + u_y^2) \\ c_s^4 + c_s^2(u_x^2 + u_y^2) + u_x^2 u_y^2 \end{bmatrix}^\top . \tag{16}$$

Similarly, the moments of the source term can be expressed as $\mathbf{R} = Q\,\boldsymbol{\Gamma}(\mathbf{u})$.

The collision in the moments' space

If the moments of the source term are chosen to be $\mathsf{R} = Q\,\boldsymbol{\Gamma}(u)$, and $\boldsymbol{\Upsilon}^{\mathrm{eq}}(\phi, u) = \phi\,\boldsymbol{\Gamma}(u)$, one can use eqs. (11) and (16) to express the collision operator in three equivalent forms,

$$\tilde{\boldsymbol{\Upsilon}}^{\star} = (1-\omega)\tilde{\boldsymbol{\Upsilon}} + \omega\boldsymbol{\Upsilon}^{\mathrm{eq}}(\phi, \mathbf{u}) + (1-\frac{\omega}{2})\mathsf{R} \tag{17}$$

$$= (1-\omega)\tilde{\boldsymbol{\Upsilon}} + \omega\boldsymbol{\Upsilon}^{\mathrm{eq}}(\tilde{\phi}, \mathbf{u}) + \mathsf{R} \tag{18}$$

$$= (1-\omega)\left(\tilde{\boldsymbol{\Upsilon}} - \boldsymbol{\Upsilon}^{\mathrm{eq}}(\tilde{\phi}, \mathbf{u})\right) + \boldsymbol{\Upsilon}^{\mathrm{eq}}(\tilde{\phi} + Q, \mathbf{u}) \tag{19}$$

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$$
\begin{aligned}
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&= (1-\omega)\tilde{\boldsymbol{\Upsilon}} + \omega\boldsymbol{\Upsilon}^{\mathrm{eq}}(\tilde{\phi}, \mathbf{u}) + \mathsf{R} && (18)\\
&= (1-\omega)\left(\tilde{\boldsymbol{\Upsilon}} - \boldsymbol{\Upsilon}^{\mathrm{eq}}(\tilde{\phi}, \mathbf{u})\right) + \boldsymbol{\Upsilon}^{\mathrm{eq}}(\tilde{\phi} + Q, \mathbf{u}) && (19)
\end{aligned}
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