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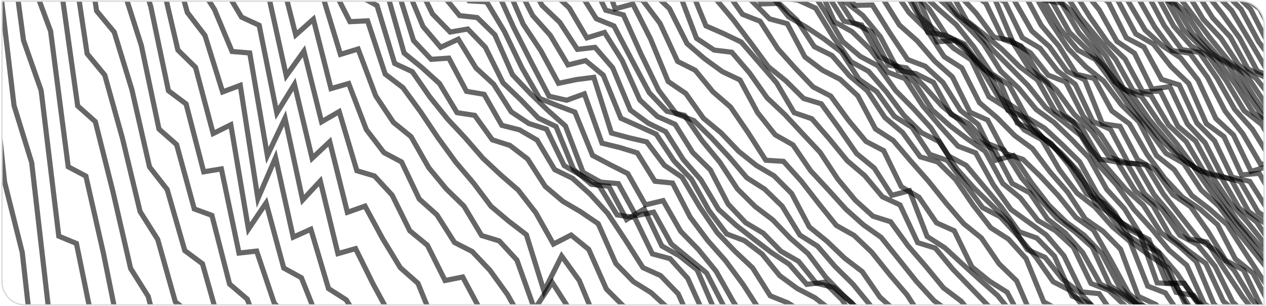
Temporal large eddy simulation with lattice Boltzmann methods

Groupe de travail "Schémas de Boltzmann sur réseau" à l’Institut Henri Poincaré (Online)

Stephan Simonis | November 24, 2021



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Motivation

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Why pair lattice Boltzmann methods (LBM) with temporal large eddy simulation (TLES)?

- LBM parallelizable/node-local
- TLES local in space
- Benefits of LES but preserve locality
- Classical advantages of causal time-domain filtering [Pru08]

Agenda

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Novelties:

- New combination of methods MRT LBM TLES
- Investigation of numerics for resulting scheme (canonical 3D test: Taylor–Green)
- Comparison to TLES with spectral element method (SEM)

This is joint work:

- S. Simonis, D. Oberle, M. Gaedtke, P. Jenny, M. J. Krause, *Temporal large eddy simulation with lattice Boltzmann methods*, 2021, Preprint submitted to J. Comput. Phys.
- S. Simonis, M. Haussmann, L. Kronberg, W. Dörfler, M. J. Krause, 2021, *Linear and brute force stability of orthogonal moment multiple-relaxation-time lattice Boltzmann methods applied to homogeneous isotropic turbulence*, Phil. Trans. R. Soc. A 379:20200405, DOI: 10.1098/rsta.2020.0405

Target equation

Approximate d-dimensional force-free incompressible Navier–Stokes equations (NSE).

NSE

$$\begin{cases} \nabla \cdot \boldsymbol{u} = 0 & \text{in } \Omega \times I, \\ \partial_t \boldsymbol{u} + \frac{1}{\rho} \nabla p + \nabla \cdot (\boldsymbol{u} \otimes \boldsymbol{u}) - \nu \Delta \boldsymbol{u} = 0 & \text{in } \Omega \times I, \\ \boldsymbol{u}(\cdot, 0) \equiv \boldsymbol{u}_0 & \text{in } \Omega, \end{cases} \tag{1}$$

where $\Omega \subseteq \mathbb{R}^d$ periodically embedded,
$I \subseteq \mathbb{R}_{\geq 0}$ denotes time,
$\boldsymbol{u}$ velocity with initial value $\boldsymbol{u}_0$,
p pressure,
$\nu > 0$ given viscosity,
ρ constant density.

Temporal direct deconvolution

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Temporal direct deconvolution model (TDDM) [OPJ20]:

- Eulerian time-domain filtering (function g, filter kernel G, filter width $\Theta > 0$, filtered quantity $\overline{\cdot}$)

$$\bar{g}(t;\Theta) = \int_{-\infty}^{t} G(t'-t;\Theta)\, g(t')\, \mathrm{d}t', \qquad (2)$$

- Filter operation in differential form for unfiltered quantity Υ (use exponential filter kernel)

$$\frac{\partial}{\partial t}\overline{\Upsilon} = \frac{\Upsilon - \overline{\Upsilon}}{\Theta}, \qquad (3)$$

- Reverse filtering operation for direct deconvolution

$$\Upsilon = \overline{\Upsilon} + \Theta \frac{\partial \overline{\Upsilon}}{\partial t}. \qquad (4)$$

- Apply filter to NSE and obtain ODE for residual stress $T_{\alpha\beta} = \overline{u_\alpha u_\beta} - \overline{u_\alpha}\,\overline{u_\beta}$

System to approximate

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- Instead of NSE (1), approximate closed system:

Time-filtered NSE

$$\frac{\partial \bar{u}_\alpha}{\partial x_\alpha} = 0, \qquad (5)$$

$$\frac{\partial \bar{u}_\alpha}{\partial t} + \frac{\partial \bar{u}_\alpha \bar{u}_\beta}{\partial x_\beta} = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_\alpha} + \nu \frac{\partial^2 \bar{u}_\alpha}{\partial x_\beta \partial x_\beta} - \frac{\partial T_{\alpha\beta}}{\partial x_\beta}, \qquad (6)$$

Residual stress evolution equation

$$\frac{\partial T_{\alpha\beta}}{\partial t} = -\frac{T_{\alpha\beta}}{\Theta} + \Theta \frac{\partial \bar{u}_\alpha}{\partial t}\frac{\partial \bar{u}_\beta}{\partial t}. \qquad (7)$$

How to consistently couple LES models with LBM?

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- Filtered Boltzmann equation (FBE) with BGK collision (Malaspinas and Sagaut [MS12]):

$$\frac{\partial \bar{f}}{\partial t} + (\boldsymbol{\xi} \cdot \nabla) \bar{f} = -\frac{1}{\tau}\left[\bar{f} - f^{\mathrm{eq}}\left(\bar{f}\right)\right] + \frac{1}{\tau}\mathcal{R}. \tag{8}$$

- Inject Hermite expansion for the equilibrium f^{eq} into residual $\mathcal{R} = \left[\overline{f^{\mathrm{eq}}} - f^{\mathrm{eq}}\left(\bar{f}\right)\right]$, thus

$$\mathcal{R} = w(\boldsymbol{\xi}) \sum_{n=0}^{N} \mathcal{H}^{(n)}(\boldsymbol{\xi}) : \mathcal{R}^{(n)}, \quad \text{where} \begin{cases} \mathcal{R}^{(0)} & = 0, \\ \mathcal{R}^{(1)}_{\alpha} & = \mathbf{0}, \\ \mathcal{R}^{(2)}_{\alpha\beta} & = \boxed{T_{\alpha\beta}} + \eta\delta_{\alpha\beta}, \\ & \vdots \ \ulcorner \text{cutoff}. \end{cases} \tag{9}$$

- T and $\eta \equiv 0$ (incompressible & isothermal) are subgrid stress and subgrid temperature, respectively.

The final scheme: MRT LBM TLES

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Generalize to MRT (for underresolved stability [Sim+21]), hence MRT TLES LBM defined via:

Filtered lattice Boltzmann equation (FLBE) with multiple-relaxation-time (MRT) collision

$$\boldsymbol{n}\left(\boldsymbol{x}+\triangle t\xi_i, t+\triangle t\right)=\boldsymbol{n}\left(\boldsymbol{x}, t\right)-\triangle t K\left\{\left[\boldsymbol{n}\left(\boldsymbol{x}, t\right)-\boldsymbol{f}^{\mathrm{eq}}\left(\boldsymbol{n}\right)\right]+\boldsymbol{R}\left(\boldsymbol{x}, t\right)\right\}, \tag{10}$$

where

$$\boldsymbol{R}\left(\boldsymbol{x}, t\right)=\frac{1}{2c_s^4}\left(w_i\mathcal{H}^{(2)}_{i\alpha\beta}T_{\alpha\beta}\left(\boldsymbol{x}, t\right)\right)^{\mathrm{T}}_{i=0,1,\ldots,q-1}. \tag{11}$$

Discretized residual evolution

$$T_{\alpha\beta}\left(\boldsymbol{x}, t\right)=\left(1-\frac{\triangle t}{\Theta}\right)T_{\alpha\beta}\left(\boldsymbol{x}, t-\triangle t\right)+\frac{\Theta}{\triangle t}\left\{\left[\bar{u}_\alpha\left(\boldsymbol{x}, t\right)-\bar{u}_\alpha\left(\boldsymbol{x}, t-\triangle t\right)\right]\left[\bar{u}_\beta\left(\boldsymbol{x}, t\right)-\bar{u}_\beta\left(\boldsymbol{x}, t-\triangle t\right)\right]\right\}. \tag{12}$$

Taylor–Green vortex

- Initialize flow with Taylor–Green vortex (TGV) (see e.g. [Bra91; Hau+19])

$$\boldsymbol{u}_0(\boldsymbol{x}) = \begin{pmatrix} U_c \sin\left(\frac{x}{l_c}\right)\cos\left(\frac{y}{l_c}\right)\cos\left(\frac{z}{l_c}\right) \\ -U_c \cos\left(\frac{x}{l_c}\right)\sin\left(\frac{y}{l_c}\right)\cos\left(\frac{z}{l_c}\right) \\ 0 \end{pmatrix}. \tag{13}$$

- Compute kinetic energy, enstrophy, and total/resolved/model dissipation rate:

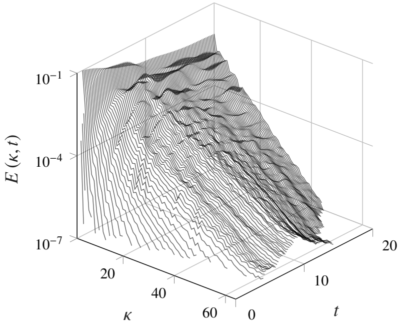
$$k(t) = \frac{1}{|\Omega|}\int_\Omega \frac{1}{2}\boldsymbol{u}^2 \mathrm{d}\boldsymbol{x}, \quad \zeta(t) = \frac{1}{|\Omega|}\int_\Omega (\nabla\times\boldsymbol{u})^2 \,\mathrm{d}\boldsymbol{x}, \tag{14}$$

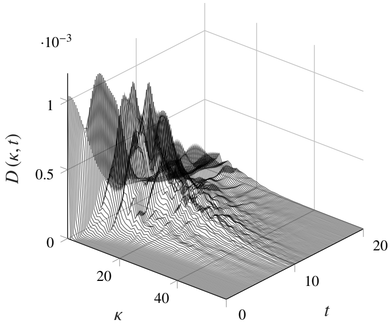
$$\epsilon_{\mathrm{tot}}(t) = -\frac{\mathrm{d}k}{\mathrm{d}t}, \quad \epsilon_{\mathrm{res}}(t) = 2\pi\nu\zeta, \quad \epsilon_{\mathrm{mod}} = \epsilon_{\mathrm{tot}} - \epsilon_{\mathrm{res}}. \tag{15}$$

- Compute energy spectrum $E(\kappa, t)$ and dissipation spectrum $D(\kappa, t) = 2\nu\kappa E(\kappa, t)$.

Reference solution

- Direct numerical simulation (DNS)
- Spectral element method (SEM) as reference
- Resolves Kolmogorov length
- E.g. spectra for $Re = 800$:





Stability of MRT LBM

Use standard equilibrium and define matrix $K = M^{-1}SM$ via:

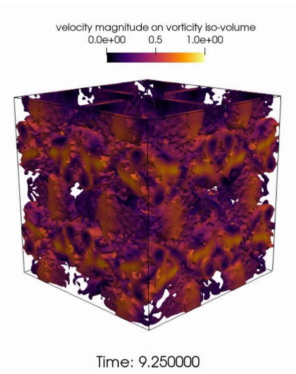
- orthogonal moments $M \in \mathrm{GL}_q(\mathbb{R})$,
- relaxation matrix $S = \mathrm{diag}(\boldsymbol{s}^{\mathrm{T}})$,
- dynamic relaxation frequency vector $\boldsymbol{s}$ for stability [Sim+21].

Orthogonal moment MRT LBM: Dynamic relaxation frequencies

moment type	physical tensor	moment order	$\tilde{\boldsymbol{s}}$ [d'H+02]	$\hat{\boldsymbol{s}}$ [CM+20]	$\boldsymbol{s}$ [Sim+21]
hydro-dynamic	ρ	0	0	0	0
	$\rho u_x, \rho u_y, \rho u_z$	1	0	0	0
	e	2	1.19	1.19 or $\frac{2c_s^2}{2\nu+c_s^2}$	s_e
	$3P_{xx}, P_{yy}-P_{zz}, P_{xy}, P_{yz}, P_{xz}$	2	$\frac{2c_s^2}{2\nu+c_s^2}$	$\frac{2c_s^2}{2\nu+c_s^2}$	s_P
kinetic	q_x, q_y, q_z	3	1.2	$\hat{s}_q$	s_q
	μ_x, μ_y, μ_z	3	1.98	$\hat{s}_\mu$	s_μ
	ε	4	1.4	1.4	s_ε
	$3\Pi_{xx}, \Pi_{yy}-\Pi_{zz}$	4	1.4	1.4	s_Π

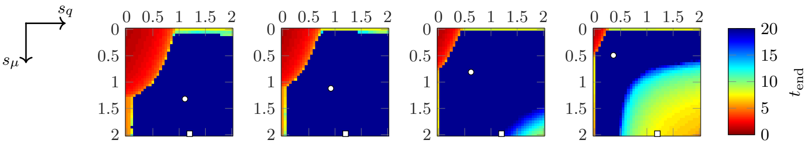
Table: Moments and corresponding relaxation frequencies and functions for $D3Q19$ MRT.

Orthogonal moment MRT LBM (no model): Brute force stability



Compute TGV simulation for $Re = 1600$, $N = 64$ until divergence occurs:

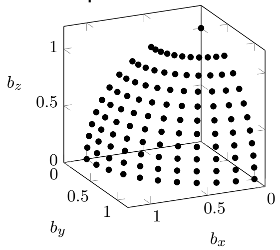
- 1 pixel = 1 simulation of TGV until $t_{\mathrm{end}} \leq 20$ for 1 specific constant relaxation matrix S
- 1 map = 41^2 simulations of three-dimensional TGV



(a) $Ma = 0.3$ (b) $Ma = 0.2$ (c) $Ma = 0.1$ (d) $Ma = 0.05$

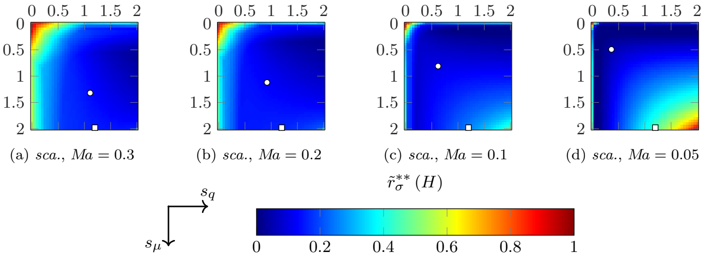
Orthogonal moment MRT LBM (no model): Von Neumann stability

$\boldsymbol{u}_{\mathrm{m}} = \mathrm{ave}(\boldsymbol{u}_0) u^{\mathrm{L}} \boldsymbol{b}$,
where $\boldsymbol{b} \in \mathcal{B}$ are nodes on unit sphere



Compute scaled normalized spectral radius $\tilde{r}_{\sigma}^{**}$ of linearized amplification matrix $H(\boldsymbol{k}, \boldsymbol{u}_{\mathrm{m}}, S) \in \mathbb{R}^{q \times q}$:

- 1 pixel = $257^3 \cdot 111$ spectral radius computations of H with QR algorithm for 1 specific constant relaxation matrix S
- 1 map = $41^2 \cdot (257^3 \cdot 111)$ max. eigenvalue computations



(a) *sca.*, $Ma = 0.3$ (b) *sca.*, $Ma = 0.2$ (c) *sca.*, $Ma = 0.1$ (d) *sca.*, $Ma = 0.05$

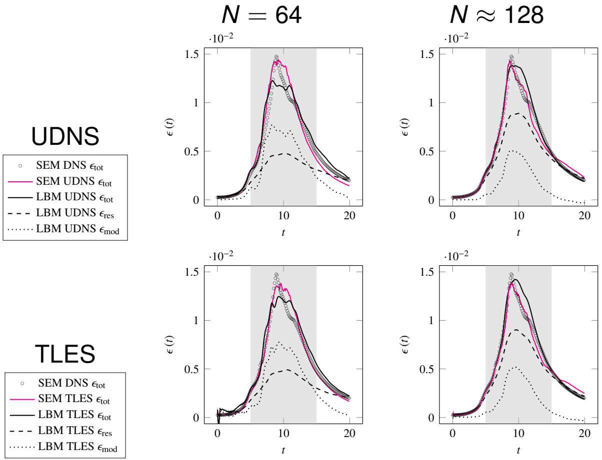
Calibration of the TDDM

Compare sequences of outputs (wrt. recovery of ϵ_{res}, ϵ_{mod}, ϵ_{tot}, E, and D) for

- $Re = 800$, $N = 64$, $Ma = 0.1$, $\Theta/\triangle t \in [5, 40]$
  $\Rightarrow$ optimal for $\Theta/\triangle t = 10$
- $Re = 800$, $N = 64$, $Ma \in [0.05, 0.2]$, $\Theta/\triangle t = 10$
  $\Rightarrow$ optimal for $Ma = 0.1$

Increase to $Re = 3000$ for the following tests ...

LBM vs SEM: Dissipation rate with and without TLES



$Re = 3000$, $Ma = 0.1$, $\Theta/\triangle t = 10$.

Key observation:

- Model enhances dissipation rate around the peak region ($t \approx 10$) towards DNS shape

LBM vs SEM: Spectra at $t = 9$ with and without TLES

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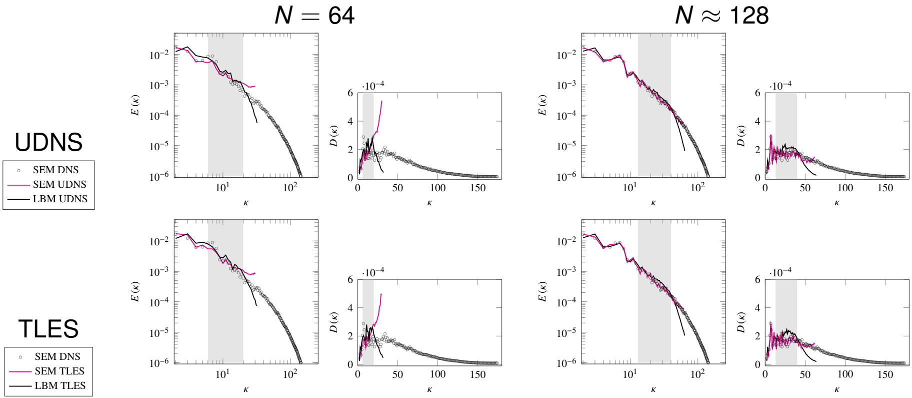

$Re = 3000$, $Ma = 0.1$, $\Theta / \triangle t = 10$.

Key observations:

- Model increases energy in intermediate wavenumbers
- Energy transfer upwards in the energy cascade

Subgrid activity and energy spectrum error

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How to measure model impact on accuracy? Geurts *et al.* [GF02]:

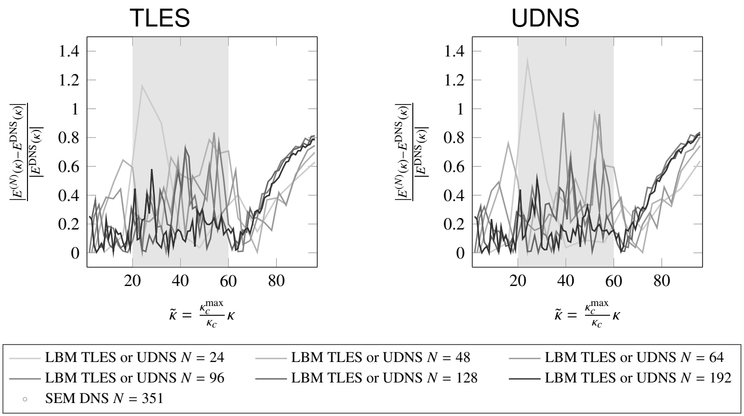
Subgrid activity

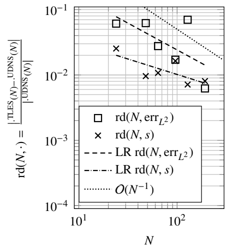
$$s(N,t) = \frac{\left|\epsilon_{\mathrm{mod}}^{(N)}(t)\right|}{\left|\epsilon_{\mathrm{tot}}^{(N)}(t)\right|}, \tag{16}$$

Energy spectrum error

$$\mathrm{err}_{L^2}(N,t) = \sqrt{\frac{\sum_{i=2}^{c}\left|E^{(N)}(\kappa_i,t) - E^{\mathrm{DNS}}(\kappa_i,t)\right|^2}{\sum_{i=2}^{c}\left|E^{\mathrm{DNS}}(\kappa_i,t)\right|^2}}. \tag{17}$$

Subgrid activity and energy spectrum error





Key observations:

- Local error peaks for low N decreased by TLES
- Model converges towards UDNS with EOC $\approx \mathcal{O}(N^{-1})$

Conclusion & Outlook

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Summary:

- First LBM TLES
- Consistent formulation
- Enhances turbulence recovery
- Retains convergence
- LBM computations were done with OpenLB [Kra+21] on the supercomputers ForHLR II and HoreKa

Possible future lines of work:

- Use other collision schemes
- Include regularization terms
- Derive compressible TDDM

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Thank you! Questions?

Announcement:

5th Spring School: LBM with OpenLB Software Lab

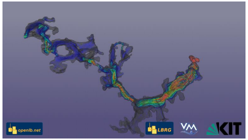
5th Spring School

Lattice Boltzmann Methods with OpenLB Software Lab

Kraków, Poland, 21st – 25th March 2022

- for scientists and industry, beginners level
- comprehensive **theoretical lectures on LBM**
- **mentored training** on case studies using *OpenLB*, **bring your own problem**
- knowledge exchange, networking at poster session, coffee breaks and excursion

350€ academia/1700€ industry for 5 days course including course material, 5x lunch, 2x dinner, coffee breaks and excursion



Executive committee

N. Hafen, **M. J. Krause**, J. E. Marquardt, **P. Madejski,** T. Kuś, N. Subramanian, M. Bujalski

Invited speakers

Timm Krüger, Tim Reis, Halim Kusumaatmaja, Francois Dubois

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organized under the honorary patronage of the dean of the Faculty of Mechanical Engineering and Robotics, Krzysztof Mendrok

1 23/04/2021 Mathias J. Krause Lattice Boltzmann Research Group, KIT

Methodological modifications

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Single-relaxation-time collision (SRT)

$$n_i\left(\boldsymbol{x}+\triangle t\boldsymbol{\xi}_i, t+\triangle t\right) = n_i\left(\boldsymbol{x}, t\right) - \frac{\triangle t}{\tau + \frac{\triangle t}{2}}\left\{\left[n_i\left(\boldsymbol{x}, t\right) - f_i^{\mathrm{eq}}\left(\boldsymbol{n}\right)\right] + R_i\left(\boldsymbol{x}, t\right)\right\} \tag{18}$$

Second order finite differenced (FD) residual evolution (2-step AB scheme)

$$\begin{aligned} T_{\alpha\beta}\left(\boldsymbol{x}, t\right) = & \left(1 - \frac{3\triangle t}{2\Theta}\right) T_{\alpha\beta}\left(\boldsymbol{x}, t-\triangle t\right) + \frac{\triangle t}{2\Theta} T_{\alpha\beta}\left(\boldsymbol{x}, t-2\triangle t\right) \\ & - \frac{\Theta}{2\triangle t}\left[\frac{1}{2}\bar{u}_\alpha\left(\boldsymbol{x}, t\right) - 2\bar{u}_\alpha\left(\boldsymbol{x}, t-\triangle t\right) + \frac{3}{2}\bar{u}_\alpha\left(\boldsymbol{x}, t-2\triangle t\right)\right]\left[\frac{1}{2}\bar{u}_\beta\left(\boldsymbol{x}, t\right) - 2\bar{u}_\beta\left(\boldsymbol{x}, t-\triangle t\right) + \frac{3}{2}\bar{u}_\beta\left(\boldsymbol{x}, t-2\triangle t\right)\right] \\ & + \frac{3\Theta}{8\triangle t}\left[\bar{u}_\alpha\left(\boldsymbol{x}, t\right) - \bar{u}_\alpha\left(\boldsymbol{x}, t-2\triangle t\right)\right]\left[\bar{u}_\beta\left(\boldsymbol{x}, t\right) - \bar{u}_\beta\left(\boldsymbol{x}, t-2\triangle t\right)\right]. \end{aligned}$$