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An Energy Stable Filtered Backward Euler Scheme for the MBE Equation with Slope Selection

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Abstract. As a promising strategy to adjust the order in the variable-order BDF algorithm, a time filtered backward Euler scheme is investigated for the molecular beam epitaxial equation with slope selection. The temporal second-order convergence in the L^2 norm is established under a convergence-solvability-stability (CSS)-consistent time-step constraint. The CSS-consistent condition means that the maximum step-size limit required for convergence is of the same order to that for solvability and stability (in certain norms) as the small interface parameter $\varepsilon \to 0^+$. Similar to the backward Euler scheme, the time filtered backward Euler scheme preserves some physical properties of the original problem at the discrete levels, including the volume conservation, the energy dissipation law and L^2 norm boundedness. Numerical tests are included to support the theoretical results.

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Key words: MBE model, time filter, energy dissipation law, error estimate.

1. Introduction

Filtering algorithm is a kind of numerical post-processing algorithm based on the original calculation code of complex system. It is widely used in computational fluid industry applications [1,4] and numerical weather forecasting [23,24] to improve numerical simulation, such as eliminating high-frequency oscillations to improve stability, reducing dispersion error to improve computational accuracy, etc. Recently, the effect of adding a simple time filter to backward Euler method is considered in [6] for the initial value problem

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$$y'(t) = f\big(t, y(t)\big) \quad \text{for} \quad t > 0, \quad y(0) = y_0.$$

Consider the uniform time level $t_k = k\tau$ for $0 \leq k \leq N$ with the time-step size $\tau := T/N$. Given a grid sequence $\{v^n\}_{n=0}^N$, denote

$$\partial_\tau v^n := \frac{1}{\tau}(v^n - v^{n-1}), \quad \partial_\tau^2 v^n := \frac{1}{\tau}\big(\partial_\tau v^n - \partial_\tau v^{n-1}\big).$$

The time filtered backward Euler (FiBE) method in [6] approximates this problem by the backward Euler method and uses a simple time filter to update the solution

$$\begin{aligned} &\text{Step1}: \quad \frac{1}{\tau}\big(y_*^n - y^{n-1}\big) = f(t_n, y_*^n) && \text{for} \quad n \geq 2, \\ &\text{Step2}: \quad y^n = y_*^n - \frac{\nu}{2}\big(y_*^n - 2y^{n-1} + y^{n-2}\big) && \text{for} \quad n \geq 2, \end{aligned}$$

where y_*^n and y^n denote unfiltered and filtered values, and ν is an algorithm parameter to be determined. The FiBE method improves the accuracy of the fully implicit method to second-order by a well-calibrated post-filter with $\nu = 2/3$. In the absence of a better approach, time filter method solves the problem of the accuracy improvement in a complex, possibly legacy code, and the approach is modular and requires the addition of only one line of additional code. Error estimation and variable time step are straightforward and the individual effect of each step is conceptually clear. Recently, this method was extended to the Navier-Stokes equations in [4]. DeCaria *et al.* [3] presented several new embedded families of high accuracy methods with low cognitive complexity and excellent stability properties.

As seen, the above time filtered approach is a promising strategy to adjust the order in variable-order and variable-step BDF algorithms for gradient flow models, see our recent analysis [7, 9–15] on the variable-step BDF2 and high-order BDF methods. As pointed out in [6], the combination of backward Euler plus a curvature reducing time filter gives another option for long-time numerical simulations although the BDF2 method is satisfactory in many applications. To this aim, the stability and convergence of the FiBE method is investigated for the molecular beam epitaxy (MBE) model with slope selection [18], which can be viewed as an L^2 gradient flow of the Ehrlich-Schwoebel energy functional

$$E[\Phi] = \int_\Omega \left[\frac{\varepsilon^2}{2}|\Delta\Phi|^2 + F(\nabla\Phi)\right] \mathrm{d}\boldsymbol{x}, \tag{1.1}$$

where

$$F(\boldsymbol{v}) = \frac{1}{4}\big(|\boldsymbol{v}|^2 - 1\big)^2$$

is a nonlinear energy density function. In recent years, many of time stepping methods, including the stabilized semi-implicit scheme [25], the Crank-Nicolson scheme [19], the convex splitting scheme [20], and operator splitting schemes [8, 16, 17, 27] have been constructed and analyzed for the MBE growth model and related nonlinear models, also see [2, 5, 7, 12, 21, 22] and references therein.

Consider the MBE model on $\Omega = (0, L)^2 \subset \mathbb{R}^2$ and $0 \le t \le T$,

$$\partial_t \Phi = -\kappa \mu, \quad \mu := \frac{\delta E}{\delta \Phi} = \varepsilon^2 \Delta^2 \Phi - \nabla \cdot f(\nabla \Phi) \tag{1.2}$$

subjected to the initial data $\Phi(\boldsymbol{x}, 0) := \Phi_0(\boldsymbol{x})$. Here the mobility coefficient $\kappa > 0$, the interface width parameter $\epsilon > 0$, Φ is a periodic height function and $f(\boldsymbol{v}) := F'(\boldsymbol{v}) = (|\boldsymbol{v}|^2 - 1)\boldsymbol{v}$ is the nonlinear bulk. As well known, the MBE system with periodic boundary conditions preserves the volume conservation $\langle \Phi(t), 1 \rangle = \langle \Phi(0), 1 \rangle$, the energy dissipation law

$$\frac{\mathrm{d}E}{\mathrm{d}t} + \kappa \|\mu\|^2 = 0, \tag{1.3}$$

and the following L^2 norm stability estimate:

$$\|\Phi\|^2 \le \|\Phi_0\|^2 + \frac{\kappa}{2} |\Omega| \, t, \tag{1.4}$$

where $|\Omega|$ denotes the volume of Ω and the norm $\|v\| := \sqrt{\langle v, v \rangle}$ is generated by the L^2 inner product

$$\langle u, v \rangle := \int_\Omega uv d\boldsymbol{x}.$$

For simplicity, we only consider the time approximation in this paper. Our theoretical results including unique solvability, stability and convergence estimates, can be easily extended to the fully discrete scheme preserving the discrete integration-by-parts formulas by using the finite difference, finite element or pseudo-spectral approximations in space. The backward Euler method reads

$$\partial_\tau \phi^n = -\kappa \mu^n, \quad \mu^n := \varepsilon^2 \Delta^2 \phi^n - \nabla \cdot f(\nabla \phi^n) \quad \text{for} \quad n \ge 1. \tag{1.5}$$

Adding an extra line of code, we get the following FiBE scheme for the MBE model (1.2):

$$\text{Step1}: \quad \frac{1}{\tau}(\phi_*^n - \phi^{n-1}) = -\kappa \mu_*^n, \quad \mu_*^n := \varepsilon^2 \Delta^2 \phi_*^n - \nabla \cdot f(\nabla \phi_*^n) \quad \text{for} \quad n \ge 2, \tag{1.6}$$

$$\text{Step2}: \quad \phi^n = \phi_*^n - \frac{1}{3}(\phi_*^n - 2\phi^{n-1} + \phi^{n-2}) \quad \text{for} \quad n \ge 2, \tag{1.7}$$

where ϕ_*^n and ϕ^n denote the unfiltered and filtered solutions, respectively. As seen, the computational cost of (1.7) is nearly negligible so that the computational cost of the FiBE method (1.6)-(1.7) is the same as that of the backward Euler scheme. Also, we will prove that the FiBE method is second-order convergent under a convergence-solvability-stability (CSS)-consistent time-step constraint, see Table 1, where the time-step constraints for the solvability, convergence and stability of the backward Euler and BDF2 schemes can be derived by following the present analysis. The CSS-consistent condition means that the maximum step-size limit required for convergence is of the same order to that for solvability and stability (in certain norms) as the small interface parameter $\varepsilon \to 0^+$, cf. [26]. The main contributions are two-fold:

Table 1: The CSS-consistent time-step conditions.

	FiBE scheme	Backward Euler scheme	BDF2 scheme
Convergence	$\tau \le 4\kappa^{-1}\epsilon^2/(3+2\sqrt{3})$	$\tau \le 2\kappa^{-1}\epsilon^2$	$\tau \le \kappa^{-1}\epsilon^2/2$
Solvability	$\tau \le 4\kappa^{-1}\epsilon^2$	$\tau \le 4\kappa^{-1}\epsilon^2$	$\tau \le 6\kappa^{-1}\epsilon^2$
Energy stability	$\tau \le 4\kappa^{-1}\epsilon^2$	$\tau \le 4\kappa^{-1}\epsilon^2$	$\tau \le 2\kappa^{-1}\epsilon^2$
L^2 norm stability	$\tau = \mathcal{O}(1)$	$\tau = \mathcal{O}(1)$	$\tau = \mathcal{O}(1)$

- The FiBE scheme (1.6)-(1.7) is uniquely solvable if the time-step size $\tau \le 4\kappa^{-1}\epsilon^2$, see Theorem 2.1. Theorem 2.2 states that the filtered solution ϕ^n is second-order convergent in the L^2 norm if the step size τ is small such that $\tau \le 4\kappa^{-1}\epsilon^2/(3+2\sqrt{3})$.
- Theorem 3.1 says that the method is unconditionally stable in the L^2 norm, while it also preserves a (modified) discrete energy dissipation law if $\tau \le 4\varepsilon^2/\kappa$, see Theorem 3.2.

The rest of the paper is organized as follows. In Section 2, we verify the volume conservation and unique solvability of the FiBE scheme (1.6)-(1.7), and establish the L^2 norm convergence. The discrete energy dissipation law and L^2 norm stability are addressed in Section 3. Some numerical tests are included in the last section to show the effectiveness of the FiBE method.

2. Solvability and L^2 norm convergence

The time discrete scheme (1.6)-(1.7) is volume conservative and uniquely solvable. Taking the inner product of (1.6) by τ and applying the Green's formula, one can check that

$$\big\langle \phi_*^k - \phi^{k-1}, 1\big\rangle = \big\langle -\kappa\tau\mu_*^k, 1\big\rangle = 0 \quad \text{for} \quad k \ge 1.$$

It leads to $\langle \phi_*^k, 1\rangle = \langle \phi^{k-1}, 1\rangle$. By using the filtering step (1.7), a simple induction yields the volume conversation law, that is,

$$\langle \phi^n, 1\rangle = \langle \phi^{n-1}, 1\rangle = \cdots = \langle \phi^0, 1\rangle, \quad n \ge 1.$$

Theorem 2.1. *If the time step size $\tau \le 4\varepsilon^2/\kappa$, the FiBE scheme* (1.6)-(1.7) *is unique solvable.*

Proof. For any fixed time-level index $n \ge 1$, let

$$\mathbb{V}^* := \big\{ z \in L^2(\Omega) \,|\, \langle z, 1\rangle = \langle \phi^{n-1}, 1\rangle \big\}$$

be a subspace of $L^2(\Omega)$. Define the following functional $G[z]$ on the space $\mathbb{V}^*$:

$$G[z] := \frac{1}{2\tau}\|z - \phi^{n-1}\|^2 + \frac{\kappa\varepsilon^2}{2}\|\Delta z\|^2 + \frac{\kappa}{4}\|\nabla z\|_{l^4}^4 - \frac{\kappa}{2}\|\nabla z\|^2.$$

Since $\|v\|_{L^4}^4 \geq 2\|v\|^2 - |\Omega|$ due to the fact $(a^2-1)^2 \geq 0$, the functional $G[z]$ is coercive on $\mathbb{V}^*$,

$$G[z] \geq \frac{1}{2\tau}\|z-\phi^{n-1}\|^2 + \frac{\kappa}{4}\|\nabla z\|_{l^4}^4 - \frac{\kappa}{2}\|\nabla z\|^2 \geq \frac{1}{2\tau}\|z-\phi^{n-1}\|^2 - \frac{\kappa}{4}\,|\Omega|\,.$$

Also, $G[z]$ is strictly convex functional on $\mathbb{V}^*$. Actually, for any $\lambda \in \mathbb{R}$ and $\psi \in \mathbb{V}^*$, one has

$$\begin{aligned}
&\frac{\mathrm{d}^2}{\mathrm{d}\lambda^2} G[z+\lambda\psi]\Big|_{\lambda=0} \\
&= \frac{1}{\tau}\|\psi\|^2 + \kappa\varepsilon^2\|\Delta\psi\|^2 + 2\kappa\|\nabla z\cdot\nabla\psi\|^2 + \kappa\big\langle |\nabla z|^2, |\nabla\psi|^2\big\rangle - \kappa\|\nabla\psi\|^2 \\
&\geq \frac{1}{\tau}\|\psi\|^2 + \kappa\varepsilon^2\|\Delta\psi\|^2 + \kappa\langle\psi,\Delta\psi\rangle \geq \left(\frac{1}{\tau} - \frac{\kappa}{4\varepsilon^2}\right)\|\psi\|^2 \geq 0,
\end{aligned}$$

where the Cauchy-Schwarz inequality and Young's inequality have been used in third step. Thus, the functional $G[z]$ has a unique minimizer ϕ_*^n, if and only if it solves the equation

$$0 = \frac{\mathrm{d}}{\mathrm{d}\lambda} G\big[z+\lambda\psi\big]\Big|_{\lambda=0} = \left\langle \frac{1}{\tau}(z-\phi^{n-1}) + \kappa\varepsilon^2\Delta^2 z - \kappa\nabla\cdot f(\nabla z), \psi \right\rangle.$$

The arbitrariness of $\psi \in \mathbb{V}^*$ implies that the unique minimizer ϕ_*^n satisfies the following Euler-Lagrange equation:

$$0 = \frac{1}{\tau}\big(\phi_*^n - \phi^{n-1}\big) + \kappa\varepsilon^2\Delta^2\phi_*^n - \kappa\nabla\cdot f(\nabla\phi_*^n),$$

which is just the backward Euler step (1.6). Then the FiBE scheme is uniquely solvable because the filtering step (1.7) is linear. This completes the proof. $\square$

To prove the L^2 norm convergence, we need the following algebraic identity, which can be verified by direct calculations. Appendix A presents a detailed proof for interesting readers.

Lemma 2.1. *For any real sequence* $\{w_n \,|\, n \geq 0\}$*, it holds that*

$$\begin{aligned}
2w_{*,n}(w_{*,n} - w_{n-1}) = &\frac{3}{4}w_n^2 + \frac{1}{4}(3w_n - 2w_{n-1})^2 \\
&- \left[\frac{3}{4}w_{n-1}^2 + \frac{1}{4}(3w_{n-1} - 2w_{n-2})^2\right] \\
&+ \frac{3}{2}(w_n - 2w_{n-1} + w_{n-2})^2 \quad \textit{for} \quad n \geq 2,
\end{aligned}$$

where

$$w_{*,n} := \frac{3}{2}w_n - w_{n-1} + \frac{1}{2}w_{n-2}.$$

From the filtering step (1.7), we have

$$\phi_*^k = \frac{3}{2}\phi^k - \phi^{k-1} + \frac{1}{2}\phi^{k-2} \quad \text{for} \quad k \geq 2, \tag{2.1}$$

so that

$$\frac{1}{\tau}\big(\phi_*^k - \phi^{k-1}\big) = \frac{3}{2}\partial_\tau \phi^k - \frac{1}{2}\partial_\tau \phi^{k-1} \triangleq D_2\phi^k \quad \text{for} \quad k \geq 2,$$

where $D_2\phi^k$ denotes the second-order two-step BDF approximation of $\partial_t \Phi$ at $t = t_k$. Thus the unfiltered step (1.6) can be written as

$$D_2\phi^k + \kappa\varepsilon^2\Delta^2\phi_*^k - \kappa\nabla \cdot f\big(\nabla\phi_*^k\big) = 0 \quad \text{for} \quad k \geq 2. \tag{2.2}$$

To simplify the error analysis, introduce an auxiliary (exact) solution

$$\Phi_*(t_k) := \frac{3}{2}\Phi(t_k) - \Phi(t_{k-1}) + \frac{1}{2}\Phi(t_{k-2}) \quad \text{for} \quad k \geq 2. \tag{2.3}$$

The unfiltered solution ϕ_*^k can be viewed as a discrete approximation of $\Phi_*(t_k)$ such that

$$\begin{aligned}\Phi_*(t_k) - \phi_*^k = &\frac{3}{2}\big[\Phi(t_k) - \phi^k\big] - \big[\Phi(t_{k-1}) - \phi^{k-1}\big] \\ &+ \frac{1}{2}\big[\Phi(t_{k-2}) - \phi^{k-2}\big] \quad \text{for} \quad k \geq 2.\end{aligned} \tag{2.4}$$

Then the time consistency error ξ_Φ^k of the first step (1.6) at $t = t_k$ is defined by

$$\begin{aligned}\xi_\Phi^k :&= \frac{1}{\tau}\big(\Phi_*(t_k) - \Phi(t_{k-1})\big) + \kappa\varepsilon^2\Delta^2\Phi_*(t_k) - \kappa\nabla \cdot f\big(\nabla\Phi_*(t_k)\big) \\ &= \frac{1}{\tau}\big(\Phi_*(t_k) - \Phi(t_{k-1})\big) - \partial_t\Phi(t_k) + \kappa\varepsilon^2\Delta^2\big[\Phi_*(t_k) - \Phi(t_k)\big] \\ &\quad - \kappa\nabla \cdot \big[f\big(\nabla\Phi_*(t_k)\big) - f\big(\nabla\Phi(t_k)\big)\big],\end{aligned}$$

where $\Phi_*(t_k)$ is defined by (2.3). Reminding the following facts,

$$\begin{aligned}\frac{1}{\tau}\big[\Phi_*(t_k) - \Phi(t_{k-1})\big] &= D_2\Phi(t_k), \\ \Phi_*(t_k) - \Phi(t_k) &= \frac{\tau^2}{2}\,\partial_\tau^2\Phi(t_k),\end{aligned}$$

it is not difficult to find that

$$\big\|\xi_\Phi^k\big\| \leq C_\phi\tau^2 \quad \text{for} \quad k \geq 2, \tag{2.5}$$

provided the solution Φ is sufficiently regular. For simplicity of presentation, we use the following notation $\|\!|v^k|\!\|$:

$$\|\!|v^k|\!\| = \big\|\!\big|[v^k, v^{k-1}]\big|\!\big\| := \sqrt{\frac{3}{4}\|v^k\|^2 + \frac{1}{4}\|3v^k - 2v^{k-1}\|^2} \quad \text{for} \quad k \geq 1. \tag{2.6}$$

With this definition (2.6) and the inequality $\sqrt{a^2+b^2} \le |a|+|b|$, it is easy to know that

$$\begin{aligned}\frac{\sqrt{3}}{2}\|v^k\| \le \|\!|v^k|\!\| &\le \frac{\sqrt{3}}{2}\|v^k\| + \frac{1}{2}\|3v^k - 2v^{k-1}\| \\ &\le \frac{3+\sqrt{3}}{2}\|v^k\| + \|v^{k-1}\| \quad \text{for} \quad k \ge 1. \end{aligned} \tag{2.7}$$

Theorem 2.2. *If the step size τ is sufficiently small such that $\tau \le 4\varepsilon^2/(3+2\sqrt{3})\kappa$, the filtered solution ϕ^n of the FiBE scheme* (1.6)-(1.7) *is convergent in the L^2 norm,*

$$\|\!|\Phi^n - \phi^n|\!\| \le 2\exp\left(\frac{3\kappa t_{n-1}}{\varepsilon^2}\right)\left(\|\!|\Phi^1 - \phi^1|\!\| + C_\phi t_{n-1}\tau^2\right) \quad \textit{for} \quad 2 \le n \le N,$$

or equivalently,

$$\|\Phi^n - \phi^n\| \le 3\exp\left(\frac{3\kappa t_{n-1}}{\varepsilon^2}\right)\left(\|\Phi^1 - \phi^1\| + \|\Phi^0 - \phi^0\| + C_\phi t_{n-1}\tau^2\right) \quad \textit{for} \quad 2 \le n \le N.$$

Proof. Let

$$e^n := \Phi(t_n) - \phi^n$$

be the error between the exact solution and the filtered solution. Eq. (2.4) shows that

$$e_*^n := \Phi_*(t_n) - \phi_*^n = \frac{3}{2}e^n - e^{n-1} + \frac{1}{2}e^{n-2} \quad \text{for} \quad n \ge 2. \tag{2.8}$$

We get the following error system:

$$\begin{aligned}&\frac{e_*^k - e^{k-1}}{\tau} + \kappa\varepsilon^2\Delta^2 e_*^k \\ &= \kappa\nabla\cdot\left(|\nabla\Phi_*(t_k)|^2\nabla\Phi_*(t_k) - |\nabla\phi_*^k|^2\nabla\phi_*^k\right) - \kappa\Delta e_*^k + \xi_\Phi^k. \end{aligned} \tag{2.9}$$

Considering the inner product of (2.9) and $2\tau e_*^k$, we obtain

$$\begin{aligned}&2\left\langle e_*^k - e^{k-1}, e_*^k\right\rangle + 2\kappa\tau\varepsilon^2\|\Delta e_*^k\|^2 \\ &= -2\kappa\tau\left\langle |\nabla\Phi_*(t_k)|^2\nabla\Phi_*(t_k) - |\nabla\phi_*^k|^2\nabla\phi_*^k, \nabla e_*^k\right\rangle \\ &\quad + 2\kappa\tau\|\nabla e_*^k\|^2 + 2\tau\left\langle \xi_\Phi^k, e_*^k\right\rangle \quad \text{for} \quad k \ge 2. \end{aligned} \tag{2.10}$$

For the first term in (2.10), Lemma 2.1 yields

$$2\left\langle e_*^k - e^{k-1}, e_*^k\right\rangle \ge \|\!|e^k|\!\|^2 - \|\!|e^{k-1}|\!\|^2 \quad \text{for} \quad k \ge 2.$$

For any vectors $\boldsymbol{u}, \boldsymbol{v} \in R^2$, we can check that

$$\left\langle |\boldsymbol{u}|^2\boldsymbol{u} - |\boldsymbol{v}|^2\boldsymbol{v}, \boldsymbol{u} - \boldsymbol{v}\right\rangle = \frac{1}{2}\left||\boldsymbol{u}|^2 - |\boldsymbol{v}|^2\right|^2 + \frac{1}{2}|\boldsymbol{u}-\boldsymbol{v}|^2\left(|\boldsymbol{u}|^2 + |\boldsymbol{v}|^2\right) \ge 0.$$

Thus the nonlinear term in the right side of (2.10) is non-positive and can be dropped. The second term at the right side of (2.10) can be estimated as

$$2\kappa\big\|\nabla e_*^k\big\|^2 \le 2\kappa\varepsilon^2\big\|\Delta e_*^k\big\|^2 + \frac{\kappa}{2\varepsilon^2}\big\|e_*^k\big\|^2.$$

Therefore, it follows from (2.10) that

$$|||e^k|||^2 \le |||e^{k-1}|||^2 + \frac{\kappa\tau}{2\varepsilon^2}\big\|e_*^k\big\|^2 + 2\tau\big\|\xi_\Phi^k\big\|\big\|e_*^k\big\| \quad \text{for} \quad k \ge 2,$$

and, by summing k from 2 to n,

$$|||e^n|||^2 \le |||e^1|||^2 + \frac{\kappa\tau}{2\varepsilon^2}\sum_{k=2}^{n}\big\|e_*^k\big\|^2 + 2\tau\sum_{k=2}^{n}\big\|\xi_\Phi^k\big\|\big\|e_*^k\big\| \quad \text{for} \quad n \ge 2. \tag{2.11}$$

By using the formula (2.8), one can check the simple fact

$$\begin{aligned} e_*^k = &\frac{6}{(\sqrt{3}+1)^2}\frac{\sqrt{3}+1}{4}\left(\frac{\sqrt{3}}{2}e^k\right) + \frac{\sqrt{3}+1}{4}\left(\frac{3}{2}e^k - e^{k-1}\right) \\ &+ \frac{1}{2}\left(\frac{\sqrt{3}}{2}e^{k-1}\right) - \frac{1}{2}\left(\frac{3}{2}e^{k-1} - e^{k-2}\right). \end{aligned}$$

We apply the inequality

$$|a| + |b| \le \sqrt{2(a^2+b^2)}$$

and the definition (2.6) to get

$$\begin{aligned} \big\|e_*^k\big\| \le &\frac{\sqrt{3}+1}{4}\left(\left\|\frac{\sqrt{3}}{2}e^k\right\| + \left\|\frac{3}{2}e^k - e^{k-1}\right\|\right) \\ &+ \frac{1}{2}\left(\left\|\frac{\sqrt{3}}{2}e^{k-1}\right\| + \left\|\frac{3}{2}e^{k-1} - e^{k-2}\right\|\right) \\ \le &\frac{\sqrt{3}+1}{2}\frac{\sqrt{2}}{2}|||e^k||| + \frac{\sqrt{2}}{2}|||e^{k-1}|||. \end{aligned} \tag{2.12}$$

By choosing some integer n_0 $(1 \le n_0 \le n)$ such that

$$|||e^{n_0}||| = \max_{1\le k\le n}|||e^k|||,$$

it is easy to get

$$\big\|e_*^k\big\| \le \frac{(\sqrt{3}+1)\sqrt{6}}{4}|||e^{n_0}|||.$$

Now we take $n := n_0$ in the estimate (2.11) to obtain

$$|||e^{n_0}|||^2 \le |||e^1|||^2 + \frac{\kappa\tau}{2\varepsilon^2}\sum_{k=2}^{n_0}\big\|e_*^k\big\|^2 + 2\tau\sum_{k=2}^{n_0}\big\|\xi_\Phi^k\big\|\big\|e_*^k\big\|$$

$$\leq \|\!|e^1\|\!|^2 + \frac{(\sqrt{3}+1)\sqrt{6}}{4}\frac{\kappa}{2\varepsilon^2}\sum_{k=2}^{n_0}\tau\big\|e_*^k\big\|\|\!|e^{n_0}\|\!| + \frac{(\sqrt{3}+1)\sqrt{6}}{2}\sum_{k=2}^{n_0}\tau\big\|\xi_\Phi^k\big\|\|\!|e^{n_0}\|\!|.$$

Then dividing both sides of the inequality by $\|\!|e^{n_0}\|\!|$ one gets

$$\|\!|e^{n_0}\|\!| \leq \|\!|e^1\|\!| + \frac{(\sqrt{3}+1)\sqrt{6}}{4}\frac{\kappa}{2\varepsilon^2}\sum_{k=2}^{n_0}\tau\big\|e_*^k\big\| + \frac{(\sqrt{3}+1)\sqrt{6}}{2}\sum_{k=2}^{n_0}\tau\big\|\xi_\Phi^k\big\|$$

such that

$$\begin{aligned}\|\!|e^{n}\|\!| \leq \|\!|e^{n_0}\|\!| &\leq \|\!|e^1\|\!| + \frac{(\sqrt{3}+1)\sqrt{6}}{4}\frac{\kappa}{2\varepsilon^2}\sum_{k=2}^{n}\tau\big\|e_*^k\big\| + \frac{(\sqrt{3}+1)\sqrt{6}}{2}\sum_{k=2}^{n}\tau\big\|\xi_\Phi^k\big\| \\ &\leq \|\!|e^1\|\!| + \frac{(3+2\sqrt{3})\kappa}{8\varepsilon^2}\tau\|\!|e^n\|\!| + \frac{3(2+\sqrt{3})\kappa}{8\varepsilon^2}\sum_{k=1}^{n-1}\tau\|\!|e^k\|\!| + \frac{(\sqrt{3}+1)\sqrt{6}}{2}\sum_{k=2}^{n}\tau\big\|\xi_\Phi^k\big\|.\end{aligned}$$

Under the time-step constraint $\tau \leq 4\varepsilon^2/(3+2\sqrt{3})\kappa$, one has

$$\begin{aligned}\|\!|e^{n}\|\!| &\leq 2\|\!|e^1\|\!| + \frac{3(2+\sqrt{3})\kappa}{4\varepsilon^2}\sum_{k=1}^{n-1}\tau\|\!|e^k\|\!| + (3+\sqrt{3})\sqrt{2}\sum_{k=2}^{n}\tau\big\|\xi_\Phi^k\big\| \\ &\leq 2\|\!|e^1\|\!| + \frac{3\kappa}{\varepsilon^2}\sum_{k=1}^{n-1}\tau\|\!|e^k\|\!| + 7\sum_{k=2}^{n}\tau\big\|\xi_\Phi^k\big\|.\end{aligned}$$

Then, with the time consistency bound (2.5), the discrete Grönwall inequality yields the first error estimate. Then the equivalence relationship (2.7) arrives at the second estimate and completes the proof. □

As seen, the filtered solution ϕ^n of the FiBE scheme (1.6)-(1.7) is second-order accurate if the first-level solution ϕ^1 is second-order accurate. Actually, the backward Euler scheme (1.5) at the first time level is adequate since in such case one has, cf. the proof of [26, Theorem 3.1],

$$\|\Phi^1 - \phi^1\| \leq 2\|\Phi^0 - \phi^0\| + C_\phi\tau^2.$$

Recalling the definition (2.8), one has

$$\begin{aligned}\big\|\Phi(t_n) - \phi_*^n\big\| &\leq \big\|\Phi(t_n) - \Phi_*^n\big\| + \big\|\Phi_*(t_n) - \phi_*^n\big\| \\ &\leq C_\phi\tau^2 + \frac{3}{2}\|e^n\| + \|e^{n-1}\| + \frac{1}{2}\|e^{n-2}\| \\ &\leq 9\exp\left(\frac{3\kappa t_{n-1}}{\varepsilon^2}\right)\big(\|\Phi^1-\phi^1\| + \|\Phi^0-\phi^0\| + C_\phi t_{n-1}\tau^2\big).\end{aligned} \tag{2.13}$$

It says that the unfiltered solution ϕ_*^n is also second-order convergent, see Table 2.

3. L^2 norm stability and energy dissipation law

The following result simulates the continuous L^2 norm estimate (1.4) at the discrete levels.

Theorem 3.1. *The FiBE scheme* (1.6)-(1.7) *is unconditionally stable in the L^2 norm,*

$$\|\!|\phi^n|\!\|^2 \le \|\!|\phi^1|\!\|^2 + \frac{\kappa}{2}|\Omega| t_{n-1} \quad \textit{for} \quad n \ge 1,$$

where the auxiliary norm $\|\!|\cdot|\!\|$ is defined by (2.6).

Proof. Taking the L^2 inner product of (1.6) with $2\tau\phi_*^n$, and using the Green's formula, one gets

$$2\left\langle \phi_*^n - \phi^{n-1}, \phi_*^n \right\rangle + 2\kappa\tau\varepsilon^2 \left\|\Delta\phi_*^n\right\|^2 + 2\kappa\tau\left\langle f(\nabla\phi_*^n), \nabla\phi_*^n \right\rangle = 0 \quad \text{for} \quad n \ge 2. \tag{3.1}$$

By Lemma 2.1, the first term can be bounded by

$$2\left\langle \phi_*^k - \phi^{k-1}, \phi_*^k \right\rangle \ge \|\!|\phi^k|\!\|^2 - \|\!|\phi^{k-1}|\!\|^2.$$

The nonlinear term is handled by

$$\left\langle f(\nabla\phi_*^n), \nabla\phi_*^n \right\rangle = \left\| |\nabla\phi_*^n|^2 - \frac{1}{2} \right\|^2 - \frac{1}{4}|\Omega| \ge -\frac{1}{4}|\Omega|.$$

Inserting the two estimates into (3.1), one has

$$\|\!|\phi^k|\!\|^2 - \|\!|\phi^{k-1}|\!\|^2 \le \frac{\kappa\tau}{2}|\Omega| \quad \text{for} \quad k \ge 2. \tag{3.2}$$

Summing this inequality from $k = 2$ to n yields the claimed result and completes the proof. □

To build up the discrete energy dissipation law for the FiBE scheme (1.6)-(1.7), we need the following algebraic identity. Appendix B presents a proof for interesting readers.

Lemma 3.1. *For any real sequence $\{w_n \,|\, n \ge 0\}$, it holds that*

$$\begin{aligned}
&2(w_{*,n} - w_{*,n-1})(w_{*,n} - w_{n-1}) \\
=& \frac{3}{2}(\delta_1 w_n)^2 + \frac{3}{4}(\delta_1 w_n - \delta_1 w_{n-1})^2 \\
&- \left[\frac{1}{2}(\delta_1 w_{n-1})^2 + \frac{1}{4}(\delta_1 w_{n-1} - \delta_1 w_{n-2})^2\right] + (\delta_1 w_{*,n})^2,
\end{aligned}$$

where

$$w_{*,n} := \frac{3}{2}w_n - w_{n-1} + \frac{1}{2}w_{n-2}, \quad \delta_1 w_n := w_n - w_{n-1}.$$

Consider the following modified energy:

$$\mathcal{E}[\phi^k] := E\big[\phi_*^k\big] + \frac{\tau}{4\kappa}\|\partial_\tau\phi^k\|^2 + \frac{\tau^3}{8\kappa}\big\|\partial_\tau^2\phi^k\big\|^2 \quad \text{for} \quad k\geq 2, \tag{3.3}$$

where $E[\phi_*^k]$ is the discrete version of energy functional (1.1),

$$E\big[\phi_*^k\big] := \frac{\varepsilon^2}{2}\big\|\Delta\phi_*^k\big\|^2 + \frac{1}{4}\big\||\nabla\phi_*^k|^2 - 1\big\|^2 \quad \text{for} \quad k\geq 2.$$

From the formula (2.1), we see that $\phi_*^k \to \phi^\infty$ as the solution ϕ^k approaches the steady state ϕ^∞, that is, $\phi^k \to \phi^\infty$. In the limit $\phi^k\to\phi^\infty$, we have $\partial_\tau\phi^k \to 0$ so that $\mathcal{E}[\phi^k]\to E[\phi^\infty]$.

Theorem 3.2. *If the time step size* $\tau \leq 4\varepsilon^2/\kappa$*, the FiBE scheme* (1.6)-(1.7) *preserves a modified energy dissipation law*

$$\mathcal{E}[\phi^n] \leq \mathcal{E}[\phi^{n-1}] \quad \textit{for} \quad n\geq 3.$$

Proof. For simplicity of presentation, denote

$$\delta_1 v^n := v^n - v^{n-1}, \quad \delta_1^2 v^n := \delta_1 v^n - \delta_1 v^{n-1}$$

for any time sequence $\{v^n \,|\, n\geq 0\}$. Taking the inner product of (1.6) by $\kappa^{-1}\delta_1\phi_*^n$, one obtains that

$$\begin{aligned}&\frac{1}{\kappa\tau}\left\langle \phi_*^n - \phi^{n-1}, \delta_1\phi_*^n\right\rangle + \varepsilon^2\big\langle \Delta\phi_*^n, \delta_1\Delta\phi_*^n\big\rangle \\ &\quad + \big\langle |\nabla\phi_*^n|^2\nabla\phi_*^n, \delta_1\nabla\phi_*^n\big\rangle - \big\langle \nabla\phi_*^n, \delta_1\nabla\phi_*^n\big\rangle = 0 \quad \text{for} \quad n\geq 3,\end{aligned} \tag{3.4}$$

where the Green's formula was used. For the first term, Lemma 3.1 yields

$$\begin{aligned}&\frac{1}{\kappa\tau}\left\langle \phi_*^n - \phi^{n-1}, \delta_1\phi_*^n\right\rangle \\ \geq\, &\frac{1}{4\kappa\tau}\|\delta_1\phi^n\|^2 + \frac{1}{8\kappa\tau}\big\|\delta_1^2\phi^n\big\|^2 - \frac{1}{4\kappa\tau}\|\delta_1\phi^{n-1}\|^2 \\ &- \frac{1}{8\kappa\tau}\big\|\delta_1^2\phi^{n-1}\big\|^2 + \frac{1}{2\kappa\tau}\big\|\delta_1\phi_*^n\big\|^2.\end{aligned}$$

For the second and fourth terms in (3.4), the identity $2a(a-b) = a^2 - b^2 + (a-b)^2$ leads to

$$\begin{aligned}\varepsilon^2\left\langle \Delta\phi_*^n, \delta_1\Delta\phi_*^n\right\rangle &= \frac{\varepsilon^2}{2}\big\|\Delta\phi_*^n\big\|^2 - \frac{\varepsilon^2}{2}\big\|\Delta\phi_*^{n-1}\big\|^2 + \frac{\varepsilon^2}{2}\big\|\delta_1\Delta\phi_*^n\big\|^2, \\ -\langle\nabla\phi_*^n, \delta_1\nabla\phi_*^n\rangle &= -\frac{1}{2}\big\|\nabla\phi_*^n\big\|^2 + \frac{1}{2}\big\|\nabla\phi_*^{n-1}\big\|^2 - \frac{1}{2}\big\|\delta_1\nabla\phi_*^n\big\|^2.\end{aligned}$$

Since

$$a^3(a-b) = \frac{1}{2}a^2\big[a^2 - b^2 + (a-b)^2\big]$$

$$= \frac{1}{4}a^4 - \frac{1}{4}b^4 + \frac{1}{4}(a^2-b^2)^2 + \frac{1}{2}a^2(a-b)^2,$$

the nonlinear term in (3.4) can be bounded by

$$\big\langle |\nabla\phi_*^n|^2\nabla\phi_*^n, \delta_1\nabla\phi_*^n\big\rangle \geq \frac{1}{4}\big\langle |\nabla\phi_*^n|^4, 1\big\rangle - \frac{1}{4}\big\langle |\nabla\phi_*^{n-1}|^4, 1\big\rangle.$$

Thus by collecting the above estimates, it follows from (3.4) that

$$\mathcal{E}[\phi^n] - \mathcal{E}[\phi^{n-1}] + \frac{1}{2\kappa\tau}\big\|\delta_1\phi_*^n\big\|^2 + \frac{\varepsilon^2}{2}\big\|\delta_1\Delta\phi_*^n\big\|^2 - \frac{1}{2}\big\|\delta_1\nabla\phi_*^n\big\|^2 \leq 0.$$

The Young's inequality shows that

$$-\frac{1}{2}\big\|\delta_1\nabla\phi_*^n\big\|^2 \geq -\frac{\varepsilon^2}{2}\big\|\delta_1\Delta\phi_*^n\big\|^2 - \frac{1}{8\varepsilon^2}\big\|\delta_1\phi_*^n\big\|^2.$$

Then we have

$$\mathcal{E}[\phi^n] - \mathcal{E}[\phi^{n-1}] + \left(\frac{1}{2\kappa\tau} - \frac{1}{8\varepsilon^2}\right)\big\|\delta_1\phi_*^n\big\|^2 \leq 0 \quad \text{for} \quad n \geq 3.$$

Then the claimed energy dissipation law follows if $\tau \leq 4\varepsilon^2/\kappa$. □

4. Numerical tests

This section presents some numerical tests of the FiBE method (1.6)-(1.7) with the Fourier pseudo-spectral approximation in space. A simple fixed-point iteration algorithm with the termination error 10^{-12} is applied to solve the resulting nonlinear equations at each time step. Since the FiBE method requires an initialization step, where the solution at previous level as the initial guess for each iteration, the fully implicit backward Euler scheme is used here to obtain the first level solution.

Example 4.1. We consider the exact solution

$$\Phi(x,y,t) = \cos(t)\sin(x)\sin(y)$$

of the MBE model (1.6)-(1.7) with a proper forcing term $g(\mathbf{x},t)$, i.e.,

$$\partial_t\Phi + \kappa\big(\epsilon^2\Delta^2\Phi - \nabla\cdot f(\nabla\Phi)\big) = g(\mathbf{x},t),$$

where the domain $\Omega = (0,2\pi)^2$ and the model parameter $\kappa = 1$, $\epsilon^2 = 0.1$.

In our computations, we set $T = 1$ and use a 128^2 spatial mesh with the uniform spacings to cover the domain Ω. Since the spatial error of the Fourier pseudo-spectral method is standard, we only examine the temporal error. The convergence order is computed by

$$\text{Order} \approx \frac{\log\big(e(N)/e(2N)\big)}{\log\big(\tau(N)/\tau(2N)\big)},$$

where the discrete L^2 norm error

$$e(N) := \max_{1\leq n\leq N}\|\Phi^n - \phi^n\|.$$

Table 2: Numerical accuracy of backward Euler, FiBE and BDF2 schemes.

N	Backward Euler		FiBE ϕ_*^n		FiBE ϕ^n		BDF2	
	$e(N)$	Order	$e(N)$	Order	$e(N)$	Order	$e(N)$	Order
40	9.28e-03	–	1.30e-04	–	5.50e-05	–	1.19e-04	–
80	4.60e-03	1.01	2.87e-05	2.18	1.58e-05	1.80	2.85e-05	2.06
160	2.29e-03	1.01	6.72e-06	2.09	4.20e-06	1.91	6.97e-06	2.03
320	1.14e-03	1.00	1.62e-06	2.05	1.08e-06	1.96	1.72e-06	2.02
640	5.72e-04	1.00	3.99e-07	2.02	2.75e-07	1.98	4.28e-07	2.01

Table 2 records the numerical results by the backward Euler, FiBE and BDF2 methods. As expected, the backward Euler method with first-order accuracy can achieve second-order time accuracy after adding an extra code. The time filtered method has the advantage of improving the first-order accuracy without increasing the computational complexity.

4.1. Simulation of coarsening dynamics

Example 4.2. We use the FiBE scheme to conduct the long-time dynamic simulations of coarsening. Consider the MBE equations (1.6)-(1.7) with the initial condition

$$\phi(\mathbf{x},0) = 0.1\big(\sin(3x)\sin(2y) + \sin(5x)\sin(5y)\big).$$

The spatial domain is set as $\Omega = (0,2\pi)^2$ and the spatial meshes is set as 128×128. The model parameters are chosen as $\kappa = 1$, $\epsilon^2 = 0.1$.

Numerical tests in [2] showed that the MBE model permits multi-scale behavior in time. We run the FiBE scheme (1.6)-(1.7) with time-step size $\tau = 10^{-3}$ until $T = 30$. In Fig. 1, the snapshots of solution profiles are taken at time $t = 0, 0.05, 2.5, 5.5, 8, 30$, respectively. Time snapshots of the evolution of the model with slope selection are in accordance with the previous observations in [2]. We plot two discrete energy curves in Fig. 2, where $E(t_n) := E[\phi^n]$ is the original energy calculated by the filtered solution ϕ^n and $\mathcal{E}(t_n) := \mathcal{E}[\phi^n]$ is the modified energy defined in (3.3). It is clearly seen that both the modified energy and the free energy decay monotonically in the coarsening process.

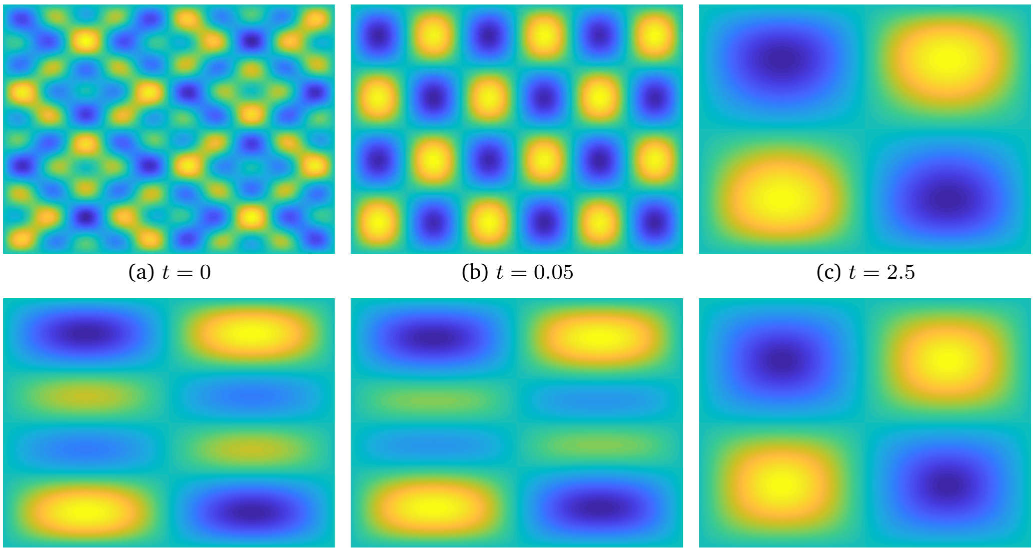
Appendix A. Proof of Lemma 2.1

Define

$$\delta_1 w_n := w_n - w_{n-1}, \quad \delta_1^2 w_n := \delta_1 w_n - \delta_1 w_{n-1}.$$

One has

$$\begin{aligned} w_{*,n} &= \frac{3}{2}w_n - w_{n-1} + \frac{1}{2}w_{n-2} = w_n + \frac{1}{2}\delta_1^2 w_n, \\ w_{*,n} - w_{n-1} &= \delta_1 w_n + \frac{1}{2}\delta_1^2 w_n. \end{aligned}$$



(a) $t = 0$ (b) $t = 0.05$ (c) $t = 2.5$

(d) $t = 5.5$ (e) $t = 8$ (f) $t = 30$

Figure 1: The snapshot of ϕ at the time $t = 0, 0.05, 2.5, 5.5, 8, 30$.

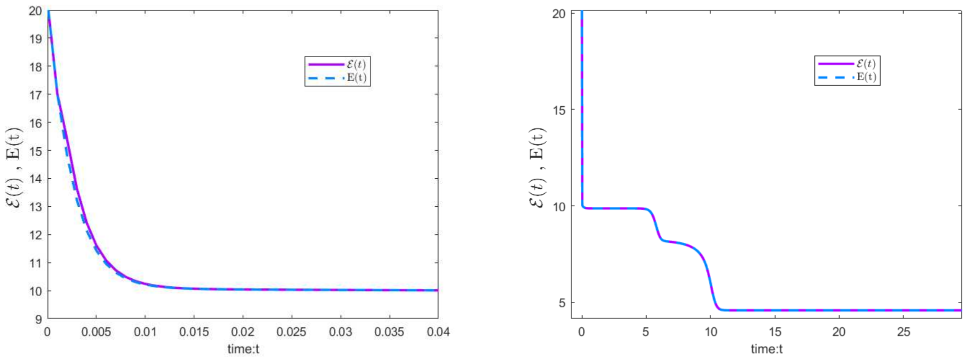


Figure 2: Time evolutions of original energy $E(t)$ and modified energy $\mathcal{E}(t)$.

Then we derive that

$$
\begin{aligned}
& 4w_{*,n}(w_{*,n} - w_{n-1}) \\
= & \left(2w_n + \delta_1^2 w_n\right)\left(2\delta_1 w_n + \delta_1^2 w_n\right) \\
= & 4w_n \delta_1 w_n + 2\delta_1 w_n \left(\delta_1^2 w_n\right) + 2w_n \delta_1^2 w_n + \left(\delta_1^2 w_n\right)^2 \\
= & 4w_n \delta_1 w_n + 4\delta_1 w_n \left(\delta_1^2 w_n\right) + 2w_{n-1} \delta_1^2 w_n + \left(\delta_1^2 w_n\right)^2.
\end{aligned} \tag{A.1}
$$

By using the identity

$$
2a(a-b) = a^2 - b^2 + (a-b)^2,
$$

we have

$$
4w_n \delta_1 w_n = 2w_n^2 - 2w_{n-1}^2 + 2(\delta_1 w_n)^2,
$$

$$
\begin{aligned}
4\delta_1 w_n(\delta_1^2 w_n) &= 2(\delta_1 w_n)^2 - 2(\delta_1 w_{n-1})^2 + 2\big(\delta_1^2 w_n\big)^2, \\
2w_{n-1}\delta_1^2 w_n &= 2w_{n-1}\delta_1 w_n - 2w_{n-1}\delta_1 w_{n-1} \\
&= w_n^2 - w_{n-1}^2 - (\delta_1 w_n)^2 - w_{n-1}^2 + w_{n-2}^2 - (\delta_1 w_{n-1})^2.
\end{aligned}
$$

Thus it follows from (A.1) that

$$
\begin{aligned}
&4w_{*,n}(w_{*,n} - w_{n-1}) \\
&= 3w_n^2 - 4w_{n-1}^2 + w_{n-2}^2 + 3(\delta_1 w_n)^2 - 3(\delta_1 w_{n-1})^2 + 3\big(\delta_1^2 w_n\big)^2 \\
&= \big[3w_n^2 - w_{n-1}^2 + 3(\delta_1 w_n)^2\big] - \big[3w_{n-1}^2 - w_{n-2}^2 + 3(\delta_1 w_{n-1})^2\big] + 3\big(\delta_1^2 w_n\big)^2 \\
&\triangleq 2G[w_n, w_{n-1}] - 2G[w_{n-1}, w_{n-2}] + 3\big(\delta_1^2 w_n\big)^2,
\end{aligned}
$$

where the functional G is non-negative due to the following fact:

$$
G[a,b] := \frac{3}{2}a^2 - \frac{1}{2}b^2 + \frac{3}{2}(a-b)^2 = 3a^2 - 3ab + b^2 = \frac{3}{4}a^2 + \frac{1}{4}(3a-2b)^2.
$$

It completes the proof. □

Appendix B. Proof of Lemma 3.1

With the notations in Appendix A, one has

$$
\begin{aligned}
w_{*,n} + w_{*,n-1} - 2w_{n-1} &= \delta_1 w_n + \frac{1}{2}\delta_1^2 w_n + \frac{1}{2}\delta_1^2 w_{n-1}, \\
w_{*,n} - w_{*,n-1} &= \delta_1 w_n + \frac{1}{2}\delta_1^2 w_n - \frac{1}{2}\delta_1^2 w_{n-1}.
\end{aligned}
$$

By using the identity

$$
2a(a-b) = a^2 - b^2 + (a-b)^2,
$$

one gets

$$
\begin{aligned}
&2(\delta_1 w_{*,n})(w_{*,n} + w_{*,n-1} - 2w_{n-1}) \\
&= 2\left(\delta_1 w_n + \frac{1}{2}\delta_1^2 w_n\right)^2 - \frac{1}{2}\big(\delta_1^2 w_{n-1}\big)^2 \\
&= 2(\delta_1 w_n)^2 + 2\delta_1 w_n\big(\delta_1^2 w_n\big) + \frac{1}{2}\big(\delta_1^2 w_n\big)^2 - \frac{1}{2}\big(\delta_1^2 w_{n-1}\big)^2 \\
&= 3(\delta_1 w_n)^2 - (\delta_1 w_{n-1})^2 + \frac{3}{2}\big(\delta_1^2 w_n\big)^2 - \frac{1}{2}\big(\delta_1^2 w_{n-1}\big)^2.
\end{aligned}
$$

Thus we derive that

$$
\begin{aligned}
&4(w_{*,n} - w_{n-1})(\delta_1 w_{*,n}) \\
&= 4w_{*,n}(\delta_1 w_{*,n}) - 4w_{n-1}(\delta_1 w_{*,n})
\end{aligned}
$$

$$
\begin{aligned}
&= 2w_{*,n}^2 - 2w_{*,n-1}^2 + 2(\delta_1 w_{*,n})^2 - 4w_{n-1}(\delta_1 w_{*,n}) \\
&= 2(\delta_1 w_{*,n})^2 + 2(w_{*,n} + w_{*,n-1} - 2w_{n-1})(\delta_1 w_{*,n}) \\
&= 3(\delta_1 w_n)^2 + \frac{3}{2}\big(\delta_1^2 w_n\big)^2 - (\delta_1 w_{n-1})^2 - \frac{1}{2}\big(\delta_1^2 w_{n-1}\big)^2 + 2(\delta_1 w_{*,n})^2.
\end{aligned}
$$

It leads to the claimed identity of Lemma 3.1. □

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