A HIGHLY EFFICIENT AND ACCURATE NEW SAV APPROACH FOR GRADIENT FLOWS

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Abstract. We present several essential improvements to the powerful scalar auxiliary variable (SAV) approach [23, 24]. Firstly, by using the introduced scalar variable to control both the nonlinear and the explicit linear terms, we are able to reduce the number of linear equations with constant coefficients to be solved at each time step from two to one, so the computational cost of the new SAV approach is essentially half of the original SAV approach while keeping all its other advantages. This technique is also extended to the multiple SAV approach. Secondly, instead of discretizing the dynamical equation for the auxiliary variable, we use a first-order approximation of the energy balance equation, which allows us to construct high-order unconditionally energy stable SAV schemes with uniform, and more importantly, variable time step sizes, enabling us to construct, for the first time, high-order unconditionally stable adaptive time-stepping BDF schemes. Representative numerical examples are provided to demonstrate the improved efficiency and accuracy of the proposed method.

1. Introduction

Dissipative physical systems are ubiquitous in the real world, due to the second law of thermodynamics. It is highly desirable for numerical methods targeted on such systems to preserve the discrete energy dissipation law. As such, many efforts to develop energy stable numerical methods have been devoted to this longstanding and active research area. These includes, but not limited to, the average vector field (AVF) method [8, 22], the convex splitting method [4, 5, 12, 13], the stabilization method [26, 33], the Lagrange multiplier method [14] and more recently, the invariant energy quadratization (IEQ) method [27, 32, 15] and the scalar auxiliary variable (SAV) method [23, 24, 16]. Among them, the SAV method is a particular powerful tool for the design of unconditionally energy-stable first- and second-order schemes for a large class of gradient flows. The aim of this paper is to present some essential improvements on the highly efficient SAV approach.

In order to motivate our improvements, we briefly review below the SAV approach for the general form of gradient flows:

$$\frac{\partial \phi}{\partial t} = -\mathcal{G} \mu,$$

where $\phi$ is the unknown function, $\mathcal{G}$ is a positive operator that gives rise to the dissipative mechanism of the system, e.g. $\mathcal{G} = I$ in the $L^2$ gradient flow and $\mathcal{G} = -\nabla^2$ in the $H^{-1}$...
gradient flow, and $\mu$ is the so-called chemical potential
\begin{equation}
\mu = \frac{\delta E_{\text{tot}}}{\delta \phi} = \mathcal{L}\phi + U(\phi),
\end{equation}
with respect to the free energy
\begin{equation}
E_{\text{tot}}(\phi) = \frac{1}{2}(\phi, \mathcal{L}\phi) + E_1(\phi),
\end{equation}
where $\mathcal{L}$ is a non-negative linear operator and $E_1(\phi)$ is a nonlinear functional. For the sake of conciseness, homogeneous Neumann or periodic boundary conditions are assumed throughout the paper such that all boundary terms will vanish when integration by parts are performed.

The key for the SAV approach is to introduce a scalar variable $r(t)$ defined by
\begin{equation}
r(t) = \sqrt{E_1[\phi] + C_0},
\end{equation}
and its associated dynamical equation
\begin{equation}
\frac{dr}{dt} = \frac{1}{2}\sqrt{E_1[\phi] + C_0} \int_{\Omega} U(\phi) \frac{\partial \phi}{\partial t} d\Omega,
\end{equation}
where $U(\phi) = \frac{\delta E_1}{\delta \phi}$.

Then, a first-order SAV scheme with explicit treatment for all nonlinear terms is as follows:
\begin{align}
\phi^{n+1} - \phi^n &= -G\mu^{n+1}, \\
\mu^{n+1} &= \mathcal{L}\phi^{n+1} + \frac{r^{n+1}}{\sqrt{E_1[\phi^n] + C_0}} U(\phi^n), \\
\frac{r^{n+1} - r^n}{\Delta t} &= \frac{1}{2\sqrt{E_1[\phi^n] + C_0}} \int_{\Omega} U(\phi^n) \frac{\phi^{n+1} - \phi^n}{\Delta t} d\Omega.
\end{align}

One can eliminate $\mu^{n+1}$ and $r^{n+1}$ from the above coupled linear scheme to obtain a linear equation for $\phi$ only:
\begin{equation}
(I + \Delta t G\mathcal{L})\phi^{n+1} = \phi^n - r^{n+1} \Delta t G\left(\frac{U[\phi^n]}{\sqrt{E_1[\phi^n] + C_0}}\right).
\end{equation}

Setting $\phi^{n+1} = \phi_1^{n+1} + \phi_2^{n+1}$, we find that $\phi_1^{n+1}$ and $\phi_2^{n+1}$ are solutions of the following two linear equations with constant coefficients
\begin{align}
(I + \Delta t G\mathcal{L})\phi_1^{n+1} &= \phi^n, \\
(I + \Delta t G\mathcal{L})\phi_2^{n+1} &= -\Delta t G\left(\frac{U[\phi^n]}{\sqrt{E_1[\phi^n] + C_0}}\right).
\end{align}

Once $\phi_1^{n+1}$ and $\phi_2^{n+1}$ are known, we can determine $r^{n+1}$ explicitly from (1.5c) (see more details in [23, 24, 30].

The above SAV approach enjoys the following remarkable properties:

- it requires only the solution of two linear systems with constant coefficients at each time step (efficiency);
- the first- and second-order SAV schemes are unconditionally energy-stable (stability);
- it only requires the nonlinear energy functional $E_1(\phi)$ be bounded from below, so it is applicable to a large class of gradient flows (flexibility).

Our aim in this paper is to propose some new essential improvements on the SAV approach to make it even more efficient and flexible in the sense that

- it only requires solving one linear system with constant coefficients at each time step;
it does not require the nonlinear energy functional \( E_1(\phi) \) be bounded from below, and applicable to more general gradient flows, even to general dissipative systems;

- and more importantly, it is extendable to higher-order BDF type schemes with unconditional stability and amenable to higher-order adaptive time stepping.

The rest of the paper is organized as follows. In Section 2, we describe the construction of the new SAV scheme for gradient flows in a general form. In Section 3, we construct the higher order unconditionally energy stable scheme. In Section 4, adaptive time stepping strategy for our unconditionally energy stable schemes will be studied. In Section 5, we provide ample numerical examples to demonstrate the performance of our proposed method and comparisons with the original SAV method will be reported. Section 6 concludes the discussions with some closing remarks.

2. A NEW SAV ENERGY-STABLE SCHEME

The SAV approach requires solving two linear equations at each time step. However, we observe that the two equations for \( \phi^{n+1} \) and \( \phi_0^{n+1} \) in (1.7) are different only on the right hand side. This motivates us to employ the auxiliary variable to control not only the nonlinear energy functional \( E \), but also the explicit term \( \phi^n \), i.e., replace the temporal derivative in (1.5a) by 

\[
\frac{\phi^{n+1} - \phi^n}{\Delta t} \quad \text{or} \quad \frac{\theta \Delta t \xi^{n+1} \phi^n}{\sqrt{E_1[\phi^n] + C_0}}.
\]

Consequently, this gives rise to the counterpart of equation (1.6)

\[
(I + \Delta t G \mathcal{L})\phi^{n+1} = r^{n+1} \left( \frac{\phi^n}{\sqrt{E_1[\phi^n] + C_0}} - \Delta t G \left( \frac{U[\phi^n]}{\sqrt{E_1[\phi^n] + C_0}} \right) \right), \tag{2.1}
\]

which requires only the solution of the single equation

\[
(I + \Delta t G \mathcal{L})\bar{\phi}^{n+1} = \frac{\phi^n}{\sqrt{E_1[\phi^n] + C_0}} - \Delta t G \left( \frac{U[\phi^n]}{\sqrt{E_1[\phi^n] + C_0}} \right), \tag{2.2}
\]

and then determine \( \phi^{n+1} \) and \( r^{n+1} \) from \( \phi^{n+1} = r^{n+1} \bar{\phi}^{n+1} \) and (1.5c).

However, such a naive treatment on the temporal derivative term could not lead to even first-order convergence due to the fact that \( \frac{\phi^{n+1} - \phi^n}{\Delta t} \) is no longer a first-order approximation of \( \frac{\partial \phi}{\partial t} \big|_{n+1} \). Specifically, assume that \( r^{n+1} \) is approximated such that

\[
\frac{r^{n+1}}{\sqrt{E_1[\phi^n] + C_0}} = 1 + O(\Delta t),
\]

we have

\[
\frac{\phi^{n+1} - \xi^{n+1} \phi^n}{\Delta t} = \frac{\phi^{n+1} - \phi^n}{\Delta t} + \frac{1 - \xi^{n+1}}{\Delta t} \phi^n = \frac{\partial \phi}{\partial t} \big|_{n+1} + O(\phi^n), \tag{2.3}
\]

where \( \xi^{n+1} := \frac{r^{n+1}}{\Delta t} \frac{1}{\sqrt{E_1[\phi^n] + C_0}} \). Actually, in order to achieve first-order approximation of \( \frac{\partial \phi}{\partial t} \big|_{n+1} \) using the novel formula (2.3), \( \xi^{n+1} \) need to be approximated such that \( \xi^{n+1} = 1 + O(\Delta t^k) \), \( k \geq 2 \).

This inspires us to replace the controlling factor \( \xi^{n+1} = \frac{r^{n+1}}{\sqrt{E_1[\phi^n] + C_0}} \) by

\[
\theta + (1 - \theta) \xi^{n+1}, \tag{2.4}
\]

where \( \theta \) is a given constant such that \( \theta = 1 + O(\Delta t) \). In this way, it is direct to observe that

\[
\frac{\phi^{n+1} - \theta + (1 - \theta) \xi^{n+1} \phi^n}{\Delta t} = \frac{\phi^{n+1} - \phi^n}{\Delta t} + \frac{1 - \theta}{\Delta t} \left( 1 - \xi^{n+1} \right) \phi^n = \frac{\partial \phi}{\partial t} \big|_{n+1} + O(\Delta t). \tag{2.5}
\]
More generally, for any \( \theta = 1 + O(\Delta t^m) \) and \( \xi^{n+1} = 1 + O(\Delta t^n) \), we have
\[
\theta + (1 - \theta)\xi^{n+1} = 1 + O(\Delta t^{n+m}).
\] (2.6)

This observation makes it possible to achieve high-order convergence of \( \phi^{n+1} \) with lower-order approximation for \( \xi^{n+1} \).

The novel approximation (2.5) brings about significant issues in devising energy-stable schemes. In order to overcome this obstacle, we adopt some ideas from the recently proposed gPAV method in [28]. Specifically, in [28] it is suggested to (i) use a shifted total energy \( E[\phi] = E_{tot}[\phi] + C_0 \) instead of \( E_1[\phi] \) in equation (1.3) to define the scalar auxiliary variable; (ii) use the energy balance equation of the gradient flow (1.1) instead of equation (1.4) to construct the dynamical equation of the auxiliary variable, i.e. we adopt the following equation as the dynamical equation
\[
dE[\phi] = \int_\Omega \delta E \frac{\partial \phi}{\partial t} d\Omega = -\langle \delta E, \delta \phi \rangle - (\mu, \mathcal{G}\mu) \leq 0;
\] (2.7)

and (iii) a delicate treatment of the dynamical equation to preserve the positiveness of the auxiliary variable in the discrete level. With the help of these intuitive thoughts, we are ready to construct new unconditionally energy-stable schemes, which require solving only one linear equation with constant coefficients at each time step.

We define a shifted total energy by
\[
E[\phi] = E_{tot}[\phi] + C_0 = \frac{1}{2} (\phi, \mathcal{L}\phi) + E_1(\phi) + C_0,
\] (2.8)

where \( C_0 \) is a chosen scalar such that \( E[\phi] > 0 \) for all \( \phi \). Note that for a physically meaningful system, the total energy \( E_{tot} \) is bounded from below, thus such a \( C_0 \) is always available. In spirit of the recent work [28], we introduce a scalar auxiliary variable \( R(t) := E[\phi] \), which satisfies the following dynamical equation
\[
\frac{dR(t)}{dt} = -\langle \mu, \mathcal{G}\mu \rangle. \] (2.9)

Define \( \xi(t) = \frac{R(t)}{E[\phi(t)]} \) and note that \( \xi(t) \equiv 1 \) at the continuous level, we can reformulate the system (1.1)-(1.2) into the following equivalent form
\[
\frac{\partial \phi}{\partial t} = -\mathcal{G}\mu, \quad \frac{dR}{dt} = -\xi(\mu, \mathcal{G}\mu),
\] (2.10)

where \( \theta(t) \) can be an arbitrary function at the continuous level. Our new first-order scheme for (2.10) is as follows:
\[
\phi^{n+1} - [\theta^n + (1 - \theta^n)\xi^{n+1}]\phi^n = -G\mu^{n+1}, \quad \mu^{n+1} = \mathcal{L}\phi^{n+1} + [\theta^n + (1 - \theta^n)\xi^{n+1}]U(\phi^n), \quad \xi^{n+1} = \frac{R^{n+1}}{E[\phi^{n+1}]}, \quad \frac{R^{n+1} - R^n}{\Delta t} = -\xi^{n+1}(\mu^{n+1}, \mathcal{G}\mu^{n+1}).
\] (2.11)
where $\theta^n$, $\phi^{n+1}$ and $\tilde{\mu}^{n+1}$ are to be specified below, together with the initial conditions

$$
\phi^0 = \phi_0(x,t), \quad R^0 = E[\phi_0].
$$

Combining equations (2.11a) and (2.11b) leads to the following linear equation

$$(I + \Delta tG\mathcal{L})\phi^{n+1} = \left(\theta^n + (1 - \theta^n)\xi^{n+1}\right)\left(\phi^n - \Delta tG(U[\phi^n])\right).$$

Setting

$$\phi^{n+1} = \left(\theta^n + (1 - \theta^n)\xi^{n+1}\right)\tilde{\phi}^{n+1},$$

in the above, we find that $\tilde{\phi}^{n+1}$ is determined by

$$(I + \Delta tG\mathcal{L})\tilde{\phi}^{n+1} = \phi^n - \Delta tG(U[\phi^n]).$$

Once $\tilde{\phi}^{n+1}$ is known, we define

$$\tilde{\mu}^{n+1} = L\tilde{\phi}^{n+1} + U(\tilde{\phi}^{n+1}).$$

Note that $\tilde{\phi}^{n+1}$ can be viewed as an approximation of $\phi(t^{n+1})$ by a direct semi-implicit method. Thus, $\tilde{\phi}^{n+1}$ and $\tilde{\mu}^{n+1}$ are first-order approximations of $\phi^{n+1}$ and $\mu^{n+1}$. Inserting equation (2.11c) into equation (2.11d) leads to

$$\xi^{n+1} = \frac{R^n}{E[\phi^{n+1}] + \Delta t(L\tilde{\mu}^{n+1},G\tilde{\mu}^{n+1})}.$$  

It remains to specify $\theta^n$ which should be chosen such that $\theta^n = 1 + \mathcal{O}(\Delta t)$ for first-order consistency. While theoretically, $\theta^n = 1 + \mathcal{O}(\Delta t)$ suffices to have the desired order of accuracy and leads to stable schemes, our numerical results indicate that $\theta^n = \xi^n$, which obviously satisfies the order requirement, leads to more accurate and robust results.

To summarize, the scheme (2.11a)-(2.11d) can be implemented as follows:

- solve $\tilde{\phi}^{n+1}$ from (2.15);
- set $\tilde{\mu}^{n+1} = L\tilde{\phi}^{n+1} + U(\tilde{\phi}^{n+1})$ and compute $\xi^{n+1}$ from (2.17);
- update $\phi^{n+1} = (\theta^n + (1 - \theta^n)\xi^{n+1})\tilde{\phi}^{n+1}$, and go to the next time step.

We observe that the above procedure only requires solving one linear equation with constant coefficients as in a standard semi-implicit scheme. As for the stability, we have the following result:

**Theorem 2.1.** Given $R^n \geq 0$, we have $R^{n+1}, \xi^{n+1} \geq 0$, and the scheme (2.11a)-(2.11d) is unconditionally energy stable in the sense that

$$R^{n+1} - R^n = -\Delta t\xi^{n+1}(\tilde{\mu}^{n+1},G\tilde{\mu}^{n+1}) \leq 0.$$  

**Proof.** In light of equation (2.7), $(\tilde{\mu}^{n+1},G\tilde{\mu}^{n+1}) \geq 0$. Given that $R^n \geq 0$, since $E[\phi^{n+1}] > 0$, we derive from (2.17) that $\xi^{n+1} \geq 0$. We then conclude from (2.11d). 

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3. Extension to higher-order

The proposed method can be extended to construct high-order unconditionally energy-stable schemes when coupled with $k$-step backward differentiation formula (BDF$k$). The essential idea resides in that we can achieve overall $k$th order accuracy for $\phi$ by using just a first-order approximation for $\xi$, if we choose $\theta^n$ such that $\theta^n + (1 - \theta^n)\xi^{n+1}$ is a $(k+1)$th order approximation to 1, thanks to (2.5). Actually, for any $\theta^n = 1 + \mathcal{O}(\Delta t^p)$ and $\xi^{n+1} = 1 + \mathcal{O}(\Delta t^q)$, we have that

$$\theta^n + (1 - \theta^n)\xi^{n+1} = 1 + \mathcal{O}(\Delta t^{p+q}).$$

(3.1)
3.1. A recurrence formula for $\theta^n$. As discussed in the first-order case, the proposed scheme tends to be more accurate and robust when $\theta^n$ is computed from $\xi^n$. In what follows, we provide a recurrence formula to effectively construct $\theta^n$ from $\xi^n$ such that $\theta^n + (1 - \theta^n)\xi^{n+1}$ is sufficient to achieve $k$th order convergent scheme for $\phi$ at $t^{n+1}$.

Given $\xi^n$ and let $l$ be an integer to be specified, we define $\theta^n$ by the following recursion:

$$
\begin{align*}
\gamma_0 &= \xi^n + (1 - \xi^n)\xi^n, \\
\gamma_1 &= \gamma_0 + (1 - \gamma_0)\gamma_0, \\
\gamma_2 &= \gamma_1 + (1 - \gamma_1)\gamma_1, \\
&\vdots \\
\theta^n &= \gamma_l = \gamma_{l-1} + (1 - \gamma_{l-1})\gamma_{l-1}.
\end{align*}
$$

(3.2)

One can easily check that the following result holds.

**Lemma 3.1.** If $\xi^n$ and $\xi^{n+1}$ are first-order approximations to 1, i.e. $\xi^n, \xi^{n+1} = 1 + O(\Delta t)$, then

$$
\theta^n + (1 - \theta^n)\xi^{n+1} = 1 + O(\Delta t^{1+2^{l+1}}),
$$

where $\theta^n$ is obtained by (3.2).

Thus, to achieve an overall $k$th order scheme for $\phi$, it suffices to choose the smallest non-negative integer $l$ satisfying

$$
l \geq \frac{\ln k}{\ln 2} - 1.
$$

(3.4)

For example, for $k = 2, 3, 4, l$ can be chosen as 0, 1, 1, respectively.

3.2. A $k$th order energy-stable scheme. Combining the idea from the previous section for the first-order scheme, the above recurrence relation for constructing $\theta^n$ and the classical $k$-step backward differentiation formula, we arrive at a new $k$th order BDF$k$ scheme:

$$
\begin{align*}
\frac{\alpha \phi^{n+1} - \theta^n + (1 - \theta^n)\xi^{n+1}}{\Delta t} \hat{\phi}^n &= -G\mu^{n+1}, \\
\mu^{n+1} &= L\phi^{n+1} + (\theta^n + (1 - \theta^n)\xi^{n+1})U(\phi^{n+1}), \\
\xi^{n+1} &= \frac{R^{n+1}}{E(\phi^{n+1})}, \\
\frac{R^{n+1} - R^n}{\Delta t} &= -\xi^{n+1}(\bar{\mu}^{n+1}, G\bar{\mu}^{n+1}),
\end{align*}
$$

(3.5)

where $\theta^n$ is obtained from (3.2). Here, $\alpha, \hat{\phi}^n$ and $\phi^{*,n+1}$ in equation (3.5) are defined as follows:

**BDF2:**

$$
\alpha = \frac{3}{2}, \quad \hat{\phi}^n = 2\phi^n - \frac{1}{2}\phi^{n-1}, \quad \phi^{*,n+1} = 2\phi^n - \phi^{n-1};
$$

(3.6)

**BDF3:**

$$
\alpha = \frac{11}{6}, \quad \hat{\phi}^n = 3\phi^n - \frac{3}{2}\phi^{n-1} + \frac{1}{3}\phi^{n-2}, \quad \phi^{*,n+1} = 3\phi^n - 3\phi^{n-1} + \phi^{n-2};
$$

(3.7)

**BDF4:**

$$
\alpha = \frac{25}{12}, \quad \hat{\phi}^n = 4\phi^n - 3\phi^{n-1} + \frac{4}{3}\phi^{n-2} - \frac{1}{4}\phi^{n-3}, \quad \phi^{*,n+1} = 4\phi^n - 6\phi^{n-1} + 4\phi^{n-2} - \phi^{n-3}.
$$

(3.8)
We can also use BDF5 and BDF6, but for the sake of brevity, we omit the detailed formula here.

Note that the solution algorithm for the new BDF\(k\) scheme is the same as the first-order scheme presented in Section 2. In each time step, it requires only the solution of one linear equation with constant coefficients, making the proposed method highly efficient. The new BDF\(k\) scheme also enjoys the same stability as the first-order scheme, namely, we can prove the following result using exactly the same procedure as in Section 2.

**Theorem 3.2.** Given \(R^n \geq 0\), we have \(R^{n+1}, \xi^{n+1} \geq 0\), and the scheme (3.5a)-(3.5d) for any \(k \geq 2\) is unconditionally energy stable in the sense that
\[
R^{n+1} - R^n = -\Delta t \xi^{n+1}(\bar{\mu}^{n+1}, G\bar{\mu}^{n+1}) \leq 0.
\] (3.9)

**Remark 3.1.** Note that the stability is built into the scheme in (3.5d), independent of the actual scheme used in (3.5a) and (3.5b). In principle, we can use any linear multistep schemes in place of (3.5a) and (3.5b).

### 4. Adaptive time-stepping strategy for SAV BDF\(k\) schemes

To achieve satisfactory numerical results in real simulations efficiently, it is supposed to use small time steps when the energy and solution of gradient flows vary drastically while using relatively larger time steps when they vary slightly. However, for conditionally stable schemes, the allowable time step is often dictated by the stability constraint, not by accuracy. One salient feature of an unconditionally energy stable scheme is that it allows us to employ an appropriate adaptive time-stepping strategy [9, 17, 21, 31]. Note that time-adaptivity strategy has been applied to first-order and second-order Crank-Nicolson SAV schemes in [11, 19, 24]. There are essential difficulties to apply adaptive time stepping to other schemes, particularly other second- or higher-order schemes. The main reason is that one does not have robust unconditionally stable second- or higher-order schemes with variable step sizes. In a recent work [9], the authors developed a stabilized second-order BDF scheme with variable step sizes that is stable if \(\tau^{n+1} \leq \gamma^* \tau^n\) where \(\{\tau^k\}\) are the time step sizes and \(\gamma^* \approx 1.5\) for optimal convergence. To the best of our knowledge, there is no unconditionally stable third- or higher-order BDF scheme with variable step sizes.

However, as stated in Remark 3.1, we can replace (3.5a) and (3.5b) by any linear multistep schemes without affecting the stability provided by (3.9). In particular, we can replace them by the BDF\(k\) schemes (along with \(k\)th order extrapolation formula for nonlinear terms) with variable step sizes which we shall derive in the Appendix.

It is crucial to figure out a good indicator for adaptive time-stepping schemes, which suggests us to adjust the time step at reasonable moments. Some observations from abundant numerical experiments are as follows:

(i) to achieve an accurate result, \(\xi^{n+1}\) has to be a good approximation to 1;

(ii) \(\xi^{n+1}\) starts to deviate from 1 when oscillation or inaccuracy turns to happen, while adopting a smaller time step can avoid such situation.

These observations suggest us that \(|1 - \xi^{n+1}|\) is a suitable indicator for the time-adaptivity procedure. Roughly speaking, we should decrease the time step whenever \(|1 - \xi^{n+1}|\) is bigger than a given tolerance while we can maintain a relatively large time step whenever \(|1 - \xi^{n+1}|\) is small enough.

Based on these observations, we provide an adaptive time-stepping algorithm for the proposed BDF\(k\) SAV scheme. Given a default safety coefficient \(\rho\), a reference tolerance
tol, the minimum time steps $\tau_{\text{min}}$ and the maximum time steps $\tau_{\text{max}}$, the adaptivity speed tunable constant $r$, we can update the time step size by the following formula

$$A_{dp}(e, \tau) = \rho\left(\frac{tol}{e}\right)^r \tau.$$ (4.1)

The corresponding algorithm is summarized as follows:

**Algorithm 1:** Time step adaptive procedure

**Given:** the previous time step $\tau_n$.

**step 1.** compute $\xi_n$ from previous step with time step $\tau_n$;

**step 2.** calculate $e_n = |1 - \xi_n|$;

**step 3. if** $e_n > tol$, **then**

recalculate time step $\tau_n \leftarrow \max\{\tau_{\text{min}}, \min\{A_{dp}(e_n, \tau_n), \tau_{\text{max}}\}\}$;

**goto** step 1

**step 4. else** update time step $\tau_{n+1} \leftarrow \max\{\tau_{\text{min}}, \min\{A_{dp}(e_n, \tau_n), \tau_{\text{max}}\}\}$;

**step 5. endif**

**Remark 4.1.** It is suggested in [34] that when $R^n$ has an obvious deviation from $E[\phi^n]$, a reset of $R^n = E[\phi^n]$ can be prescribed to improve the long time accuracy of the numerical scheme. This strategy could also be incorporated into the time-adaptivity algorithm. Specifically, $R^n$ is reset to $E[\phi^n]$ when $\tau_{n+1}/\tau_n$ is less than a threshold value.

The proposed time-stepping strategy will be applied to the simulations of Allen-Cahn and Cahn-Hilliard equations in the next section to show its advantages to achieve high accuracy with low computational cost.

### 5. Representative numerical examples

In this section, we provide ample numerical results to validate the accuracy and efficiency of our proposed method. Comparisons with the original SAV approach [23, 24] will be reported and the efficiency of the time-adaptivity technique for high-order schemes will be addressed.

Let us consider two typical types of gradient flow, i.e. the Allen-Cahn equation [11] and the Cahn-Hilliard equation [6, 7]. Given the free energy

$$E_{\text{tot}}[\phi] = \int_\Omega \frac{\lambda}{2} |\nabla \phi|^2 + E_1[\phi] d\Omega, \quad E_1[\phi] = \frac{\lambda}{4\eta^2} (1 - \phi^2)^2,$$ (5.1)

the chemical potential in (1.2) takes the form

$$\mu = \frac{\delta E_{\text{tot}}}{\delta \phi} = -\lambda \nabla^2 + U[\phi], \quad U[\phi] = \frac{\lambda}{\eta^2} \phi(\phi^2 - 1).$$ (5.2)

The Allen-Cahn equation corresponds to the $L^2$ gradient flow with $G = m_0 I$, while the Cahn-Hilliard equation corresponds to the $H^{-1}$ gradient flow with $G = -m_0 \nabla^2$ in equation (1.1).

**Remark 5.1.** Although we consider only the Allen-Cahn and the Cahn-Hilliard equations in the forthcoming numerical experiments, it is worthwhile to point out that our proposed approach is directly applicable to gradient flow problems where the nonlinear part of the free energy contains spatial derivatives, i.e., the molecular beam epitaxy model [11].
Example 1. (Convergence rate of the new SAV/BDFk scheme for the Allen-Cahn and Cahn-Hilliard equations) Consider the Allen-Cahn and Cahn-Hilliard equations in the computational domain $\Omega = [0, 2] \times [0, 2]$ with a contrived exact solution
\[
\phi(x, t) = \cos(\pi x) \cos(\pi y) \sin(t)/(1 + 10t^2),
\]
and correspondingly, the external source term $f(x, t)$ satisfying $\phi_t = -\mathcal{G} \mu + f$. Fourier spectral method $[25]$ for spatial discretization is employed throughout this section. $N_x$ and $N_y$ denote the number of Fourier collocation points along $x$ and $y$ axis, respectively. In the simulations, we set $(N_x, N_y) = (40, 40)$ with which the spatial discretization error is negligible compared with time discretization error. Other parameters are $\lambda = 0.01$, $m_0 = 0.01$, $\eta = 0.05$ and $C_0 = 0$. The algorithm for the new SAV/BDF$k$ ($k = 1, 2, 3, 4$) is employed to numerically integrate the governing equations in time from $t = 0$ to $t = 1$. The $L^2$ errors of $\phi$ at $t = 1$ are plotted respectively in Figure 5.1 (a)-(b) for the Allen-Cahn equation and Figure 5.2 (a)-(b) for the Cahn-Hilliard equation, where we can observe the expected convergence rate of the field variable $\phi$ for all cases.

Recall that $R(t) = E[\phi]$ in the continuous level and the evolution equation of $R(t)$ is stemmed from this equation. The discretization $E[\phi]$ of $R(t)$ leads to a first order approximation of $E[\phi]$. Consequently, $\xi_n^{n+1} = \frac{ER_n^{n+1}}{E[\phi_n^{n+1}]}$ is a first order approximation of 1. We depict the $L^\infty$ error of $\xi_n^{n+1}$ to 1 for the Allen-Cahn and Cahn-Hilliard equations in Figure 5.1 (c)-(d) and Figure 5.2 (c)-(d), respectively. As expected, it can be observed that $\xi_n^{n+1}$ converges to 1 with a first order convergence rate for all cases. Moreover, this observation implies that $\xi_n^{n+1}$ can serve as an indicator of the accuracy of the simulations. If the difference of $\xi_n^{n+1}$ from 1 is small, then the simulation tends to be more accurate. Otherwise, when $\xi_n^{n+1}$ deviates significantly from 1, the simulation is no longer accurate.

Example 2. (Spinodal decomposition for the Allen-Cahn equation) Consider the spinodal decomposition of a homogeneous mixture into two coexisting phases governed by the Allen-Cahn equation as another test of the algorithms developed herein. The computational domain is $[0, 2] \times [0, 2]$ and the initial phase field is given by an uniformly distributed datas between $[-0.5, 0.5]$. We adopt $(N_x, N_y) = (512, 512)$, $\lambda = 1$, $m_0 = 10^{-4}$, $\eta = 0.005$ and $C_0 = 0$ in the forthcoming simulations. The new SAV/BDF2 scheme is employed to numerically integrate this problem.

In Figure 5.3, we depict a temporal sequence of snapshots of the interfaces formed between the two phases. Figure 5.4 shows the time histories of the total energy $E_{\text{tot}}[\phi]$ obtained by the current method and the original SAV method using various time steps $\Delta t = 10^{-1}, 10^{-2}, 10^{-3}$. A reference solution obtained with $\Delta t = 10^{-4}$ using the original SAV scheme is also included for comparison. It can be observed in Figure 5.4 (a) that all the energy history curves decrease dramatically at the beginning and level off gradually, indicating the stability of the proposed method. In Figure 5.4 (b), we zoom in the energy history curves at the region $t \in [0, 0.1]$. It shows that the results obtained by the current method and the original SAV method overlap with each other for the same time step size. This implies that the proposed method provides almost the same accuracy with the original SAV method, but with halved computational cost. It also indicates that to achieve acceptable accuracy, the step size should be chosen no bigger than $\Delta t = 10^{-3}$.

Example 3. (Application of adaptive time-stepping strategy to example 2) Next, we use the spinodal decomposition governed by the Allen-Cahn equation to demonstrate the performance of the time adaptivity. The setup is the same as Example 2. The proposed SAV/BDF$k$ schemes with variable time steps using $l = 0, 1, 1$ in the recurrence relation (3.2)
for $k = 2, 3, 4$, respectively, are employed to numerically integrate this problem. We choose $\rho = 0.9$, $tol = 10^{-3}$ and $r = 0.25$ in equation (4.1). The minimum time step is taken as $\tau_{\text{min}} = 10^{-6}$, while the maximum time step is take as $\tau_{\text{max}} = 10^{-3/k}$, $k = 2, 3, 4$, respectively, such that when $\tau_{\text{max}}$ is employed, the errors for BDF$^k$ schemes ($k = 2, 3, 4$) are of the same level. The initial time step is taken as $\tau_{\text{min}}$.

In Figure 5.5 (a), we depict the energy history curves obtained by BDF$^k$ ($k = 2, 3, 4$) schemes for long time simulations, and it can be seen that the curves essentially overlap with each other. Correspondingly, the snapshot of the interfaces between these two phases at $t = 300$ are compared in Figure 5.5 (b)-(d) and no noticeable difference can be observed.

In order to demonstrate the efficiency of the time-adaptivity technique, we plot in Figure 5.6-5.8 the time history curves of the time steps and time step ratios between two successive steps in the time window $t \in (0, 3)$, where rapid changes of the phase field variable occur. It can be seen that the time steps gradually increases for all these three solvers and the average time steps in these period are $1.6 \times 10^{-2}$, $2.0 \times 10^{-2}$ and $2.1 \times 10^{-2}$. Note that in Example 2, for BDF2 scheme with a fixed time step, it takes at least $\Delta t = 10^{-3}$ to obtain reasonable numerical results. We also record the total wall time of this simulation computed from $t = 0$.
Figure 5.2. (Example 1.) Temporal convergence test for the Cahn-Hilliard equation using the new SAV/BDFk ($k = 1, 2, 3, 4$). (a)-(b) $L^2$ errors of $\phi$ as a function of $\Delta t$; (c)-(d) $L^\infty$ errors of $\xi$ as a function of $\Delta t$.

to $t = 300$ with BDF2 scheme using a fixed time step $\Delta t = 10^{-3}$, which is 19970.2 seconds. While equipped with the time-adaptivity technique, the total wall time for the BDF2-BDF4 schemes reduces drastically to 929.0 seconds, 318.9 seconds and 429.6 seconds, respectively. The speedups in these simulations are noticeable, compared with the solver without time adaptivity. In [9], it is point out that the variable step BDF2 scheme is stable if $\tau_{n+1} \leq \gamma^* \tau_n$ and $\gamma^* \approx 1.5$ for optimal convergence. While with the current method, we are not restricted by this constraint and the maximum time step ratios are observed to be as large as 22, 41, 41 for $k = 2, 3, 4$.

Example 4. (Merging of an array of circles for the Cahn-Hilliard equation) We consider, as another test problem, the merging of a rectangular array of $9 \times 9$ circles governed by the Cahn-Hilliard equation. The computational domain is $[0, 2] \times [0, 2]$ and the initial phase field is given by

$$
\phi_0(x, t) = 80 - \sum_{i=1}^{9} \sum_{j=1}^{9} \tanh \left( \sqrt{(x-x_i)^2 + (y-y_j)^2 - R_0} \right) \sqrt{2\eta},
$$

(5.4)
where \( R_0 = 0.085, x_i = 0.2 \times i \) and \( y_j = 0.2 \times j \) for \( i, j = 1, 2, ..., 9 \). We adopt \((N_x, N_y) = (512, 512), \lambda = 1, m_0 = 10^{-6}, \eta = 0.01\) and \( C_0 = 0 \) in the simulations.

In Figure 5.9, we plot a temporal sequence of snapshots of the interfaces formed between the two phases using the BDF3 scheme with variable time steps using \( \rho = 0.95, tol = 10^{-3}, r = 0.57, \tau_{\text{min}} = 10^{-6} \) and \( \tau_{\text{max}} = 10^{-1} \) in equation (4.1).
In order to investigate the influence of the parameter $tol$ to the accuracy and efficiency of the new SAV/BDF$k$ ($k = 2, 3, 4$) schemes with time-adaptivity, we depict in Figure 5.10 the $L^2$-errors of $\phi$ as a function of the average of the time step sizes. These errors are obtained through comparing the numerical solutions with a reference solution computed by the new SAV/BDF2 scheme with a fixed small $\Delta t = 10^{-5}$ at $t = 1$. It can be seen that a better accuracy is achieved when we adopt a smaller $tol$.

Figure 5.11 is a demonstration of the stability of the proposed scheme. The time histories of the modified energy $R(t)$ obtained by large time step sizes $\Delta t = 2, 5$ are depicted. At these large time step sizes, we can no longer expect the results to be accurate. But it can be observed that the modified energy decays and remains to be positive for long time simulations.

In Figure 5.12 we depict a comparison of the time histories of $\xi^{n+1}$ obtained by the new BDF2 schemes with $\theta^n = 1 - (\Delta t)^2$ and $\theta^n = \xi^n + (1 - \xi^n)\xi^n$ (see the recurrence relation (3.2)). As discussed before, the difference between $\xi^{n+1}$ and the unit value can be used to
indicate the accuracy of the computation. Thus, this comparison shows the influence of these two different choices of \( \theta_n \) to the performance of the proposed scheme. It can be observed in Figure 5.12 (a) that when \( \Delta t = 10^{-3} \) is used, \( \xi^{n+1} \) obtained by both choices are close to 1 and the history curves of \( \xi^{n+1} \) overlap with each other. While when a relatively larger \( \Delta t = 0.006 \) in Figure 5.12 (b) is employed, \( \xi^{n+1} \) obtained by the scheme with a constant \( \theta_n \) deviates more from 1, indicating a larger numerical error, compared with the one obtained by the scheme with \( \theta_n = \xi^n + (1 - \xi^n)\xi^n \).

**Example 5. (An improved multiple SAV method for one-component Bose-Einstein condensates)** We consider the ground state solution of one-component Bose-Einstein condensates in two dimensions [2] [3] [34] as an example to show how our current method can reduce the number of linear equations to be solved in each time step from three to two, comparing with the classical MSAV [10] [34] approach.
A NEW SAV METHOD FOR GRADIENT FLOWS

Figure 5.9. (Example 4.) Merging of an array of circles governed by the Cahn-Hilliard equation. Simulations are obtained with the proposed SAV/BDF3 schemes with time-adaptivity technique.

Figure 5.10. (Example 4.) $L^2$-errors of $\phi$ as a function of the average of $\Delta t$ obtained by (a) the BDF2 scheme, (b) the BDF3 scheme, and (c) the BDF4 scheme, respectively. The time-adaptivity technique is employed with $tol = 10^{-1}, 10^{-2}, 10^{-3}$. The parameters $(r, \rho)$ in equation (4.1) are set to be $(0.75, 0.85), (0.57, 0.95), (0.7, 0.85)$ for the BDF2-BDF4 schemes, respectively.

Similar with [34], we consider the penalized energy

$$E(\phi) = \frac{1}{2}(\phi, \mathcal{L}\phi) + \frac{1}{2} \int_{\Omega} F(|\phi|^2)d\Omega + \frac{1}{4\varepsilon} \left( \int_{\Omega} |\phi|^2d\Omega - 1 \right)^2. \quad (5.5)$$
Here, \( F(\phi) = \frac{\beta}{2} \phi^2 \), \( \mathcal{L} = -\frac{1}{2} \nabla^2 + V(x, y) \phi \) with \( V(x, y) \geq 0 \) and \( \epsilon \ll 1 \). Correspondingly, the governing equation for this gradient flow problem takes the form
\[
\frac{\partial \phi}{\partial t} = -\frac{\delta E}{\delta \phi} = -\mathcal{L} \phi - F'(|\phi|^2) \phi - \frac{1}{\epsilon} (||\phi||^2 - 1) \phi, \tag{5.6}
\]
and subject to the constraints
\[
\int_{\Omega} |\phi(x, t)|^2 \, d\Omega = 1, \tag{5.7a}
\]
\[
\lim_{|x| \to \infty} \phi(x, t) = 0. \tag{5.7b}
\]
In our new MSAV approach, we introduce two scalar auxiliary variables
\[
R_1(t) = E_1(\phi), \quad R_2(t) = E_2(\phi). \tag{5.8}
\]
where
\[ E_1 = \frac{1}{2} (\phi, \mathcal{L}\phi) + \frac{1}{2} \int_{\Omega} F(|\phi|^2) d\Omega, \quad E_2 = \frac{1}{4\varepsilon} \left( \int_{\Omega} |\phi|^2 d\Omega - 1 \right)^2. \] (5.9)

With the same spirit to improve the single SAV approach in Section 2, we employ one of the introduced auxiliary variables to control not only the nonlinear term, but also the explicit linear term, and consequently, we are only required to solve two linear equations at each time step. The first order new MSAV scheme can be written as

\[ \frac{\phi^{n+1} - [\theta_1^n + (1 - \theta_1^n)\xi_1^{n+1}]\phi^n}{\Delta t} = -\mu^{n+1}, \] (5.10a)

\[ \mu^{n+1} = \mathcal{L}\phi^{n+1} + [\theta_1^n + (1 - \theta_1^n)\xi_1^{n+1}]U_1(\phi^n) + [\theta_2^n + (1 - \theta_2^n)\xi_2^{n+1}]U_2(\phi^n), \] (5.10b)

\[ \xi_1^{n+1} = \frac{R_1^{n+1}}{E_1[\phi^{n+1}]}, \quad \xi_2^{n+1} = \frac{R_2^{n+1}}{E_2[\phi^{n+1}]}, \] (5.10c)

\[ \frac{R_1^{n+1} - R_1^n}{\Delta t} = -\frac{R_1^{n+1} + R_2^{n+1}}{E_1[\phi^{n+1}] + E_2[\phi^{n+1}]}(\mathcal{L}\phi^{n+1} + U_1(\phi^{n+1}), \bar{\mu}^{n+1}), \] (5.10d)

\[ \frac{R_2^{n+1} - R_2^n}{\Delta t} = -\frac{R_1^{n+1} + R_2^{n+1}}{E_1[\phi^{n+1}] + E_2[\phi^{n+1}]}(U_2(\phi^{n+1}), \bar{\mu}^{n+1}), \] (5.10e)

where \( \bar{\mu}^{n+1} = \mathcal{L}\phi^{n+1} + U_1(\phi^{n+1}) + U_2(\phi^{n+1}), \) \( \theta_i = 1 + \mathcal{O}(\Delta t) \) for \( i = 1, 2, \) and \( \phi^{n+1} \) is defined similar as the single SAV case and

\[ U_1(\phi) = F'(|\phi|^2)\phi, \quad U_2(\phi) = \frac{1}{\varepsilon}(\|\phi\|^2 - 1)\phi. \] (5.11)

The initial condition is chosen as

\[ \phi_0(x, y) = \frac{(\gamma_x\gamma_y)^{1/4}}{\pi^{1/2}} e^{-((\gamma_x x^2 + \gamma_y y^2)/2} \] (5.12)

with two different potential functions:

**Case 1.** A harmonic oscillator potential

\[ V(x, y) = \frac{1}{2}(\gamma_x x^2 + \gamma_y y^2). \] (5.13)

**Case 2.** A harmonic oscillator potential and a potential of a stirrer corresponding to a far-blue detuned Gaussian laser beam

\[ V(x, y) = \frac{1}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2) + \omega_0 e^{-\delta((x-r_0)^2 + y^2)}. \] (5.14)

The parameters are chosen as: \( \gamma_x = 1, \gamma_y = 4 \) and \( \beta = 200 \) in case 1 and \( \gamma_x = 1, \gamma_y = 1, \omega_0 = 4, \delta = r_0 = 1 \) and \( \beta = 200 \) in case 2. We then solve case 1 by spectral-Galerkin method on \( \Omega_1 = [-8, 8] \times [-4, 4] \) and case 2 on \( \Omega_2 = [-8, 8] \times [-8, 8] \). In both cases, we choose \( (N_x, N_y) = (40, 40), \varepsilon = 10^{-4}, \) time steps \( \Delta t = 10^{-4} \) and impose the homogeneous Dirichlet boundary condition.

We plot the ground state solutions of both cases in Figure 5.13 and compare the chemical potential and the energy of the ground states with the results obtained by original MSAV method in [34] and by TSSP method in [3] in Tables 1 and 2, where we denote

\[ x_{\text{rms}} = \|x\phi\|_{L^2(\Omega)}, \quad y_{\text{rms}} = \|y\phi\|_{L^2(\Omega)}, \] (5.15)
and

$$\mu_\beta(\phi) = \int_\Omega \left( \frac{1}{2} |\nabla \phi(x)|^2 + V(x)|\phi(x)|^2 + \beta |\phi(x)|^4 \right) d\Omega$$

$$= E_\beta(\phi) + \frac{\beta}{2} |\phi(x)|^4 d\Omega.$$ 

We observe from Tables 1 and 2 that the results by our new SAV schemes are consistent with the results obtained by using the original SAV and TSSP methods.

**Figure 5.13.** Ground state solutions of one-component Bose-Einstein condensates

<table>
<thead>
<tr>
<th>Scheme</th>
<th>$x_{\text{rms}}$</th>
<th>$y_{\text{rms}}$</th>
<th>$E_\beta$</th>
<th>$\mu_\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>TSSP</td>
<td>2.2734</td>
<td>0.6074</td>
<td>11.1563</td>
<td>16.3377</td>
</tr>
<tr>
<td>MSAV</td>
<td>2.2812</td>
<td>0.6096</td>
<td>11.1560</td>
<td>16.3002</td>
</tr>
<tr>
<td>New MSAV</td>
<td>2.2710</td>
<td>0.6064</td>
<td>11.1621</td>
<td>16.2514</td>
</tr>
</tbody>
</table>

**Table 1.** Case 1: $\gamma_x = 1$, $\gamma_y = 4$ and $\beta = 200$

<table>
<thead>
<tr>
<th>Scheme</th>
<th>$x_{\text{rms}}$</th>
<th>$y_{\text{rms}}$</th>
<th>$E_\beta$</th>
<th>$\mu_\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>TSSP</td>
<td>1.6951</td>
<td>1.7144</td>
<td>5.8507</td>
<td>8.3269</td>
</tr>
<tr>
<td>MSAV</td>
<td>1.6978</td>
<td>1.7169</td>
<td>5.8506</td>
<td>8.3189</td>
</tr>
<tr>
<td>New MSAV</td>
<td>1.6933</td>
<td>1.7124</td>
<td>5.8455</td>
<td>8.3202</td>
</tr>
</tbody>
</table>

**Table 2.** Case 2: $\gamma_x = 1$, $\gamma_y = 1$, $\omega_0 = 4$, $\delta = r_0 = 1$ and $\beta = 200$

**Remark 5.2.** Some remarks are in order:

1. Same as the single SAV approach mentioned in section 2, one can easily prove the scheme (5.10) is unconditionally energy stable in the sense that $R_1^n + R_2^n \geq 0$ for every $n$, and

$$\frac{(R_1^{n+1} + R_2^{n+1}) - (R_1^n + R_2^n)}{\Delta t} + \frac{R_1^{n+1} + R_2^{n+1}}{E_1[\bar{\phi}^{n+1}] + E_2[\bar{\phi}^{n+1}]} (\bar{\mu}^{n+1} - \overline{\mu}^{n+1}) \leq 0. \quad (5.17)$$
2. The new MSAV scheme \([5,10]\) only requires solving two instead of three linear equations, compared with in the original MSAV scheme in \([34]\). In general, if we introduce \(K\) auxiliary variables, our new MSAV scheme requires only the solution of \(K\) linear equations, while the original SAV scheme requires to solve \(K + 1\) linear equations. Hence, the new MSAV schemes is more efficient.

3. We can also construct higher-order unconditionally energy stable MSAV schemes based on the approach presented in Section 3.

6. Concluding remarks

We presented in this paper several essential improvements over the original SAV approach, making our new SAV approach even more efficient, flexible and amenable to higher-order. More precisely, our new SAV approach enjoys the following additional advantages:

(1) For the case with single SAV, our new method only requires solving one linear equation with constant coefficients, reducing half of the computational cost of the original SAV approach. In other words, the computational cost of the new SAV approach, being unconditionally energy stable, is essentially the same as that of the semi-implicit approach which is only conditionally stable. Furthermore, the new approach does not require the nonlinear part of the free energy to be bounded from below, making it more flexible than the original SAV approach.

(2) While the original SAV approach only leads to first- and second-order unconditionally stable BDF type schemes, the new SAV approach allows us to construct higher-order unconditionally energy stable schemes with any multistep schemes. In particular, we are able to construct, for the first time, unconditionally energy stable higher-order time adaptive schemes based on the BDF\(k\) scheme with variable step sizes.

(3) For the cases where \(K\) SAVs are needed, our new method requires solving \(K\) linear equations with constant coefficients, as opposed to \(K + 1\) linear equations by the original MSAV approach.

The SAV method is not limited to the realm of gradient flow. The idea of introducing a scalar auxiliary variable has been extended to many non-gradient flow type problems, e.g. Navier Stokes equation \([18,20]\), two phase flows \([29]\) and chemo-repulsion model \([28]\) et. al. Although we only focus on gradient flow problems in the current paper, the proposed method can be in principle extended to general dissipative systems. We will explore this issue in our future work.

Appendix A. Backward differentiation formula for variable time step sizes

Given a successive of variable time steps

\[
\tau^{n+1} = t^{n+1} - t^n, \quad \tau^n = t^n - t^{n-1}, \quad \tau^{n-1} = t^{n-1} - t^{n-2}, \quad \tau^{n-2} = t^{n-2} - t^{n-3}, \ldots, \tag{1.1}
\]

the corresponding \(\alpha\), \(\hat{\phi}^n\) and \(\phi^{*,n+1}\) in equation (3.5) for BDF\(k\) scheme with \(k\)th order extrapolation can be derived by Taylor expansion. More precisely, let us denote

\[
\begin{align*}
x_1 &= -\tau^{n+1}, \\
x_2 &= -\tau^{n+1} - \tau^n, \\
x_3 &= -\tau^{n+1} - \tau^n - \tau^{n-1}, \\
x_4 &= -\tau^{n+1} - \tau^n - \tau^{n-1} - \tau^{n-2}, \\
&\quad \ldots
\end{align*} \tag{1.2}
\]
Then, for \( k = 2, 3, 4 \), the formulae are given below:

**BDF2:**

\[
\alpha = \gamma^{-1}, \quad \phi^n = \gamma^{-1}(a\phi^n + b\phi^{n-1}), \quad \phi^{*,n+1} = A\phi^n + B\phi^{n-1},
\]

where

\[
\gamma = \frac{x_2}{x_1 + x_2}, \quad a = -\frac{x_2^2}{x_1^2 - x_2^2}, \quad b = \frac{x_1^2}{x_1^2 - x_2^2}, \quad A = -\frac{x_2}{x_1 - x_2}, \quad B = \frac{x_1}{x_1 - x_2}.
\]

**BDF3**

\[
\alpha = \gamma^{-1}, \quad \phi^n = \gamma^{-1}(a\phi^n + b\phi^{n-1} + c\phi^{n-2}), \quad \phi^{*,n+1} = A\phi^n + B\phi^{n-1} + C\phi^{n-2},
\]

where

\[
\gamma = \frac{x_2 x_3}{x_1 x_2 + x_1 x_3 + x_2 x_3}, \quad a = \frac{x_2^2 x_3^2}{(x_1 - x_2)(x_1 - x_3)(x_1 x_2 + x_1 x_3 + x_2 x_3)}, \quad b = -\frac{x_1^2 x_3^2}{(x_1 - x_2)(x_2 - x_3)(x_1 x_2 + x_1 x_3 + x_2 x_3)},
\]

\[
c = \frac{x_2^2 x_3^2}{(x_1 - x_3)(x_2 - x_3)(x_1 x_2 + x_1 x_3 + x_2 x_3)},
\]

and

\[
A = \frac{x_2 x_3}{(x_1 - x_2)(x_1 - x_3)}, \quad B = -\frac{x_1 x_3}{(x_1 - x_2)(x_2 - x_3)}, \quad C = \frac{x_1 x_2}{(x_1 - x_3)(x_2 - x_3)}.
\]

**BDF4**

\[
\alpha = \gamma^{-1}, \quad \phi^n = \gamma^{-1}(a\phi^n + b\phi^{n-1} + c\phi^{n-2} + d\phi^{n-3}), \quad \phi^{*,n+1} = A\phi^n + B\phi^{n-1} + C\phi^{n-2} + D\phi^{n-3},
\]

where

\[
\gamma = \frac{23 23}{23 23}, \quad a = -\frac{23 23}{23 23}, \quad b = \frac{23 23}{23 23}, \quad c = -\frac{23 23}{23 23}, \quad d = \frac{23 23}{23 23},
\]

and

\[
A = -\frac{x_2 x_3 x_4}{(x_1 - x_2)(x_1 - x_3)(x_1 - x_4)}, \quad B = \frac{x_1 x_3 x_4}{(x_1 - x_2)(x_2 - x_3)(x_2 - x_4)},
\]

\[
C = -\frac{x_1 x_2 x_4}{(x_1 - x_3)(x_2 - x_3)(x_3 - x_4)}, \quad D = \frac{x_1 x_2 x_3}{(x_1 - x_4)(x_2 - x_4)(x_3 - x_4)}.
\]

The formulae for higher-order BDF\( k \) \( (k \geq 5) \) with variable step sizes can also be derived similarly. We omit the detail here for brevity.
REFERENCES


