B-METHODS FOR THE NUMERICAL SOLUTION OF EVOLUTION PROBLEMS WITH BLOW-UP SOLUTIONS PART I: VARIATION OF THE CONSTANT

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Abstract. In the last two decades, the field of geometric numerical integration and structure-preserving algorithms has focused on the design of numerical methods that preserve properties of Hamiltonian systems, evolution problems on manifolds and problems with highly oscillatory solutions. In this paper, we show that a different geometric property, namely the blow-up of solutions in finite time, can also be taken into account in the numerical integrator, giving rise to geometric methods we call B-methods. We give a first systematic approach for deriving such methods for scalar and systems of semi- and quasi-linear parabolic and hyperbolic partial differential equations. We show both analytically and numerically that B-methods have substantially better approximation properties than standard numerical integrators as the solution approaches the blow-up time.

Key words. Geometric Integration, Blow-up Solutions, Non-Linear Partial Differential Equations, Nonlinear Systems of Equations

AMS subject classifications. 65M12,65M15,65L06,65H10

1. Introduction. It is well known that nonlinear partial differential equations (PDEs) can develop singular solutions even when the initial and boundary data are smooth. In this paper, we are interested in equations whose solutions exhibit "blow-up", i.e., become unbounded in finite time. One example is the following quasilinear equation, which arises in plasma physics, see [40, 41]:

$$u_t = \Delta u^m + \alpha u^m \quad \text{in } \Omega \subset \mathbb{R}^d,\ t > 0, \quad m > 1. \tag{1.1}$$

Here, Δ denotes the Laplacian operator in d-dimensional space, $d = 2$ or 3. It is shown in [41] that when α is larger than the smallest eigenvalue of $-\Delta$, then the solution becomes unbounded at some finite time $t = T$. Nonlinear PDEs with blow-up solutions are also used to model phenomena such as combustion [21, 14, 30, 32], turbulent flow [36], nonlinear optics [35, 38, 39] and population dynamics [43, 25]. The blow-up of solutions typically indicates the collapse of some approximation used to derive the model, so it is important to know the blow-up time T and the rate of growth prior to blow-up, so that one has the chance to adjust the physical model before blow-up occurs. Because of the nonlinear nature of the equations, this analysis is generally done on a case-by-case basis, see [34, 44, 23, 45, 24, 19, 3, 16, 13]. For more recent overviews, see [4, 20].

A particularly well-studied class is the semilinear equation

$$u_t = \Delta u + F(u), \tag{1.2}$$

where $F(u)$ is a convex function that is non-negative for $u \geq 0$. In combustion models, the function $F(u)$ represents nonlinear heat generation, and different choices have been made. In the solid-fuel or Frank-Kamenetskii model of combustion, one

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chooses $F(u) = \delta e^u$ with $\delta > 0$, see [6]. Another classical choice is $(u+\alpha)^p$ for $\alpha \geq 0$ and $p > 1$ [18, 28, 29]. For these choices, theoretical results such as existence and uniqueness for short time are available, as well as estimates of the blow-up time T and the growth rate near blow-up. For instance, for $F(u) = \delta e^u$ and homogeneous Dirichlet boundary conditions, the following results are known, see [7, 5]:

- Let λ_1 be the smallest eigenvalue of the negative Laplacian operator in Ω. Suppose $m > 0$ is such that $\delta e^u > \lambda_1 u$ whenever $u \geq m$. Then if the initial data $u(x, 0)$ satisfies $m \leq u(x, 0) \leq M$, the solution $u(x, t)$ becomes infinite as $t \to T$, where
$$e^{-M} \leq T \leq \int_m^\infty \frac{du}{\delta e^u - \lambda_1 u}.$$
- The solution satisfies
$$u(x,t) - \ln \frac{1}{T-t} \to 0 \qquad \text{as } t \to T^-$$
uniformly on $|x| \leq C(T-t)^{1/2}$, $C \geq 0$.

If more precise estimates on the blow-up time and rate of growth are required, we must resort to solving the PDEs numerically. This involves choosing appropriate discretization schemes in both space and time. For spatial discretizations, one way of maintaining accuracy is to adapt the spatial mesh in time, so that there are always enough mesh points near the singularity as it develops. If one fixes the number of mesh points so that only their locations change in time, we obtain the so-called r-adaptive moving mesh methods, for which a vast literature exists; we refer to the paper [10], the textbook [27] and the references therein for more details. The choice of time discretization is also a determining factor in solution accuracy. In principle, any numerical ODE solver can be used (Runge-Kutta, Linear Multistep, General Linear Methods) to obtain an approximate solution of (1.2) in time. For example, we may use Backward Euler with time step h to discretize in time and obtain

$$u_{n+1} - u_n = h(\Delta u_{n+1} + F(u_{n+1})). \tag{1.3}$$

However, how fast the numerical solution converges to the continuous one depends on the size of u and its derivatives, both of which are large for blow-up problems. Thus, convergence can be very slow, and the numerical solution for a given time step size h may not exhibit blow-up at the right time (or may not even blow up at all!). It is therefore important to use numerical methods that can reproduce the blow-up behavior and yield the same blow-up time and growth rate as the continuous solution. The goal of this paper is to introduce a systematic way of constructing numerical methods that preserve these important properties.

The area of research aimed at developing numerical methods that preserve specific properties of the underlying differential equation is known as geometric numerical integration. Much progress has been made over the last decade in this area, see the research monograph [26] and references therein. There are for example symmetric methods for time reversible problems, symplectic or energy conserving methods for Hamiltonian problems, methods on manifolds and also specialized methods for highly oscillatory problems. Considering blow-up as a geometric property seems however to be new, and existing methods in the literature have been derived in an ad hoc manner. For instance, in [37], Le Roux proposed a very unusual time stepping scheme for solving (1.1)[1]:

$$(m-1)^{-1}(u_n^{1-m}u_{n+1}^m - u_{n+1}) = h(\Delta u_{n+1}^m + \alpha u_{n+1}^m), \tag{1.4}$$

Under some weak hypotheses, she proved that this time discretization leads to numerical solutions with the same blow-up behavior as the exact solution. Her derivation uses two essential ingredients: she noted that the evolution problem without the spatial operator has a closed form solution, and then used an ad hoc change of variables to devise a time stepping scheme based on this closed form solution.

The goal of this paper is to present systematic ways of obtaining such specialized numerical time stepping schemes that capture the geometric property of blow-up as soon as the non-linear term dominates. We call these methods B-methods as a reminder of the main application to PDEs with blow-up solutions. Just like Le Roux, our schemes are also based on the exact solution of the underlying ODE, but we present a systematic approach, based on the variation of constants technique in the solution of ODEs, to incorporate these exact solutions to obtain B-methods for the underlying PDE. There is also a second approach for deriving B-methods, based on operator splitting. This will be the subject of a companion paper [8].

This paper is structured as follows: in Section 2, we show how to use the variation-of-constants approach to construct B-methods for solving quasilinear parabolic equations. We also present a simple truncation error analysis to illustrate why we should expect more accurate solutions. In Section 3, we analyze one of our B-methods in detail. In particular, we prove for a class of semilinear PDEs that our B-Method is well-defined at least up to a final time T_f that is close to the analytical blow-up time T_b. In Section 4, we show that our B-method produces solutions that have the same geometric blow-up properties as the underlying PDE. Since B-methods generally require solving a system of nonlinear algebraic equations, Section 5 is devoted to the discussion of iterative methods that can be used to solve such systems. We then show numerical experiments in Section 6, and present our conclusions in Section 7.

2. Construction of B-Methods. We start by assuming that we have access to an exact representation of the solution of the non-linear ODE $u_t = f(u)$, which we will use as a basis for constructing B-methods. (For implementation purposes, this exact representation may be replaced by a very accurate numerical approximation.) The goal is to derive a numerical method for the perturbed equation

$$u_t = f(u) + \epsilon\ell(u). \tag{2.1}$$

The function $\epsilon\ell(u)$ will eventually become the spatial differential term, which becomes small relative to $f(u)$ near blow-up time. The derivation is based on the method of variation of the constant, which can be used to solve inhomogenous ordinary differential equations. We modify this approach to obtain a B-method for the model problem (2.1) as follows. Suppose $U = U(t, C)$ is the general solution of $U_t = f(U)$, with C being the constant of integration. We then seek a solution u of (2.1) of the form $u = U(t, C(t))$, i.e., we allow the constant to vary with time. Differentiating leads to

$$u_t = U_t + U_C C_t = f(u) + \epsilon\ell(u).$$

[1]"We have to construct a scheme whose solution has the same propoerties as the solution of the theoretical problem"

Since U satisfies the equation $U_t = f(U(t,C)) = f(u)$, the two terms always cancel in the above equation, so we get for C the differential equation

$$C_t = \frac{\epsilon\ell(u)}{U_C(t,C)}. \tag{2.2}$$

Now we can apply a standard numerical method to (2.2), e.g. Forward Euler with time step $h := t_{n+1} - t_n$, and obtain

$$C_{n+1} - C_n = h \cdot \frac{\epsilon\ell(u_n)}{U_C(t_n, C_n)}. \tag{2.3}$$

Applying the inverse transform $C = U^{-1}(t,u)$ yields the time integration method

$$U^{-1}(t_{n+1}, u_{n+1}) - U^{-1}(t_n, u_n) = h \cdot \frac{\epsilon\ell(u_n)}{U_C(t_n, U^{-1}(t_n, u_n))}, \tag{2.4}$$

which we will call the Variation-of-Constant Forward Euler (VCFE) method. The Backward Euler variant, called the VCBE method, can be derived similarly.

2.1. Derivation for a Model Problem. To be more concrete, let us illustrate the construction of various B-methods on the quasilinear parabolic problem

$$\begin{cases} u_t &= \Delta u^m + \delta F(u), & \Omega \times (0,T), \\ u &= 0, & \partial\Omega \times (0,T), \\ u(x,0) &= u_0(x), & \Omega, \end{cases} \tag{2.5}$$

where $\delta > 0$ is a constant parameter. For our later convenience, we define the functions

$$g(u) = \int_u^\infty \frac{ds}{F(s)}, \qquad G = g^{-1},$$

so that $g'(u) = -1/F(u)$. (We assume for the moment that the integral in $g(u)$ converges; a detailed discussion is deferred to Section 3.) If we let $U(t,C) = G(C - \delta t)$, then

$$U_t = -\delta G'(C - \delta t) = -\frac{\delta}{g'(G(C - \delta t))} = \delta F(U),$$

so U is indeed the solution operator of the ODE $U_t = \delta F(U)$. We further note the relations

$$g(U) = C - \delta t \iff C = g(U) + \delta t,$$
$$U_C(t,C) = G'(C - \delta t) = \frac{1}{g'(G(C - \delta t))} = -F(U).$$

We can now write the different discretizations of (2.2) in terms of the functions F and g. In this paper, the following variation-of-constants variants will be considered: Forward Euler (VCFE), Backward Euler (VCBE), Trapezoidal Rule (VCTR) and

Midpoint Rule (VCMR). Denoting again the step size by $h := t_{n+1} - t_n$, we get

$$\text{(2.6)} \qquad \text{VCFE}: \qquad g(u_{n+1}) - g(u_n) + \delta h = -\frac{h\Delta u_n^m}{F(u_n)},$$

$$\text{(2.7)} \qquad \text{VCBE}: \qquad g(u_{n+1}) - g(u_n) + \delta h = -\frac{h\Delta u_{n+1}^m}{F(u_{n+1})},$$

$$\text{(2.8)} \qquad \text{VCTR}: \qquad g(u_{n+1}) - g(u_n) + \delta h = -\frac{h}{2}\left[\frac{\Delta u_n^m}{F(u_n)} + \frac{\Delta u_{n+1}^m}{F(u_{n+1})}\right],$$

$$\text{(2.9)} \qquad \text{VCMR}: \qquad g(u_{n+1}) - g(u_n) + \delta h = -\frac{h\Delta u_{n+1/2}^m}{F(u_{n+1/2})},$$

where $u_{n+1/2} = G\left(\frac{g(u_n)+g(u_{n+1})}{2}\right)$. To derive the corresponding scheme for a specific function $F(u)$, it suffices to calculate the respective function $g(u)$: for example, for $F(u) = u^m$, $m > 1$, we have $g(u) = (m-1)^{-1}u^{1-m}$, so the VCBE method becomes

$$\frac{1}{m-1}(u_{n+1}^{1-m} - u_n^{1-m}) + \delta h = -\frac{h\Delta u_{n+1}^m}{u_{n+1}^m}, \qquad n = 0, 1, 2, \ldots$$

After some algebraic manipulations, we see that this is identical to Le Roux's scheme (1.4). Unlike the ad hoc derivation by Le Roux, the Variation of Constants approach is not limited to quasilinear parabolic equations: in Section 6, we will derive B-methods for the wave equation and for a parabolic PDE system, and show numerical results for them.

2.2. Truncation Error Analysis. Let us see on a concrete example how the non-standard VCFE method performs on the differential equation (2.1):

$$u_t = u^2 + \epsilon\ell(u).$$

Using the same notation as in the above, we have $F(u) = u^2$, $g(u) = 1/u$, so the corresponding scheme reads

$$\frac{1}{u_{n+1}} - \frac{1}{u_n} + h = -\frac{h\epsilon\ell(u_n)}{u_n^2}.$$

In Figure 1, we compare this method with the standard Forward Euler method for the simple case of an ODE with $\epsilon = 0.1$ and $\ell(u) = \sin(u)$. To generate the graphs, we use the initial condition $u(0) = 3$ and integrate up to $T = 0.328$. The "exact" solution is computed using an adaptive ODE solver with the Dormand–Prince pair. The left panel shows the solution profile for a time-step size of $h = 0.0328$, whereas the right panel shows the error as a function of h. We see from Figure 1 that this non-standard method performs much better than the simple Forward Euler method.

To understand why VCFE generates a smaller error, we consider what happens when the reaction term dominates or, equivalently, when ϵ is small. We expand both methods in a Taylor series for h fixed and ϵ small:

$$\text{VCFE:} \qquad u_{n+1} = \frac{1}{\frac{1}{u_n} - h - h(\frac{1}{u_n})^2\epsilon\ell(u_n)} = \frac{u_n}{1-hu_n} + \frac{\ell(u_n)h\epsilon}{(1-hu_n)^2} + O(\epsilon^2)$$

$$\text{FE:} \qquad u_{n+1} = u_n + h(u_n^2 + \epsilon\ell(u_n)) = u_n(1+hu_n) + \ell(u_n)h\epsilon$$

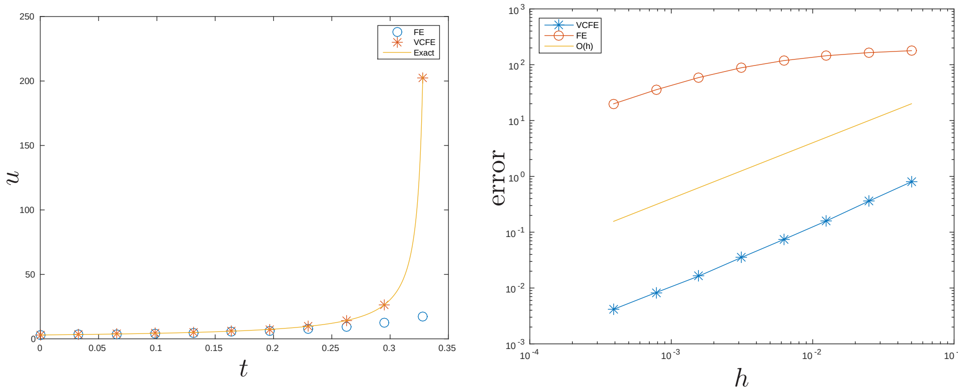

FIG. 1. *Comparison of the non-standard VCFE method to Forward Euler on the simple model problem* (2.1). *Left: solution profile close to the blow-up point. Right: error of the methods as the time step is refined.*

The local truncation error of the two methods for ϵ fixed and h small then becomes

$$\tau^{VCFE} = \left(\left(u_n^2\ell'(u_n) - 2u_n\ell(u_n)\right)\epsilon + \left(\ell'(u_n)\ell(u_n) - \tfrac{2\ell^2(u_n)}{u_n}\right)\epsilon^2\right)\tfrac{h^2}{2} + O(h^3),$$

$$\tau^{FE} = h^2u_n^3 + \left(\left(u_n^2\ell'(u_n) + 2u_n\ell(u_n)\right)\epsilon + \ell'(u_n)\ell(u_n)\epsilon^2\right)\tfrac{h^2}{2} + O(h^3).$$

Thus, the first error term is small in ϵ for VCFE, but not for standard FE because of the term $h^2u_n^3$. In other words, as the spatial part becomes $O(\epsilon)$ relative to the solution near blow-up time, VCFE has $O(\epsilon)$ truncation error for a fixed h, whereas standard FE has $O(1)$ error. This explains why VCFE gives much more accurate solutions than for the classical FE method. A similar analysis can be used to analyze the accuracy of the other VC variants.

3. Analysis of the VCBE Method for Semilinear Parabolic Problems. As B-methods are numerous and different for every model, it is not possible to study them as a whole. Thus we choose to concentrate on one selected scheme, the VCBE method, for the semilinear parabolic problem

$$\begin{cases} u_t = \Delta u + \delta F(u), & \Omega \times (0,T), \\ u = 0, & \partial\Omega \times (0,T), \\ u(x,0) = u_0(x), & \Omega, \end{cases}$$

where Ω is a bounded domain in $\mathbb{R}^d$, u_0 is a positive continuous function on $\bar{\Omega}$ and δ is a positive constant. To simplify the analysis below, we continue to use the notation $g(s) = \int_s^\infty \frac{1}{F(\sigma)}d\sigma$ and $G = g^{-1}$. Using these definitions, we can rewrite the general VCBE method as

$$g(u_{n+1}) - g(u_n) + h\delta = \frac{-h}{F(u_{n+1})}\Delta u_{n+1}. \tag{3.1}$$

To ensure that these functions are well defined, we make the following assumption on $F(s)$:

ASSUMPTION 1. *The function F is assumed to be positive, strictly increasing and strictly convex on $(0,\infty)$, belonging to $C^2([0,\infty))$ and satisfying*

$$\int_b^\infty \frac{ds}{F(s)} < \infty \qquad \textit{for every } b > 0. \tag{3.2}$$

Typical examples satisfying Assumption 1 are:
(i) $F(u) = e^u$,
(ii) $F(u) = e^u - 1$,
(iii) $F(u) = (u + \alpha)^{p+1}$, with $\alpha \geq 0$ and $p > 0$,
(iv) $F(u) = (1 + u)[\ln(1 + u)]^{p+1}$ with $p > 0$.

Under this assumption, we see that the function $g(s) = \int_s^\infty \frac{1}{F(\sigma)} d\sigma$ is continuous and strictly decreasing on $(0, \infty)$. The function $G = g^{-1}$ is continuous and strictly decreasing on $(0, M)$, where

$$M := \lim_{s\to 0} g(s) \leq \infty. \tag{3.3}$$

Note also that g and G are positive with $\lim_{s\to\infty} g(s) = 0$ and $\lim_{s\to 0} G(s) = \infty$.

In order to study (3.1), we introduce $Au := -\Delta u$ and rewrite (3.1) as $Au_{n+1} = f(x, u_{n+1})$ with

$$f(x, u) = \frac{1}{h} F(u) \left(g(u) - g(u_n(x)) + \delta h\right). \tag{3.4}$$

For our purposes, we need f to be defined and continuous at $u = 0$. This is clearly the case if $F(0) > 0$ since $g(s) = \int_s^\infty \frac{1}{F(\sigma)} d\sigma$, however if $F(0) = 0$, then it is possible to have $\lim_{b\to 0^+} g(b) = \infty$, so we need to make sure that $F(u)g(u)$ remains finite as $u \to 0^+$.

Lemma 3.1. *Let $F(s)$ satisfy Assumption 1 with $F(0) = 0$. Then $\lim_{u\to 0^+} f(x, u) = 0$, so that f can be continuously extended by setting $f(x, 0) = 0$ for all x in Ω.*

Proof. By definition, for each $c > 0$, we have $g(c) = \int_c^\infty \frac{ds}{F(s)}$, so that

$$F(c)g(c) = \int_c^\infty \frac{F(c)}{F(s)} ds = \int_c^a \frac{F(c)}{F(s)} ds + \int_a^\infty \frac{F(c)}{F(s)} ds$$

for any fixed $a \geq c$. Then, since F is increasing and $s \geq c$,

$$F(c)g(c) \leq \int_c^a 1\, ds + \int_a^\infty \frac{F(c)}{F(s)} ds = (a - c) + F(c) \int_a^\infty \frac{ds}{F(s)}.$$

The last integral is finite by condition (3.2), we call it I_a. Then we let c tend to zero. We get

$$\lim_{c\to 0^+} F(c)g(c) \leq a + F(0)I_a = a,$$

since $F(0) = 0$. So for any fixed $a > 0$, we get $\lim_{c\to 0^+} F(c)g(c) \leq a$, hence

$$\lim_{c\to 0^+} F(c)g(c) = 0,$$

and $\lim_{u\to 0^+} f(x, u) = 0$ for all $x \in \Omega$. □

By abuse of notation, we shall refer to f as its continuous extension on $[0, \infty)$.

3.1. Existence of a Solution. In this subsection, we give the conditions under which (3.1), or equivalently, $Au_{n+1} = f(x, u_{n+1})$ with f defined by (3.4), has at least one solution u_{n+1}. Amann proved in [2] that in case $f(x, 0) \geq 0$, a necessary and sufficient condition for the existence of a non-negative solution is the existence of a non-negative supersolution.

THEOREM 3.2 (Amann). *Let $f \in C^\alpha(\bar\Omega \times \mathbb{R}_+)$ be given, with $\alpha \in (0,1)$, and assume that $f(x,0) \geq 0$. Then a necessary and sufficient condition for the existence of a non-negative solution $u \in C^{2+\alpha}(\Omega)$ of the BVP*

$$\begin{aligned} Au := -\Delta u = f(x,u), &\qquad \text{in } \Omega, \\ u = 0, &\qquad \text{on } \partial\Omega, \end{aligned} \tag{3.5}$$

is the existence of a non-negative function $v \in C^{2+\alpha}(\bar\Omega)$ satisfying

$$\begin{aligned} Av \geq f(x,v), &\qquad \text{in } \Omega, \\ v \geq 0, &\qquad \text{on } \partial\Omega. \end{aligned}$$

Moreover, if this condition is satisfied, there exist a maximal non-negative solution $\hat u \leq v$ and a minimal non-negative solution $\bar u \leq v$ in the sense that, for every non-negative solution $u \leq v$ of (3.5), the inequality

$$\bar u \leq u \leq \hat u$$

holds. We use this result to prove the existence of a non-negative solution of the scheme.

THEOREM 3.3. *If the function u_n is positive in Ω, continuous in $\bar\Omega$, and satisfies*

$$\|u_n\|_\infty < G(\delta h), \tag{3.6}$$

then scheme (3.1) has a maximal nonnegative solution $\hat u \leq B_n$ with

$$B_n = G(g(\|u_n\|_\infty) - \delta h),$$

and a minimal solution $\bar u \geq 0$ and if u is a solution, then $u \in C^2(\bar\Omega)$ and satisfies $\bar u \leq u \leq \hat u$. Note that by the definition of G we have $\lim_{h\to 0} G(\delta h) = \infty$ (see Assumption 1), so that by choosing h small enough, the bound on the right-hand side of (3.6) can be made as large as desired. All the results in the rest of the paper require this condition to be satisfied, hence even when the solution can be computed further, the numerical result can become incorrect once this bound is exceeded.

Proof. As shown in Lemma 3.1, if $F(0) = 0$, we have $f(x,0) = 0$ for all $x \in \Omega$. If $F(0) > 0$, since g is decreasing, we have $g(0) - g(u_n) + \delta h > g(0) - g(u_n) \geq 0$, so we get $f(x,0) > 0$. Thus, to apply Theorem 3.2, we need to show that the constant B_n is a supersolution, that is

$$\frac{1}{h} F(B_n)\,(g(B_n) - g(u_n) + \delta h) \leq 0 \; (= AB_n),$$

and since $F(B_n) > 0$ and G is decreasing, this is equivalent to requiring that

$$B_n \geq G(g(u_n) - \delta h).$$

Hence, the constant

$$B_n = G(g(\|u_n\|_\infty) - \delta h),$$

which is well-defined if condition (3.6) is satisfied and positive by definition of G, is a supersolution. ∎

If $F(0) = 0$, the identically zero function is a solution of scheme (3.1). In this case we need to use a stronger result, proved in [9] by Brezis and Oswald, to prove the existence of a non-identically zero solution.

We consider a problem of the form

$$\begin{cases} -\Delta u &= f(x,u), & \text{in } \Omega, \\ u \geq 0, & u \not\equiv 0 & \text{in } \Omega, \\ u &= 0, & \text{on } \partial\Omega, \end{cases} \tag{3.7}$$

where $\Omega \subset \mathbb{R}^d$ is a bounded domain with smooth boundary and $f(x,u) : \Omega \times [0,\infty) \to \mathbb{R}$. Set

$$a_0(x) = \lim_{u\to 0} \frac{f(x,u)}{u},$$

and

$$a_\infty(x) = \lim_{u\to\infty} \frac{f(x,u)}{u}.$$

For $a(x) = a_0(x), a_\infty(x)$, we denote by $\lambda_1(-\Delta - a(x))$ the smallest eigenvalue of $-\Delta - a(x)$ with zero Dirichlet boundary condition. Brezis and Oswald proved the following result.

THEOREM 3.4 (Brezis and Oswald). *We suppose that the function f satisfies the following conditions:*

1. *for almost every $x \in \Omega$, the function $u \mapsto f(x,u)$ is continuous on $[0,\infty)$;*
2. *for each $u \geq 0$, the function $x \mapsto f(x,u)$ belongs to $L^\infty(\Omega)$;*
3. *there exists $K_1 > 0$ such that $f(x,u) \leq K_1(u+1)$ for almost every $x \in \Omega$, and for all $u \geq 0$;*
4. *for each $\mu > 0$, there exists $K_\mu \geq 0$ such that $f(x,u) \geq -K_\mu u$ for all $u \in [0,\mu]$, and almost every $x \in \Omega$;*
5. *we have $\lambda_1(-\Delta - a_0(x)) < 0$ and $\lambda_1(-\Delta - a_\infty(x)) > 0$. Note that in the special case where $a_0(x)$ and $a_\infty(x)$ are independent of x, this is equivalent to*

$$a_\infty < \lambda_1(-\Delta) < a_0.$$

Then problem (3.7) has a solution $u \in H_0^1(\Omega) \cap L^\infty(\Omega)$.

We will use the above theorem to show the existence of a non-identically zero positive solution to (3.7), but first we need the following lemma.

LEMMA 3.5. *Let $F(u)$ be a function satisfying Assumption 1 with $F(0) = 0$. Then*

$$\lim_{u\to\infty} \frac{F(u)}{u} = \infty, \qquad \lim_{u\to 0^+} g(u) = \infty.$$

Proof. Let $Q(u) = F(u)/u$. Then for $u > 0$,

$$Q'(u) = \frac{1}{u}\left(F'(u) - \frac{F(u)}{u}\right) > 0,$$

since F is strictly convex. So Q is an increasing function of u; to show that $\lim_{u\to\infty} Q(u) = \infty$, it suffices to show that Q is unbounded for large u. Indeed, assume on the contrary that $Q(u) \leq K_1 < \infty$ for some constant K_1. Then for any $b > 0$,

$$\int_b^\infty \frac{du}{F(u)} = \int_b^\infty \frac{du}{uQ(u)} \geq \frac{1}{K_1}\int_b^\infty \frac{du}{u} = \infty,$$

which violates condition (3.2). So Q is unbounded.

To prove the second limit, we first note that

$$\lim_{u\to 0^+} Q(u) = \lim_{u\to 0^+} \frac{F(u)-F(0)}{u} = F'(0) < \infty,$$

so there exists a constant $K_2 > 0$ such that $1/Q(u) > K_2$ for u small enough, e.g., whenever $u \in [0,\epsilon]$ for some fixed $\epsilon > 0$. Then for u in that range, we have

$$g(u) = \int_u^\infty \frac{ds}{sQ(s)} \geq K_2 \int_u^\epsilon \frac{ds}{s} = K \ln(\epsilon/u) \to \infty$$

as $u \to 0^+$. □

We are now ready to prove the existence theorem for the case of $F(0) = 0$.

THEOREM 3.6. *If the function u_n is positive in Ω, continuous in $\bar{\Omega}$, and satisfies condition (3.6), the following hold:*

1. *If $F(0) = 0$ and $F'(0) > 0$, scheme (3.1) has a non-identically zero nonnegative solution.*
2. *If $F(0) = 0$, $F'(0) = 0$ and*

$$L := \lim_{u\to 0} \frac{-F(u)}{F(u) - uF'(u)},$$

is positive, then scheme (3.1) has a non-identically zero nonnegative solution if

$$h < \frac{1}{\lambda_1(-\Delta)} L.$$

Proof. We already proved in Lemma 3.1 that the function $u \mapsto f(x,u)$ is continuous on $[0,\infty)$, so condition (1) of Theorem 3.4 holds. Moreover, since Ω is bounded, condition (2) is satisfied for all $u \geq 0$.

We now check that condition (3) and (4) of Theorem 3.4 hold. We first introduce the notation

$$c(x) = g(u_n) - \delta h.$$

To check that (3) holds, it suffices to show that $f(x,u)$ is bounded above by a constant independent of x as $u \to \infty$, since $u \mapsto f(x,u)$ is continuous on $[0,\infty)$. Because u_n satisfies condition (3.6), we have $g(\|u_n\|_\infty) > \delta h$, so there exists $\varepsilon > 0$ such that $g(\|u_n\|_\infty) > \delta h + \varepsilon$, i.e., we have

$$c(x) > \varepsilon > 0,$$

for all $x \in \Omega$. Hence

$$f(x,u) \leq \frac{F(u)}{h}(g(u) - \varepsilon),$$

and since $\lim_{u\to\infty} g(u) = 0$ and $\lim_{u\to\infty} F(u) = \infty$ (see Assumption 1), we have

$$\lim_{u\to\infty} \frac{F(u)}{h}(g(u) - \varepsilon) = -\infty.$$

Thus, condition (3) of Theorem 3.4 is satisfied with

$$K_1 = \max_{u \geq 0} \frac{F(u)}{h}(g(u) - \varepsilon).$$

We now verify condition (4). Since $F(0) = 0$ by hypothesis, we have $f(x, 0) = 0$ and the condition is satisfied for $u = 0$. For $u > 0$, the condition requires that there exist K_μ such that for all $u \in (0, \mu]$ and all $x \in \Omega$,

$$f(x, u) \geq -K_\mu u \iff g(u) \geq c(x) - \frac{hK_\mu u}{F(u)}.$$

Since g is positive, it suffices to show that the right-hand side is negative, that is,

$$K_\mu > \frac{F(u)}{u}\frac{c(x)}{h}.$$

Since u_n satisfies condition (3.6) and $\|u_n\|_\infty > 0$, we have $0 < c(x) < g(\|u_n\|_\infty) < \infty$. We also have

$$\lim_{u\to 0} \frac{F(u)}{u} = \lim_{u\to 0} \frac{F(u) - F(0)}{u} = F'(0) < \infty,$$

where the limit exists because $F \in C^2([0, \infty])$. Thus, the constant K_μ exists for all μ, and condition (4) of Theorem 3.4 is satisfied.

Finally, we verify condition (5). Because of condition (3.2) and the strict convexity of $F(u)$, Lemma 3.5 shows that

$$\lim_{u\to\infty} \frac{F(u)}{u} = \infty.$$

Together with $\lim_{u\to\infty} g(u) = 0$, we obtain

$$a_\infty(x) = \lim_{u\to\infty} \frac{F(u)}{hu}(g(u) - c(x)) = -\infty,$$

for all x. Finally if $\lim_{u\to 0} \frac{F(u)}{u} = F'(0) > 0$,

$$a_0(x) = \lim_{u\to 0} \frac{F(u)}{hu}(g(u) - c(x)) = \infty,$$

for all x, since $\lim_{u\to 0^+} g(u) = \infty$ by Lemma 3.5. On the other hand, if $F'(0) = 0$, then we use l'Hôpital's Rule to compute

$$\begin{aligned} a_0(x) &= \lim_{u\to 0} \frac{F(u)}{hu}(g(u) - c(x)) = \lim_{u\to 0} \frac{F(u)}{hu} g(u) = \frac{1}{h} \lim_{u\to 0} \frac{g(u)}{\frac{u}{F(u)}} \\ &= \frac{1}{h} \lim_{u\to 0} \frac{g'(u)}{\frac{F(u) - uF'(u)}{F^2(u)}} = \frac{1}{h} \lim_{u\to 0} \frac{-F(u)}{F(u) - uF'(u)}, \end{aligned}$$

where we used that $g' = -1/F$. So a_0 and a_∞ are both independent of x, and condition (5) of Theorem 3.4 becomes

$$-\infty < \lambda_1(-\Delta) < a_0,$$

where $a_0 = \infty$ if $F'(0) > 0$, and $a_0 = \frac{1}{h}L$ if $F(0) = 0$. ∎

Using the theorems above, we prove that the VCBE scheme (3.1) is well-defined for the functions of interest we mentioned at the beginning of this section, as long as condition (3.6) holds.

Corollary 3.7. *Let u_n satisfy condition* (3.6). *Then the equation (3.1) has a non-identically zero nonnegative solution for:*

(i) $F(u) = e^u$,
(ii) $F(u) = e^u - 1$,
(iii) $F(u) = u^{p+1}$, *if* $p > 0$ *and* $h < \frac{1}{p\lambda_1(-\Delta)}$,
(iv) $F(u) = (u+1)[\ln(u+1)]^{p+1}$, *if* $p > 0$ *and* $h < \frac{1}{p\lambda_1(-\Delta)}$.

Proof. (i) For $F(u) = e^u$, Theorem 3.3 ensures that a minimal non-negative solution $\bar{u}$ exists. We just need to show that $\bar{u} \not\equiv 0$ by checking that $u \equiv 0$ is not a solution to $Au = f(x,u)$. Indeed, we have $g(u) = e^{-u}$, so that

$$f(x,0) = \frac{1}{h}F(0)(g(0) - g(u_n(x)) + \delta h) = \frac{1 - e^{-u_n}}{h} + \delta > 0$$

whenever $\delta > 0$. Thus, $u = 0$ is not a solution to $Au = f(x,u)$, hence $\bar{u} \not\equiv 0$.

(ii) For $F(u) = e^u - 1$, we have $F(0) = 0$, $F'(0) = 1$, and $M = \lim_{u\to 0^+} g(u) = \infty$. So part (a) of Theorem 3.6 applies, and a non-identically zero, non-negative solution exists.

(iii) For $F(u) = u^{p+1}$, we have $F'(u) = (p+1)u^p$ and $F'(0) = 0$, so to obtain the existence of a non-identically zero solution, we need

$$h\lambda_1(-\Delta) < \lim_{u\to 0} \frac{-F(u)}{F(u) - uF'(u)} = \lim_{u\to 0} \frac{-u^{p+1}}{u^{p+1} - (p+1)u^{p+1}} = \frac{1}{p}.$$

(iv) Similarly, for $F(u) = (u+1)[\ln(u+1)]^{p+1}$, we have $F'(u) = [\ln(u+1)]^p[(p+1) + \ln(u+1)]$ and $F'(0) = 0$, so to obtain the existence of a non-identically zero solution, we need

$$\begin{aligned} h\lambda_1(-\Delta) &< \lim_{u\to 0} \frac{-F(u)}{F(u) - uF'(u)} \\ &= \lim_{u\to 0} \frac{-(u+1)[\ln(u+1)]^{p+1}}{(u+1)[\ln(u+1)]^{p+1} - u[\ln(u+1)]^p[(p+1) + \ln(u+1)]} \\ &= \lim_{u\to 0} \frac{-(u+1)\ln(u+1)}{\ln(u+1) - (p+1)u} = \frac{1}{p}. \end{aligned}$$

∎

3.2. Uniqueness of the Solution. A second result of Amann [2] could be used to prove the uniqueness of positive solutions when the function f is decreasing in u. However as the function f defined in (3.4) is not generally decreasing in u, we need to use a more general result by Brezis and Oswald [9].

Theorem 3.8 (Brezis and Oswald). *Consider system (3.7). If the function f satisfies the following properties*

1. *for almost every $x \in \Omega$, the function $u \mapsto f(x,u)$ is continuous on* $[0,\infty)$*;*
2. *for each $u \geq 0$, the function $x \mapsto f(x,u)$ belongs to* $L^\infty(\Omega)$*;*

3. for almost every $x \in \Omega$, the function $u \mapsto \varphi(u) := \frac{f(x,u)}{u}$ is decreasing on $(0, \infty)$;

then problem (3.7) has at most one solution and this solution is positive.

We apply this result to problem (3.1).

THEOREM 3.9. *Suppose that the function u_n is positive in Ω, continuous in $\bar{\Omega}$, and satisfies condition (3.6). If the function F satisfies the following property*

$$\left(\frac{F(u)}{u}\right)' \left(\int_u^\infty \frac{1}{F(s)}\, ds - c\right) < \frac{1}{u}, \quad \forall\, u > 0,\ \forall\, c \in (0, M - \delta h), \tag{3.8}$$

then scheme (3.1) has at most one solution and this solution is positive.

Proof. We already proved that the first two conditions of Theorem 3.8 are satisfied, so it only remains to show that the function $\varphi(u) = f(x,u)/u$ is decreasing on $(0, \infty)$ for all x. From

$$\varphi(u) = \frac{1}{h}\frac{F(u)}{u}(g(u) - g(u_n) + \delta h),$$

we get

$$\varphi'(u) = \frac{1}{h}\left(\frac{F(u)}{u}\right)'(g(u) - g(u_n) + \delta h) - \frac{1}{h}\frac{1}{u}.$$

Since $g(u_n(x)) - \delta h \in (0, M - \delta h)$, φ is decreasing if (3.8) is satisfied. ∎

Condition (3.8) is satisfied by many functions F of interest; three important examples are given in the following corollary.

COROLLARY 3.10. *We suppose that the function u_n is positive in Ω, continuous in $\bar{\Omega}$, and satisfies condition (3.6). Then the scheme has a unique positive solution for the following functions F: (i) $F(u) = e^u$, (ii) $F(u) = e^u - 1$, (iii) $F(u) = (u+\alpha)^{p+1}$, with $\alpha \geq 0$ and $p > 0$.*

Proof. If $F(u) = e^u$, condition (3.8) becomes

$$\frac{e^u(u-1)}{u^2}(e^{-u} - c) < \frac{1}{u}, \qquad \forall\, u > 0,\ \forall\, c \in (0, 1 - \delta h),$$

that is,

$$-ce^u(u-1) < 1.$$

Since the function on the left-hand side is decreasing in u and is equal to c if $u = 0$, this condition is satisfied for all $c \in (0,1)$ and $u > 0$ and Theorem 3.9 applies.

Similarly, if $F(u) = (u+\alpha)^{p+1}$, with $\alpha \geq 0$ and $p > 0$, condition (3.8) can be written as

$$\frac{[(p+1)u - (u+\alpha)](u+\alpha)^p}{u^2}\left[\frac{(u+\alpha)^{-p}}{p} - c\right] < \frac{1}{u},$$

for all $u > 0$ and $c \in (0, \frac{1}{p\alpha^p} - \delta h)$ (or $c > 0$ if $\alpha = 0$), which becomes after simplifications

$$-c[pu - \alpha](u+\alpha)^p < \frac{\alpha}{p}.$$

If $\alpha = 0$, this condition is clearly satisfied for all $u > 0$, $c > 0$. If $\alpha > 0$, the function on the left-hand side is again decreasing in u and is equal to $c\alpha^{p+1}$ when $u = 0$, so that we end up with the condition $c < 1/(p\,\alpha^p)$. In both cases, Theorem 3.9 applies.

For $F(u) = e^u - 1$, we have

$$g(u) = \int_u^\infty \frac{1}{F(s)} ds = -\ln(1 - e^{-u}),$$

which implies $M = \lim_{u \to 0^+} g(u) = \infty$. Thus, we need to check that (3.8) holds for all $u > 0$ and $c > 0$. To do this, it suffices to show that

$$\left(\frac{F(u)}{u}\right)' > 0 \qquad \text{and} \qquad \left(\frac{F(u)}{u}\right)' g(u) \le \frac{1}{u} \tag{3.9}$$

for all $u > 0$. Indeed, we calculate

$$\left(\frac{F(u)}{u}\right)' = \frac{ue^u - (e^u - 1)}{u^2} = \frac{1 - (1-u)e^u}{u^2} > \frac{1 - e^{-u}e^u}{u^2} = 0,$$

where we used the fact that $1 - u < e^{-u}$ for all $u > 0$. To prove the second inequality in (3.9), we first note that $\ln(y) \le y - 1$ for all $y > 0$. So letting $y = 1/(1 - e^{-u})$ with $u > 0$ yields

$$g(u) = -\ln(1 - e^{-u}) = \ln\left(\frac{1}{1 - e^{-u}}\right) \le \frac{1}{1 - e^{-u}} - 1 = \frac{e^{-u}}{1 - e^{-u}}.$$

Thus, we have for $u > 0$

$$\begin{aligned}
\frac{1}{u} - \left(\frac{F(u)}{u}\right)' g(u) &\ge \frac{1}{u} - \frac{1 - (1-u)e^u}{u^2} \cdot \frac{e^{-u}}{1 - e^{-u}} \\
&= \frac{u(1 - e^{-u}) - e^{-u} + (1 - u)}{u^2(1 - e^{-u})} \\
&= \frac{1 - (u+1)e^{-u}}{u^2(1 - e^{-u})} \ge \frac{1 - e^u e^{-u}}{u^2(1 - e^{-u})} = 0,
\end{aligned}$$

where we used the fact that $u + 1 \le e^u$ for all u. Hence the two inequalities in (3.9) hold, and Theorem 3.9 applies. □

We remark that the function $F(u) = (u+1)(\ln(u+1))^{p+1}$ for $p > 0$ does not satisfy the condition (3.8) of Theorem 3.9.

3.3. Minimal Time of Existence of the Solution. If the function F satisfies the hypothesis of Theorem 3.9, and either $F(0) \ne 0$ or F satisfies the hypothesis of Theorem 3.6, then it remains to show that the condition (3.6) is satisfied for a positive number of steps.

THEOREM 3.11. *If the function F satisfies the hypothesis of Theorem 3.9, and either $F(0) \ne 0$ or F satisfies the hypothesis of Theorem 3.6, the scheme (3.1) has a positive solution u_n for n such that $t_n = nh < T_1$, where*

$$T_1 = \frac{1}{\delta} g(\|u_0\|_\infty) = \int_{\|u_0\|_\infty}^\infty \frac{ds}{\delta F(s)}.$$

This theorem gives a lower bound on the numerical blow-up time equal to the one given by Kaplan in [31] for the exact solution.

Proof. We want to prove that if $t_n < T_1$, that is

$$\|u_0\|_\infty < G(\delta t_n),$$

we have $\|u_{n-1}\|_\infty < G(\delta h)$ so that u_n is well-defined. To obtain this result, we prove by induction that if $\|u_0\|_\infty < G(\delta t_n)$, then u_n is well-defined and satisfies

$$\|u_n\|_\infty \leq G(g(\|u_0\|_\infty) - \delta t_n). \tag{3.10}$$

For this, we will need in particular the following result which comes from Theorem 3.3:

$$\text{if} \quad \|u_n\|_\infty < G(\delta h), \quad \text{then } \|u_{n+1}\|_\infty \leq B_n = G(g(\|u_n\|_\infty) - \delta h). \tag{3.11}$$

By choosing $n = 0$ in (3.11), we obtain the initial step of the induction, in particular (3.10) for $n = 1$. We suppose now that for some fixed n, if $\|u_0\|_\infty < G(\delta t_n)$, then u_n is well-defined and satisfies (3.10), and we also suppose that

$$\|u_0\|_\infty < G(\delta t_{n+1}). \tag{3.12}$$

Since G is decreasing, (3.12) implies $\|u_0\|_\infty < G(\delta t_n)$ and then by induction hypothesis, we get

$$\|u_n\|_\infty \leq G(g(\|u_0\|_\infty) - \delta t_n). \tag{3.13}$$

Moreover from (3.12) we also get

$$g(\|u_0\|_\infty) > \delta t_{n+1},$$

that we write as

$$g(\|u_0\|_\infty) - \delta t_n > \delta h.$$

Inserting this estimate into (3.13), and using that G is decreasing, we obtain

$$\|u_n\|_\infty < G(\delta h),$$

which implies that u_{n+1} is well-defined. Moreover using Theorem 3.3, we have

$$\|u_{n+1}\|_\infty \leq G(g(\|u_n\|_\infty) - \delta h).$$

Since from (3.13), we get that

$$g(\|u_n\|_\infty) - \delta h \geq g(\|u_0\|_\infty) - \delta t_{n+1},$$

we obtain

$$\|u_{n+1}\|_\infty \leq G(g(\|u_0\|_\infty) - \delta t_{n+1})$$

and the induction is proved. ◻

4. Rate of Growth. For specific functions F, the rate of growth of the exact solution close to the blow-up has been determined. In this subsection, we derive similar results for the solution of scheme (3.1).

Since the solution of $y_t = \delta F(y)$ is given by $y(t) = G\left(\delta(T - t)\right)$, where T is the blow-up time, we expect

$$u(t) \sim G\left(\delta(T - t)\right),$$

close to the blow-up. In [17], Friedman and McLeod proved that if $F(u) = u^p$ (and then $G(u) = [(p-1)u]^{-1/(p-1)}$) and $\delta = 1$, solutions $u(x,t)$ with suitable initial-boundary conditions satisfy

$$(T-t)^{\frac{1}{p-1}} u(x,t) \to \frac{1}{p-1}^{\frac{1}{p-1}}, \qquad \text{as } t \to T^-,$$

provided $|x| \le C(T-t)^{1/2}$, for some $C > 0$. For $F(u) = e^u$ (and $G(u) = 1/\ln u$), $\delta = 1$ and $n = 1$ or 2, Bebernes et al. [5] proved that the solutions $u(x,t)$ satisfy

$$u(x,t) - \ln \frac{1}{T-t} \to 0, \qquad \text{as } t \to T^-,$$

uniformly on $|x| \le C(T-t)^{1/2}$, $C \ge 0$.

Similarly, if $F(u) = e^u$, we expect that the numerical solution satisfies

$$u_n(x) \sim \ln \left(\frac{1}{\delta(T^* - t_n)} \right),$$

for some T^* and for values of x close to the blow-up point, and then

$$u_{n+1}(x) - u_n(x) \sim \ln \left(\frac{1}{\delta(T^* - t_{n+1})} \right) - \ln \left(\frac{1}{\delta(T^* - t_n)} \right) = \ln \left(\frac{T^* - t_n}{T^* - t_{n+1}} \right).$$

This motivates the following theorem.

THEOREM 4.1. *Let C_0 be a constant such that*

$$C_0 \ge \delta e^{\|u_0\|_\infty} \quad \textit{and} \quad Au_0 - \delta e^{u_0} + C_0 \ge 0. \tag{4.1}$$

Note that if $Au_0 \ge 0$, we can take $C_0 = \delta e^{\|u_0\|_\infty}$.

If $t_{n+1} < T_2 := \frac{1}{C_0}$, the function u_{n+1} given by

$$Au_{n+1} - \delta e^{u_{n+1}} + \frac{1}{h}(e^{u_{n+1} - u_n} - 1) = 0, \tag{4.2}$$

satisfies for all x

$$u_{n+1}(x) \le u_n(x) + \ln \left(\frac{T_2 - t_n}{T_2 - t_{n+1}} \right).$$

Proof. First, let's prove that if $t_1 = h < T_2$, then

$$u_1 \le u_0 + \ln \left(\frac{T_2}{T_2 - h} \right). \tag{4.3}$$

The function $u_0 + \ln \left(\frac{T_2}{T_2 - h} \right)$ is a supersolution of (4.2) for $n = 0$ if

$$Au_0 \ge \delta e^{u_0} \left(\frac{T_2}{T_2 - h} \right) - \frac{1}{h} \left(\frac{T_2}{T_2 - h} - 1 \right) = \frac{1}{T_2 - h} (\delta e^{u_0} T_2 - 1).$$

Since $\frac{1}{T_2} = C_0 \ge \delta e^{\|u_0\|}$, the right-hand side is decreasing in h so in order to get a bound valid for all $h \in (0, T_2)$, we need

$$Au_0 \ge \lim_{h \to 0} \frac{1}{T_2 - h} (\delta e^{u_0} T_2 - 1) = \delta e^{u_0} - \frac{1}{T_2},$$

which is exactly condition (4.1), hence we get (4.3).

We now assume that

$$u_n \le u_{n-1} + \ln\left(\frac{T_2 - t_{n-1}}{T_2 - t_n}\right).$$

Since $\frac{1}{T_2} = C_0 \ge \delta e^{\|u_0\|}$, we have $T_2 \le \frac{1}{\delta e^{\|u_0\|}}$ and $u_0 \le \|u_0\| \le \ln(\frac{1}{\delta T_2})$, and by induction

$$\begin{aligned} u_n &\le u_{n-1} + \ln\left(\frac{T_2 - t_{n-1}}{T_2 - t_n}\right) \\ &\le \ln\left(\frac{1}{\delta(T_2 - t_{n-1})}\right) + \ln\left(\frac{T_2 - t_{n-1}}{T_2 - t_n}\right) = \ln\left(\frac{1}{\delta(T_2 - t_n)}\right). \end{aligned} \tag{4.4}$$

The function $u_n + \ln\left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right)$ is a supersolution of the scheme (4.2) if

$$Au_n - \delta e^{u_n}\left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right) + \frac{1}{h}\left(\frac{T_2 - t_n}{T_2 - t_{n+1}} - 1\right) \ge 0. \tag{4.5}$$

Since u_n is solution of

$$Au_n = \delta e^{u_n} - \frac{1}{h}(e^{u_n - u_{n-1}} - 1),$$

and the induction hypothesis gives

$$e^{u_n - u_{n-1}} \le \frac{T_2 - t_{n-1}}{T_2 - t_n},$$

condition (4.5) is satisfied if

$$\delta e^{u_n}\left(1 - \frac{T_2 - t_n}{T_2 - t_{n+1}}\right) - \frac{1}{h}\left(\frac{T_2 - t_{n-1}}{T_2 - t_n} - 1\right) + \frac{1}{T_2 - t_{n+1}} \ge 0,$$

which simplifies to

$$\delta e^{u_n} \le \frac{1}{T_2 - t_n},$$

which is exactly (4.4). ∎

If $F(u) = (u + \alpha)^{p+1}$, we expect the numerical solution to satisfy

$$u_n \sim \left(\frac{1}{\delta(T^* - t_n)}\right)^{1/p},$$

for some T^*, so that

$$\frac{u_{n+1}}{u_n} \sim \left(\frac{\delta(T^* - t_n)}{\delta(T^* - t_{n+1})}\right)^{1/p} = \left(\frac{T^* - t_n}{T^* - t_{n+1}}\right)^{1/p}.$$

THEOREM 4.2. *Suppose there exists a constant C_0 that satisfies*

$$C_0 \ge \delta p(\|u_0\|_\infty + \alpha)^p, \quad \textit{and} \quad Au_0 - \delta(u_0 + \alpha)^{p+1} + \frac{C_0}{p}(u_0 + \alpha) \ge 0. \tag{4.6}$$

Note that if $Au_0 \geq 0$, we can take $C_0 = \delta p(\|u_0\|_\infty + \alpha)^p$.

If $t_{n+1} < T_2 := \frac{1}{C_0}$, the function u_{n+1} given by

$$hAu_{n+1} = (u_{n+1} + \alpha)^{p+1} \left[\frac{1}{p(u_{n+1} + \alpha)^p} - \frac{1}{p(u_n + \alpha)^p} + \delta h \right], \tag{4.7}$$

satisfies for all x

$$u_{n+1}(x) + \alpha \leq \left(\frac{T_2 - t_n}{T_2 - t_{n+1}} \right)^{1/p} (u_n(x) + \alpha). \tag{4.8}$$

Proof. First, we need to show that

$$v_1 := (u_0 + \alpha) \left(\frac{T_2}{T_2 - h} \right)^{1/p} - \alpha$$

is a supersolution, so that u_1 satisfies (4.8) for $n = 0$. The condition for having a supersolution means

$$hAv_1 \geq (v_1 + \alpha) \left[\frac{1}{p} \left[1 - \left(\frac{v_1 + \alpha}{u_0 + \alpha} \right)^p \right] + \delta h (v_1 + \alpha)^p \right]. \tag{4.9}$$

Since the Laplacian is such that $\Delta\chi = 0$ whenever χ is constant with respect to x, the left-hand side of (4.9) can be rewritten as

$$hAv_1 = -h\Delta v_1 = -h\Delta(v_1 + \alpha) = \left(\frac{T_2}{T_2 - h} \right)^{1/p} hAu_0.$$

The right-hand side of (4.9) can be written as

$$\begin{aligned} &\left(\frac{T_2}{T_2 - h} \right)^{1/p} (u_0 + \alpha) \left[\frac{1}{p} \left[1 - \frac{T_2}{T_2 - h} \right] + \delta h (u_0 + \alpha)^p \left(\frac{T_2}{T_2 - h} \right) \right] \\ = &\left(\frac{T_2}{T_2 - h} \right)^{\frac{p+1}{p}} (u_0 + \alpha) \left[-\frac{h}{pT_2} + \delta h (u_0 + \alpha)^p \right]. \end{aligned}$$

Thus, v_1 is a supersolution if

$$Au_0 \geq \left(\frac{T_2}{T_2 - h} \right) (u_0 + \alpha) \left[-\frac{C_0}{p} + \delta (u_0 + \alpha)^p \right].$$

Since we assumed that $C_0 \geq \delta p(u_0 + \alpha)^p$, the term inside the square brackets is negative, so the right-hand side is a decreasing function of h. Thus, v_1 is a supersolution for all $0 < h < T_2$ if

$$Au_0 + (u_0 + \alpha) \left[\frac{C_0}{p} - \delta (u_0 + \alpha)^p \right] \geq 0,$$

i.e., if the second condition in (4.6) holds. We now assume the induction hypothesis

$$u_n + \alpha \leq (u_{n-1} + \alpha) \left(\frac{T_2 - t_{n-1}}{T_2 - t_n} \right)^{1/p},$$

and we prove that

$$v_{n+1} := (u_n + \alpha)\left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right)^{1/p} - \alpha$$

is a supersolution of (4.7), so that $u_{n+1} \le v_{n+1}$. We see that

$$\begin{aligned} Av_{n+1} &= -\Delta(v_{n+1} + \alpha) = -\left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right)^{1/p} \Delta u_n \\ &= \left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right)^{1/p} \left[\frac{1}{ph}(u_n + \alpha)\left(1 - \left(\frac{u_n + \alpha}{u_{n-1} + \alpha}\right)^p\right) + \delta(u_n + \alpha)^{p+1}\right]. \end{aligned}$$

Now by the induction hypothesis, we have

$$\left(\frac{u_n + \alpha}{u_{n-1} + \alpha}\right)^p \le \frac{T_2 - t_{n-1}}{T_2 - t_n},$$

so that

$$\begin{aligned} Av_{n+1} &\ge \left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right)^{1/p} \left[\frac{1}{ph}(u_n + \alpha)\left(1 - \frac{T_2 - t_{n-1}}{T_2 - t_n}\right) + \delta(u_n + \alpha)^{p+1}\right] \\ &= \left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right)^{1/p} (u_n + \alpha)\left[-\frac{1}{p(T_2 - t_n)} + \delta(u_n + \alpha)^p\right]. \end{aligned}$$

Note that the term between the square brackets is negative, since by induction we have

$$(u_0 + \alpha)^p \le \frac{1}{\delta p T_2} \implies (u_n + \alpha)^p \le \frac{1}{\delta p (T_2 - t_n)}.$$

On the other hand, if we replace u_{n+1} in the right-hand side of (4.7) with v_{n+1}, then we get

$$\begin{aligned} &\frac{1}{ph}(v_{n+1} + \alpha)\left[1 - \left(\frac{v_{n+1} + \alpha}{u_n + \alpha}\right)^p\right] + \delta(v_{n+1} + \alpha)^{p+1} \\ &= \frac{1}{ph}(u_n + \alpha)\left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right)^{1/p}\left[1 - \left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right)\right] + \delta\left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right)^{\frac{p+1}{p}} (u_n + \alpha)^{p+1} \\ &= \left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right)^{1/p}\left[-\frac{u_n + \alpha}{p(T_2 - t_{n+1})} + \delta\left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right)(u_n + \alpha)^{p+1}\right] \\ &= \left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right)^{\frac{p+1}{p}} (u_n + \alpha)\left[-\frac{1}{p(T_2 - t_n)} + \delta(u_n + \alpha)^p\right] \\ &\overset{(*)}{\le} \left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right)^{\frac{1}{p}} (u_n + \alpha)\left[-\frac{1}{p(T_2 - t_n)} + \delta(u_n + \alpha)^p\right] \le Av_{n+1}, \end{aligned}$$

where the inequality $(*)$ is due to the fact that $(T_2 - t_n)/(T_2 - t_{n+1}) > 1$ and that the term inside the square bracket is non-positive. Thus, v_{n+1} is a supersolution, so we have

$$u_{n+1} + \alpha \le v_{n+1} + \alpha = (u_n + \alpha)\left(\frac{T_2 - t_n}{T_2 - t_{n+1}}\right)^{1/p},$$

as required. □

5. Computation of the Numerical Solution. To implement the VCBE scheme, it remains to solve the nonlinear algebraic system (3.1) for u_{n+1} when u_n is given. This is equivalent to solving $Au_{n+1} = f(x, u_{n+1})$ with $A = -\Delta$ and

$$f(x,u) = \frac{1}{h}F(u)(g(u) - g(u_n(x)) + \delta h),$$

as defined in (3.4). In section 5.1, we propose the following fixed-point iteration method to solve $Au_{n+1} = f(x, u_{n+1})$: for $k = 1, 2, \dots$, we solve

$$\left\{ \begin{array}{rcll} -\Delta v_k - \varphi(x)v_k & = & f(x, v_{k-1}) - \varphi(x)v_{k-1}, & \text{in } \Omega, \\ v_k & = & 0, & \text{on } \partial\Omega. \end{array} \right. \tag{5.1}$$

where the preconditioning function $\varphi \in C^\gamma(\bar{\Omega})$ is non-positive and satisfies (5.3). We show how to choose φ for given functions F and u_n so that the iteration (5.1) is well defined and convergent. In fact, we show that the iteration converges monotonically to the solution u_{n+1} if we start with a specific constant initial guess. A second possibility for solving $Au_{n+1} = f(x, u_{n+1})$ is to use Newton's method. We show in Section 5.2 that for our examples of interest, the method converges if we start with a constant supersolution.

5.1. Fixed-point iteration. The iteration scheme (5.1) was first presented by Courant and Hilbert in [11]; however we present the results in the form given by Keller in [33]. The proof of the following theorem follows the proofs of Theorems 4.1 and 4.2 in [33].

THEOREM 5.1 (Keller). *Consider the problem*

$$\left\{ \begin{array}{rcll} -\Delta u & = & f(x,u), & \textit{in } \Omega, \\ u & = & 0, & \textit{on } \partial\Omega. \end{array} \right. \tag{5.2}$$

Suppose there exist two constants $M \geq 0$ and $m \leq 0$ and a non-positive function $\varphi(x) \in C^\gamma(\bar{\Omega})$ such that the function f satisfies $f(x,u) \in C^\gamma(\bar{\Omega} \times [m, M])$, $f(x, m) \geq 0$ and $f(x, M) \leq 0$ on Ω, and

$$\frac{f(x,z_1) - f(x,z_2)}{z_1 - z_2} \geq \varphi(x) \quad \textit{on } \Omega, \quad \textit{for all } z_1, z_2 \in [m, M], \quad z_1 \neq z_2. \tag{5.3}$$

If $v_0(x) \in C^\gamma(\bar{\Omega})$ is a supersolution (resp. subsolution) of problem (5.2), with $m \leq v_0(x) \leq M$, then problem (5.2) has at least one solution $u(x) \in C^{2+\gamma}(\bar{\Omega})$, with $m \leq u(x) \leq M$ and given by

$$u(x) = \lim_{n\to\infty} v_n(x),$$

where the monotone non-increasing (resp. non-decreasing) sequence $\{v_n(x)\}$ is defined by (5.1).

Proof. The operator L defined by $Lu = \Delta u + \varphi(x)u$ is elliptic, with $\varphi(x) \leq 0$, and $\varphi \in C^\gamma(\bar{\Omega})$, $f \in C^\gamma(\bar{\Omega} \times [m, M])$, so from Schauder's theory (see Theorem 6.14 in [22]), problem (5.1) has a unique solution lying in $C^{2+\gamma}(\bar{\Omega})$. Hence the sequence $\{v_k\}$ is well-defined and $v_k \in C^{2+\gamma}(\bar{\Omega})$ for all $k \geq 1$.

We only prove the monotonicity of the sequence for the case where v_0 is a supersolution so that the sequence $\{v_k\}$ satisfies

$$m \leq \cdots \leq v_k(x) \leq \cdots \leq v_0(x) \leq M, \tag{5.4}$$

because the proof is similar if v_0 is a subsolution. First, we show that $v_1 \le u_0$ on $\bar{\Omega}$. We have from (5.1),

$$-\Delta(v_1 - v_0) - \varphi(x)(v_1 - v_0) = f(x, v_0) - \varphi(x)v_0 + \Delta v_0 + \varphi(x)v_0 = f(x, v_0) + \Delta v_0,$$

which is negative since v_0 is a supersolution of problem (5.2). Thus we have $L(v_1 - v_0) \ge 0$ and from the strong maximum principle (see Theorem 2.1 of [33]) we obtain $v_1 - v_0 \le 0$ on $\bar{\Omega}$.

By hypothesis, we have $m \le v_0 \le M$. We then suppose that $m \le v_k(x) \le M$ and we show that $v_{k+1} \ge m$ on $\bar{\Omega}$. Choosing $z_1 = v_k$ and $z_2 = m$ in (5.3), we obtain

$$\frac{f(x, v_k) - f(x, m)}{v_k - m} \ge \varphi(x),$$

which gives, since $v_k \ge m$,

$$f(x, v_k) - \varphi(x)v_k \ge f(x, m) - \varphi(x)m.$$

Using (5.1), it becomes

$$-\Delta v_{k+1} \ge f(x, m) + \varphi(x)(v_{k+1} - m).$$

Since $f(x, m) \ge 0$ and $\varphi(x) \le 0$ by hypothesis, we have $\Delta v_{k+1} \le 0$ on $\Omega \cap \{x \in \bar{\Omega} \mid v_{k+1}(x) \le m\}$. Using Theorem 2.2 of [33], which is a consequence of the maximum principle, we obtain $v_{k+1} \ge m$ on $\bar{\Omega}$.

Finally, we need to show that if $m \le v_k(x) \le v_{k-1}(x) \le M$ on $\bar{\Omega}$, we have $v_{k+1} \le v_k$ on $\bar{\Omega}$. We consider

$$-\Delta(v_{k+1} - v_k) - \varphi(x)(v_{k+1} - v_k) = f(x, v_k) - f(x, v_{k-1}) - \varphi(x)(v_k - v_{k-1}).$$

Since $v_k - v_{k-1} \le 0$, choosing $z_1 = v_k$ and $z_2 = v_{k-1}$ in (5.3) leads to

$$-\Delta(v_{k+1} - v_k) - \varphi(x)(v_{k+1} - v_k) \le 0,$$

and using as above Theorem 2.1 of [33], we obtain $v_{k+1} \le v_k$ on $\bar{\Omega}$.

Hence the monotonicity of the sequence $\{v_k(x)\}$ is established, together with (5.4). As the sequence is monotone and uniformly bounded, it converges to some function $\hat{u}$ defined by

$$\hat{u}(x) = \lim_{k \to \infty} v_k(x).$$

To show that $\hat{u}$ belongs to $C^{2+\gamma}(\bar{\Omega})$ and is a solution of (5.2), we will use the Compactness Theorem 12.2 in [1], however we first need to show that the convergence is uniform on $\bar{\Omega}$.

From Morrey's inequality (see Section 5.6.2 in [12]), we have

$$\max_{x,\xi \in \bar{\Omega}} \frac{|v_k(x) - v_k(\xi)|}{|x - \xi|^\alpha} \le K_0 \|v_k\|_{1,p}\,, \tag{5.5}$$

for some constant K_0 independent of v_k, and $\alpha = 1 - \frac{d}{p}$, for any $p \ge d$ (recall that $\Omega \subset \mathbb{R}^d$). Moreover, the following estimate, taken from [42],

$$\|u\|_{s,p} \le K_1(\|Au\|_{s-2,p} + \|u\|_{s-2,p}),$$

leads to, using (5.1) and letting $s = 2$,

$$\|v_k\|_{2,p} \leq K_1(\|f(x, v_{k-1}) - \varphi(x)v_{k-1}\|_{0,p} + \|v_k\|_{0,p}).$$

Since $f \in C^\gamma(\bar{\Omega} \times [m, M])$, $\varphi \in C^\gamma(\bar{\Omega})$ and $u_k(x) \leq M$ on $\bar{\Omega}$ for all k, there exists a constant K_2 such that

$$\|v_k\|_{2,p} \leq K_2, \qquad \text{for all } k \geq 0.$$

Hence inequality (5.5) becomes

$$\max_{x,\xi\in\bar{\Omega}} \frac{|v_k(x) - v_k(\xi)|}{|x - \xi|^\alpha} \leq K_0 K_2,$$

and the v_k are uniformly Hölder continuous, from which the equicontinuity and the uniform convergence of $\{v_k(x)\}$ to $\hat{u}(x)$ follow.

Thus we can apply the Compactness Theorem 12.2 of [1] with $L_i = L$ for all i and $F_i = -f(x, v_{i-1}) + \varphi(x)v_{i-1}$ which converges uniformly to $-f(x, \hat{u}) + \varphi(x)\hat{u}$. Hence a subsequence of $\{v_k\}$ converges to a solution of (5.1) that belongs to $C^{2+\gamma}(\bar{\Omega})$ and this solution must be $\hat{u}$ by monotonicity of the sequence $\{v_k\}$. ∎

It remains to choose $\varphi(x)$ such that condition (5.3) holds.

THEOREM 5.2. *Let F satisfy Assumption 1. Suppose $g(\|u_n\|_\infty) > \delta h$, i.e., the hypothesis of Theorem 3.3 holds, so that a solution to* (3.1) *exists. Let $B_n = G(g(\|u_n\|_\infty) - \delta h) > 0$ be defined as in Theorem 3.3. Then for*

$$\varphi(x) = f_u(x, B_n) = \frac{1}{h}\left[F'(B_n)(g(B_n) - g(u_n(x)) + \delta h) - 1\right],$$

we have $\varphi(x) \leq 0$, and the fixed-point iteration (5.1) *with initial iterate $v_0 = B_n$ converges to a solution u_{n+1} of* (3.1).

For our specific examples, the choice of $\varphi(x)$ is as follows:

(i) $F(u) = e^u$: we have $g(u) = e^{-u}$, so that

$$f_u(x, B_n) = -\frac{1}{h} e^{B_n}(g(u_n(x)) - \delta h).$$

(ii) $F(u) = e^u - 1$: we have $g(u) = -\ln(1 - e^{-u})$, so that

$$f_u(x, B_n) = \frac{1}{h}\left[e^{B_n}\left(\ln\frac{1 - e^{-u_n}}{1 - e^{-B_n}} + \delta h\right) - 1\right].$$

(iii) $F(u) = (u + \alpha)^{p+1}$: we have $g(u) = \frac{1}{p}(u + \alpha)^{-p}$, so that

$$f_u(x, B_n) = \frac{1}{h}\left[\frac{1}{p} - (p + 1)(B_n + \alpha)^p(g(u_n) - \delta h)\right].$$

Proof. First, since g is a decreasing function, we have

$$g(B_n) = g(\|u_n\|_\infty) - \delta h \leq g(u_n) - \delta h,$$

so that $g(B_n) - g(u_n(x)) + \delta h \leq 0$. This, together with the fact that $F'(B_n) \geq 0$ (since F is an increasing function), proves that $\varphi(x) \leq 0$. Next, we show that (5.3) holds. By the mean value theorem for derivatives, we have for $z_1, z_2 \in [0, B_n]$ that

$$\frac{f(x, z_1) - f(x, z_2)}{z_1 - z_2} = f_u(x, z^*),$$

with $0 < z^* < B_n$. Thus, it suffices to show that $\frac{\partial f}{\partial u}(x, z^*) \geq \varphi(x)$ for all $z^* \in (0, B_n)$. Indeed, letting $c(x) = g(u_n(x)) - \delta h$, we have

$$\begin{aligned} f_u(x, z^*) &= \frac{1}{h}F'(z^*)(g(z^*) - c(x)) + \frac{1}{h}F(z^*)g'(z^*) \\ &= \frac{1}{h}F'(z^*)(g(z^*) - c(x)) - \frac{1}{h} \qquad \text{(since } g'(u) = -1/F(u)\text{)} \\ &\geq \frac{1}{h}F'(z^*)(g(B_n) - c(x)) - \frac{1}{h} \qquad \text{(since } F'(z^*) \geq 0 \text{ and } g \text{ is decreasing)} \\ &\geq \frac{1}{h}F'(B_n)(g(B_n) - c(x)) - \frac{1}{h} \qquad \text{(since } F \text{ is convex and } g(B_n) - c(x) \leq 0\text{)} \\ &= f_u(x, B_n) = \varphi(x). \end{aligned}$$

Since we have already proved in Theorem 3.3 that $f(x, 0) \geq 0$ and $f(x, B_n) \leq 0$, it suffices to apply Theorem 5.1 with $m = 0$, $M = B_n$ and $v_0 = B_n$ to conclude that the iteration (5.1) converges to a solution of (3.1). ∎

5.2. Newton's method. One can also use Newton's method to implement the nonlinear schemes. We prove next the convergence of Newton's method under certain conditions on F. Using another result of Keller [33], we prove that if f satisfies the hypotheses of Theorem 5.1 and f_u is decreasing and if the first iterate w_0 is a supersolution, then Newton's method converges monotonically to the solution of the problem.

Theorem 5.3 (Keller). *Suppose that f satisfies the hypothesis of Theorem 5.1 and*

$$f_u(x, u) \in C^\gamma(\bar{\Omega} \times [m, M]),$$

and

$$f_u(x, z_1) \geq f_u(x, z_2), \quad \forall\, x \in \Omega,\ 0 \leq z_1 \leq z_2 \leq M.$$

Then the unique solution $u(x) \in [m, M]$ of problem (5.2) is given by

$$u(x) = \lim_{k \to \infty} w_k(x),$$

where $\{w_k(x)\}$, the Newton iterates, form a monotone non-increasing sequence defined by

$$\begin{aligned} Aw_{k+1} - f_u(x, w_k)w_{k+1} &= f(x, w_k) - f_u(x, w_k)w_k, && \text{in } \Omega, \\ w_{k+1} &= 0 && \text{on } \partial\Omega, \end{aligned} \tag{5.6}$$

with an initial iterate w_0 satisfying $Aw_0 \geq f(w_0)$ and $f_u(x, w_0) \leq 0$ in Ω and $w_0 \geq 0$ on $\partial\Omega$.

We proved in Corollaries 3.7 and 3.10 that two important examples of functions F satisfy the hypotheses of Theorem 3.11. We now show that they also satisfy the hypotheses of Theorem 5.3 with $m = 0$ and $M = B_n$.

Corollary 5.4. *If $F(u) = e^u$ or $F(u) = (u + \alpha)^{p+1}$, the solution of (5.2) can be obtained by Newton's iteration (5.6), with $w_0 = B_n$.*

Proof. If $F(u) = e^u$, we have $f_u(x, u) = -\frac{1}{h}(g(u_n) - \delta h)e^u \in C^\gamma(\bar{\Omega} \times [0, B_n])$. Since $g(u_n) - \delta h$ is positive, f_u is negative and decreasing in u, so Theorem 5.3 applies with $w_0 = B_n$.

Similarly, if $F(u) = (u+\alpha)^{p+1}$, we have

$$f_u(x,u) = \frac{1}{ph} - \frac{1}{h}(p+1)(g(u_n) - \delta h)(u+\alpha)^p \in C^\gamma(\bar{\Omega} \times [0, B_n]),$$

which is decreasing in u and since B_n satisfies $g(B_n) \leq g(u_n) - \delta h$, that is

$$(g(u_n) - \delta h)(B_n + \alpha)^p \geq \frac{1}{p},$$

we have $f_u(x, B_n) \leq -1/h$. Hence we can apply Theorem 5.3 with $w_0 = B_n$. □

Remark. By comparing the forms of (5.1) and (5.6), we see that the fixed point iteration is in fact a *modified* Newton iteration where the Jacobian is always evaluated at the initial iterate $v_0 = B_n$, instead of being updated after each iteration.

6. Numerical Results. In this section, we compare the error of the numerical solutions obtained by B-methods with that obtained by classical methods. We first consider methods for the scalar parabolic problem (2.5), for which B-methods have been derived in Section 2.1. We consider the semilinear ($m = 1$) case in Section 6.1 and the quasilinear ($m > 1$) case in Section 6.2. We then consider the solution of a semilinear parabolic system in Section 6.3 and that of a wave equation with a superlinear source term in Section 6.4. For these problems, we also show how to derive B-methods using the Variation of Constants principle. Unless otherwise specified, we use a fixed time-step size h for all experiments, and the reference solution is computed using `ode45`, an adaptive integrator in MATLAB that implements the Dormand–Prince pair. All errors reported correspond to the L^∞ distance between this reference solution and the respective approximate solution, taken at a final time T_f that will be specified in each case. We also report running times for each method, as observed on a desktop computer with an Intel 3.4GHz dual-core processor and 8Gb of RAM.

6.1. Semilinear Parabolic Equation. We consider the semilinear parabolic equation (2.5) for $m = 1$ and $F(u) = e^u$ on the interval $\Omega = [-1, 1]$. We set $\delta = 3$ and $u_0(x) = \cos(\pi x/2)$, which is concave on the whole interval. Using adaptive methods, we determine the blow-up time to be $T_b \approx 0.1664$. We compute the solution up to $T_f = 0.1660$ using the Forward Euler, Backward Euler, Midpoint and Trapezoidal rules, as well as their B-method counterparts. For first-order methods, we used $h =$ 0.00005, 0.000025, 0.0000125, 0.000008 and 0.000005. For second-order methods, we used $h = 0.0002$, 0.000125, 0.0001, 0.00005 and 0.000025. The error at $t = T_f$ is reported in Table 1 and plotted in Figure 2. As expected, the slopes of the lines corresponding to first-order methods are approximately one, whereas the slopes of the lines corresponding to second-order methods are close to two. We observe that the error of B-methods is approximately 10 times smaller for first-order methods, about 25 times smaller for the midpoint rule and about 50 times smaller for the trapezoidal rule. In Figure 3, we plot the solution profile up to $T_f = 0.1663$ with a time-step size of $h = 0.0001$. It is clear from the plot that the B-methods lead to much more accurate solutions than their standard counterparts, even after taking the additional computational cost into account. For this example, the VCFE solution for $h = 2.5 \times 10^{-5}$ is about 5 times more accurate than the standard FE solution at $h = 8 \times 10^{-6}$, even though the running times are similar (99 vs. 90 milliseconds). Similarly, for the same amount of computation, accuracy improved by about a factor of 10 for the VCBE/BE pair, 6 for VCMR/MR and 10 for the VCTR/TR pair.

TABLE 1
Error at $T_f = 0.1660$ for first and second order methods applied to the semilinear equation with $F(u) = e^u$. The numbers inside brackets indicate running times in milliseconds.

Timestep	5e-005	2.5e-005	1.25e-005	8e-006	5e-006
FE	0.277 (34)	0.152 (32)	0.08 (59)	0.0522 (90)	0.0331 (143)
BE	0.468 (270)	0.194 (500)	0.0904 (905)	0.0565 (1347)	0.0347 (2055)
VCFE	0.019 (57)	0.00956 (99)	0.0048 (198)	0.00307 (308)	0.00192 (488)
VCBE	0.0195 (342)	0.0097 (633)	0.00483 (1225)	0.00309 (1897)	0.00193 (3018)
Timestep	0.0002	0.000125	0.0001	5e-005	2.5e-005
MR	0.00833 (75)	0.00324 (108)	0.00207 (133)	0.000516(265)	0.000129 (471)
TR	0.0407 (138)	0.0152 (208)	0.00961 (257)	0.00237 (506)	0.000591 (926)
VCMR	0.00033 (154)	0.00013 (232)	8.36e-005(287)	2.1e-005 (572)	5.25e-006(1005)
VCTR	0.000733(233)	0.000287(363)	0.000184 (451)	4.6e-005 (902)	1.15e-005(1797)

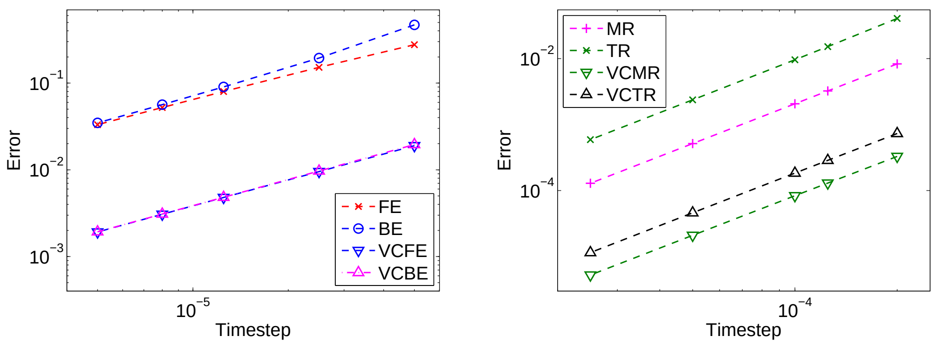

FIG. 2. *Error at $T_f = 0.1660$ for B-methods applied to the semilinear equation with $F(u) = e^u$, with different values of h. Left: first-order methods, right: second-order methods.*

6.2. Quasilinear Equation. We now consider the quasilinear equation

$$u_t = \Delta u^2 + 8u^3, \tag{6.1}$$

on $\Omega = [-1, 1]$ with the same initial condition as above: $u_0(x) = \cos(\pi x/2)$. The blow-up time is approximately $T_b \approx 0.1128$. We computed the solution up to $T_f = 0.1000$, using the step sizes $h = 0.000125$, 0.00008, 0.00005, 0.000025 and 0.0000125 for first-order methods and $h = 0.0005$, 0.00025, 0.000125, 0.00008 and 0.00005 for second-order methods. The errors and running times are listed in Table 2 and plotted in Figure 4. We observe that the B-methods obtained by variation of the constant are much more accurate than standard methods: for the same step size, the errors are 10 times smaller for first-order methods. The difference is even more remarkable among second-order methods, with the trapezoidal rule (VCTR) reducing the error by a factor of about 25, and the midpoint rule (VCMR) by more than a factor of 50, compared with their classical counterparts. If we consider the error achieved for similar running times, we see that the B-methods improve accuracy by 4-5 times for the VCFE/FE and VCBE/BE pairs, nearly 10 times for VCMR/MR and about twice for the VCTR/TR pairs.

6.3. Semilinear Parabolic System. In [16] and [15], Friedman and Giga considered parabolic systems of the form $u_t - u_{xx} = f(v)$, $v_t - v_{xx} = g(u)$, where f and g are positive, increasing and superlinear. They showed that the solutions exhibit a

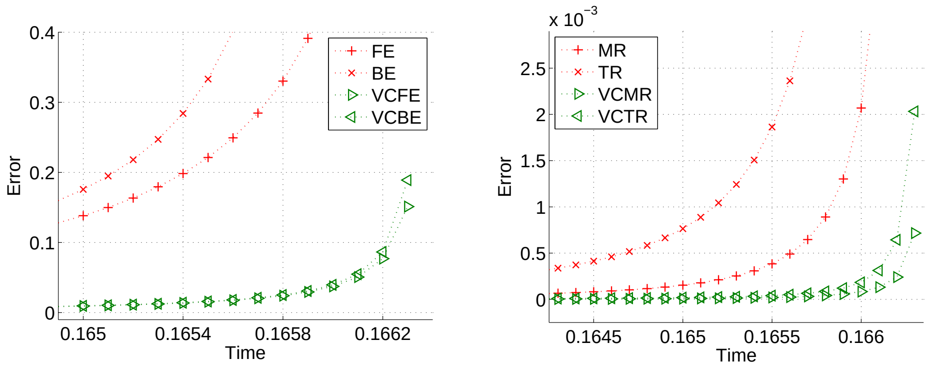

FIG. 3. *Error for first and second-order methods applied to the semilinear equation with* $F(u) = e^u$*, for time steps close to* $T_f = 0.1663$.

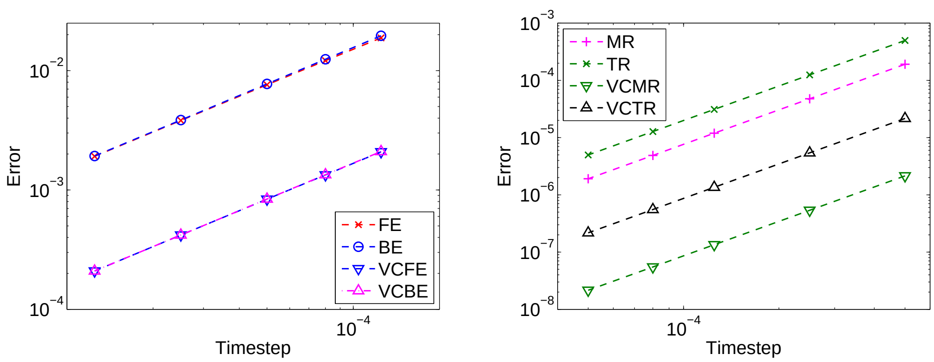

FIG. 4. *Error at* $T_f = 0.1000$ *for B-methods applied to the quasilinear equation* (6.1)*, with different values of* h*. Left: first-order methods, right: second-order methods.*

single-point blow-up. In this section, we derive B-methods for the simple case

$$\left\{\begin{array}{ll} u_t & = \Delta u + \delta e^v, \\ v_t & = \Delta v + \gamma e^u. \end{array}\right. \tag{6.2}$$

We first solve the nonlinear system of ordinary differential equations

$$\left\{\begin{array}{ll} y'(t) & = \delta e^{z(t)}, \\ z'(t) & = \gamma e^{y(t)}, \end{array}\right. \tag{6.3}$$

to get

$$\left\{\begin{array}{ll} y(t) & = \ln K - \ln[1 - \delta e^{Kt+D}] - \ln \gamma, \\ z(t) & = \ln K - \ln[1 - \delta e^{Kt+D}] + Kt + D, \end{array}\right. \tag{6.4}$$

where K and D are constants of integration. To derive B-methods using variation of the constants, we set

$$\left\{\begin{array}{ll} u(x,t) & = \ln K(x,t) - \ln[1 - \delta e^{K(x,t)t+D(x,t)}] - \ln \gamma, \\ v(x,t) & = \ln K(x,t) - \ln[1 - \delta e^{K(x,t)t+D(x,t)}] + K(x,t)t + D(x,t), \end{array}\right. \tag{6.5}$$

and compute the derivatives

$$u_t = \frac{K_t}{K} + \frac{\delta e^{D+tK}(D_t + K + tK_t)}{1 - \delta e^{D+tK}} = \frac{K_t}{K} + \frac{\delta e^{D+tK}(D_t + tK_t)}{1 - \delta e^{D+tK}} + \delta e^v,$$

TABLE 2

Error at $T_f = 0.1000$ for first and second-order methods applied to the quasilinear equation (6.1). Running times in milliseconds are given in brackets.

Timestep	0.000125	8e-005	5e-005	2.5e-005	1.25e-005
FE	0.0188 (31)	0.0121 (13)	0.00762 (18)	0.00383 (34)	0.00192 (66)
BE	0.0196 (87)	0.0125 (116)	0.00774 (185)	0.00386 (360)	0.00192 (669)
VCFE	0.00209 (20)	0.00134 (21)	0.000837 (31)	0.000419 (60)	0.000209 (118)
VCBE	0.0021 (147)	0.00134 (204)	0.000839 (280)	0.000419 (500)	0.00021 (953)

Timestep	0.0005	0.00025	0.000125	8e-005	5e-005
MR	0.000191 (39)	4.78e-005(56)	1.19e-005(110)	4.89e-006(170)	1.91e-006(273)
TR	0.000499 (33)	0.000125 (44)	3.11e-005(82)	1.28e-005(127)	4.98e-006(203)
VCMR	2.15e-006(89)	5.37e-007(135)	1.34e-007(241)	5.5e-008 (347)	2.15e-008(508)
VCTR	2.17e-005(90)	5.42e-006(137)	1.35e-006(245)	5.55e-007(352)	2.17e-007(512)

and

$$\begin{aligned} v_t &= \frac{K_t}{K} + \frac{\delta e^{D+tK}(D_t + K + tK_t)}{1-\delta e^{D+tK}} + D_t + K + tK_t, \\ &= \frac{K_t}{K} + \frac{\delta e^{D+tK}(D_t + tK_t)}{1-\delta e^{D+tK}} + D_t + tK_t + \frac{K}{1-\delta e^{D+tK}}, \\ &= \frac{K_t}{K} + \frac{\delta e^{D+tK}(D_t + tK_t)}{1-\delta e^{d+tK}} + D_t + tK_t + \gamma e^u. \end{aligned}$$

So for u and v to satisfy the system (6.2), we need

$$\begin{cases} \Delta u = \frac{K_t}{K} + \frac{\delta e^{Kt+D}}{1-\delta e^{Kt+D}}(tK_t + D_t), \\ \Delta v = \Delta u + tK_t + D_t, \end{cases}$$

which leads to the system

$$\begin{cases} K_t &= \frac{K}{1-\delta e^{Kt+D}}\left(\Delta u - \delta e^{Kt+D}\Delta v\right), \\ D_t &= \Delta v - \Delta u - \frac{tK}{1-\delta e^{Kt+D}}\left(\Delta u - \delta e^{Kt+D}\Delta v\right), \end{cases} \tag{6.6}$$

where u and v are given by (6.5). We also need to invert the system (6.5) to obtain K and D as functions of u and v:

$$\begin{cases} K &= \gamma e^u - \delta e^v, \\ D &= v - u - \ln\gamma + \delta t e^v - \gamma t e^u. \end{cases}$$

The various B-methods can now be obtained by discretizing (6.6) and expressing K and D in terms of u and v. For example, the VCBE method is given by

$$\gamma(e^{u_{n+1}} - e^{u_n}) - \delta(e^{v_{n+1}} - e^{v_n}) = h(\gamma e^{u_{n+1}}\Delta u_{n+1} - \delta e^{v_{n+1}}\Delta v_{n+1}),$$

and

$$\begin{aligned} (v_{n+1} - v_n + &\delta t_{n+1} e^{v_{n+1}} - \delta t_n e^{v_n}) - (u_{n+1} - u_n + \gamma t_{n+1} e^{u_{n+1}} - \gamma t_n e^{u_n}) \\ &= h(\Delta v_{n+1} - \Delta u_{n+1}) - h t_{n+1}(\gamma e^{u_{n+1}}\Delta u_{n+1} - \delta e^{v_{n+1}}\Delta v_{n+1}). \end{aligned}$$

We now present the results of numerical experiments for the system (6.2) with $\delta = 3$ and $\gamma = 5$. The initial conditions are $u_0(x) = \cos(\pi x/2)$ and $v_0(x) = \cos(\pi x/2)$ on

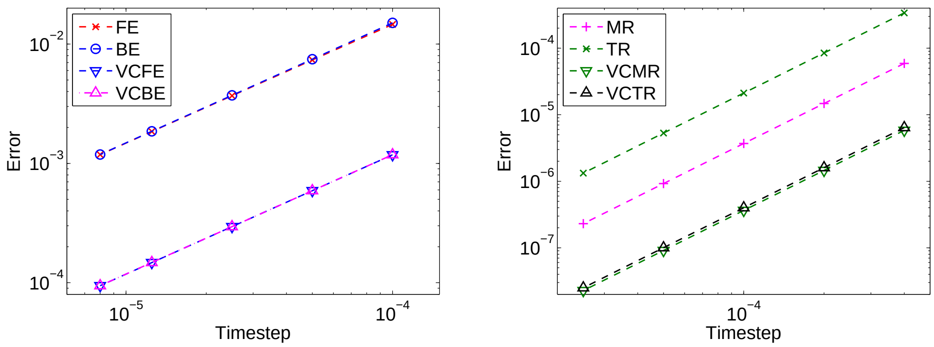

FIG. 5. *Error at $T_f = 0.1100$ for B-methods applied to the system of semilinear equations with different values of h. Left: for first-order methods, right: for second-order methods.*

$\Omega = [-1, 1]$. The blow-up time is approximately $T_b \approx 0.1181$. To obtain the data for Table 3 and Figure 5, we computed the solution up to $T_f = 0.1100$, using the step sizes $h = 0.0001, 0.00005, 0.000025, 0.0000125$ and 0.000008 for first-order methods and $h = 0.0004, 0.0002, 0.0001, 0.00005$ and 0.000025 for second-order methods. Once again, we observe that the B-methods perform much better than their standard counterparts for the same time step size. It is interesting to note that while the standard midpoint rule produces errors that are about five times smaller than the standard trapezoidal rule, the corresponding B-methods produce errors that are nearly identical to each other. If we compare the accuracy achieved for the same computational effort, we see that VCFE and VCMR are about 2-3 times more accurate than standard FE and MR, whereas VCBE is about 10 times more accurate than BE. Remarkably, VCTR yields a forty-fold improvement in accuracy over standard TR for the same running time!

TABLE 3
Error at $T_f = 0.1100$ for first and second-order methods applied to the system of semilinear equations. We report in brackets the running times in milliseconds.

Timestep	0.0001	5e-005	2.5e-005	1.25e-005	8e-006
FE	0.0146 (31)	0.00736 (21)	0.00369 (35)	0.00185 (68)	0.00118 (107)
BE	0.015 (568)	0.00747 (1101)	0.00372 (2197)	0.00186 (3941)	0.00119 (5751)
VCFE	0.00118 (51)	0.00059 (84)	0.000295 (164)	0.000148 (326)	9.45e-005(513)
VCBE	0.00118 (715)	0.000591 (1217)	0.000295 (2099)	0.000148 (3922)	9.45e-005(5966)

Timestep	0.0004	0.0002	0.0001	5e-005	2.5e-005
MR	5.91e-005(152)	1.48e-005(283)	3.69e-006(554)	9.23e-007(1106)	2.31e-007(2103)
TR	0.000339 (188)	8.48e-005(346)	2.12e-005(679)	5.3e-006 (1359)	1.32e-006(2709)
VCMR	5.82e-006(342)	1.46e-006(650)	3.64e-007(1299)	9.1e-008 (2250)	2.28e-008(3858)
VCTR	6.4e-006 (233)	1.6e-006 (440)	4e-007 (878)	1e-007 (1523)	2.5e-008 (2608)

6.4. Wave Equation. Finally, we consider the wave equation

$$u_{tt} = \Delta u + \delta e^u, \tag{6.7}$$

which is equivalent to the PDE system

$$\begin{cases} u_t = v, \\ v_t = \Delta u + \delta e^u. \end{cases} \tag{6.8}$$

To derive B-methods based on Variation of Constants, we consider the ODE

$$y_{tt} = \delta e^y.$$

If we multiply both sides by $2y_t$ and integrate with respect to t, we get

$$(y_t)^2 = 2\delta e^y + C_1. \tag{6.9}$$

This equation has two general solutions depending on the sign of C_1, namely

$$y(t) = \begin{cases} \ln \frac{2K^2}{\delta \sinh^2(D+Kt)}, & C_1 = 4K^2 > 0 \\ \ln\left(\frac{2K^2}{\delta} \sec^2(D+Kt)\right), & C_1 = -4K^2 < 0 \end{cases}.$$

Here, we will focus on the case $C_1 = -4K^2 < 0$, since the other branch has only one singularity at $D + Kt \to 0$ and is less likely to cause blow up. Thus, we consider a solution $u(x,t)$ to (6.7) of the form

$$u(x,t) = G(t, K(x,t), D(x,t)) = \ln\left(\frac{2K^2}{\delta} \sec^2(D+Kt)\right), \tag{6.10}$$

where we define, by analogy to (6.9),

$$K = \frac{1}{2}\sqrt{2\delta e^u - v^2}$$

with $v = u_t$, which is well defined whenever $2\delta e^u > (u_t)^2$. Then differentiating the above gives

$$K_t = \frac{1}{4\sqrt{2\delta e^u - v^2}}(2\delta e^u u_t - 2vv_t) = \frac{1}{8K}(2\delta e^u v - 2v(\Delta u + \delta e^u)) = -\frac{v\Delta u}{4K}. \tag{6.11}$$

We can now obtain the differential equation for $D(x,t)$ by differentiating (6.10):

$$\begin{aligned} u_t &= \frac{\delta}{2K^2 \sec^2(D+Kt)}\left[\frac{4KK_t}{\delta}\sec^2(D+Kt) + \frac{4K^2}{\delta}\sec^2(D+Kt)\tan(D+Kt)(D_t + tK_t + K)\right] \\ &= 2\left[\frac{K_t}{K} + (D_t + tK_t + K)\tan(D+Kt)\right]. \end{aligned}$$

This yields

$$D_t = \frac{1}{\tan(D+Kt)}\left(\frac{v}{2} - \frac{K_t}{K}\right) - K - tK_t, \tag{6.12}$$

where we have substituted v for u_t on the left hand side. But from (6.10) and the definition of K, we see that

$$\tan(D+Kt) = \sqrt{\sec^2(D+Kt) - 1} = \left(\frac{\delta e^u}{2K^2} - 1\right)^{1/2} = \frac{v}{2K}.$$

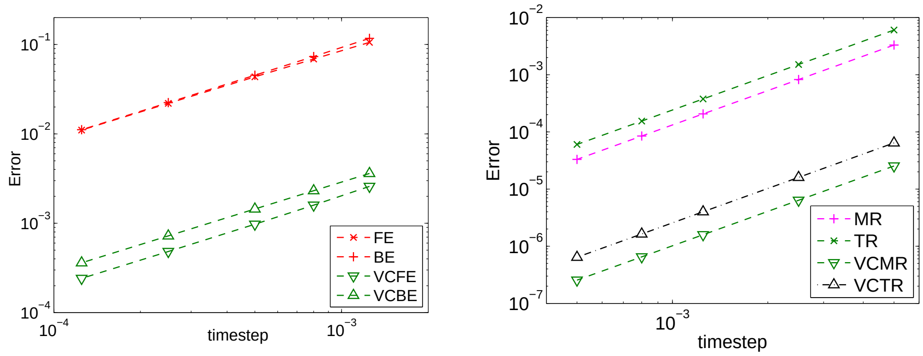

FIG. 6. *Error at $T_f = 0.600$ for B-methods applied to the wave equation (6.7) with different values of h. Left: first-order methods, right: second-order methods.*

Substituting this and (6.11) into (6.12) yields

$$D_t = \frac{\Delta u}{4K}(2 + tv). \tag{6.13}$$

It now suffices to discretize (6.11) and (6.13) to obtain the various B-methods. For example, the VCBE method becomes

$$\begin{cases} K(u_{n+1}, v_{n+1}) - K(u_n, v_n) = -\dfrac{hv_{n+1}\Delta u_{n+1}}{4K(u_{n+1}, v_{n+1})}, \\ D(t_{n+1}, u_{n+1}, v_{n+1}) - D(t_n, u_n, v_n) = \dfrac{h(2 + t_{n+1}v_{n+1})\Delta u_{n+1}}{4K(u_{n+1}, v_{n+1})}, \end{cases}$$

where

$$K(u, v) = \frac{1}{2}\sqrt{2\delta e^u - v^2}, \qquad D(t, u, v) = \arctan\left(\frac{v}{\sqrt{2\delta e^u - v^2}}\right) - \frac{t}{2}\sqrt{2\delta e^u - v^2}.$$

To test our schemes numerically, we solve (6.7) with $\delta = 5$ on $\Omega = [-1, 1]$ and homogeneous boundary conditions. The initial conditions are $u_0(x) = \cos(\pi x/2)$ and $u_{t0} = 0.1$. The blow-up time can be approximated by $T_b = 0.643$. To generate Figure 6, we computed the solution up to $T_f = 0.6$, using step sizes $h = 0.00125$, 0.0008, 0.0005, 0.00025 and 0.000125 for first-order methods and $h = 0.005$, 0.0025, 0.00125, 0.0008 and 0.0005 for second-order methods. The errors are shown in Table 4. Again, our B-methods perform very well: for first-order methods, we reduced the error by about 20 to 30 times, and for second-order methods, the error is between 80 and 125 times smaller. If we consider the accuracy achieved for a fixed amount of running time, we see that VCFE leads to a roughly tenfold improvement over FE, and the VCBE, VCMR and VCTR methods lead to improvements by a factor of 12, 10 and 4 respectively.

7. Conclusions. We presented in this paper a systematic approach for deriving numerical integrators which are very accurate for semi- and quasi-linear parabolic and hyperbolic partial differential equations exhibiting blow-up in finite time. We call this new class of geometric integration methods B-methods, where B stands for blow-up. Our construction is applicable as long as one can solve the ODE that results after dropping the spatial derivatives; thus, our procedure can be used to derive B-methods

Table 4
Error at $T_f = 0.600$ for first and second-order methods applied to the wave equation (6.7). *Running times in milliseconds are reported in brackets.*

Timestep	0.00125	0.0008	0.0005	0.00025	0.000125
FE	0.106 (5)	0.0688 (6)	0.0435 (9)	0.022 (17)	0.011 (31)
BE	0.117 (173)	0.0735 (243)	0.0453 (345)	0.0224 (668)	0.0112 (1292)
VCFE	0.00259 (17)	0.00160 (25)	0.000977 (39)	0.000484 (79)	0.000242 (151)
VCBE	0.00361 (344)	0.00231 (517)	0.00145 (816)	0.000723 (1518)	0.000361 (2713)

Timestep	0.005	0.0025	0.00125	0.0008	0.0005
MR	0.00331 (38)	0.000827 (58)	0.000207 (115)	8.46e-005(176)	3.31e-005(275)
TR	0.00608 (21)	0.00151 (39)	0.000378 (75)	0.000155 (115)	6.04e-005(178)
VCMR	2.53e-005(88)	6.35e-006(160)	1.59e-006(312)	6.51e-007(481)	2.54e-007(765)
VCTR	6.41e-005(93)	1.6e-005 (171)	4e-006 (334)	1.64e-006(516)	6.4e-007 (812)

for many other nonlinear partial differential equations that were not considered in this paper. Because of their construction, which takes the blow-up behavior into account, all these methods will behave substantially better close to blow-up, while their behavior before blow-up is similar to classical time stepping schemes.

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