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Asymptotic Mesh Independence of Newton's Method Revisited

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Asymptotic Mesh Independence of Newton's Method Revisited *

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Abstract

The paper presents a new affine invariant theory on asymptotic mesh independence of Newton's method for discretized nonlinear operator equations. Compared to earlier attempts, the new approach is both much simpler and more intuitive from the algorithmic point of view. The theory is exemplified at collocation methods for ODE boundary value problems and at finite element methods for elliptic PDE problems.

Keywords: asymptotic mesh independence, Newton's method, affine invariance

AMS classification (2000): 65J15, 65L10, 65N30

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Introduction

The term 'mesh independence' characterizes the observation that finite dimensional Newton methods, when applied to a nonlinear PDE on successively finer discretizations with comparable initial guesses, show roughly the same convergence behavior on all sufficiently fine discretizations. The 'mesh independence principle' has been stated and even exploited for mesh design in papers by Allgower and Böhmer [1] and McCormick [14]. Further theoretical investigations of the phenomenon have been given in the paper [2] by Allgower, Böhmer, Potra, and Rheinboldt. Those papers, however, lacked certain important features in the theoretical characterization that actually prohibited their application to discretized PDEs. This drawback has been avoided in the affine invariant theoretical study by Deuflhard and Potra in [9]; from that analysis, the modified term 'asymptotic mesh independence' naturally emerged. The present paper suggests a different approach, which is also affine invariant, but much simpler and more natural from the algorithmic point of view.

The paper is organized as follows. In Section 1 we first revisit the theoretical approaches given up to now to treat mesh independence for operator equations. In Section 2 we compare discrete versus continuous Newton methods, again in affine invariant terms; in contrast to the earlier treatment in [9], we only use terminology that naturally arises from the algorithmic point of view, such as Newton sequences and approximation errors. The new theory is then exemplified at collocation methods for ODE boundary value problems and at finite element methods for elliptic PDEs (Section 3).

1 Preliminary Considerations

Let a nonlinear operator equation be denoted by

$$F(x) = 0 \ ,$$

where $F : D \to Y$ is defined on a convex domain $D \subset X$ of a Banach space X with values in a Banach space Y. Throughout the paper we assume the existence of a unique solution x^* of this operator equation. The corresponding ordinary Newton method in Banach space may be written as

$$F'(x^k)\Delta x^k = -F(x^k) \ , \quad x^{k+1} = x^k + \Delta x^k \ , \quad k = 0, 1, \dots \ , \tag{1}$$

assuming, of course, that the derivatives are invertible. In each Newton step, the linearized operator equation must be solved, which is why this approach is often also called *quasilinearization*. For F, we assume that Theorem 1 from [8] holds, an affine invariant version of the classical Newton-Mysovskikh theorem, whose essence we recall here for the purpose of later reference.

Theorem 1.1. *Let $F : D \to Y$ be a continuously differentiable mapping with $D \subset X$ convex. Let $\| \cdot \|$ denote the norm in the domain space X. Suppose that $F'(x)$ is invertible for each $x \in D$. Assume that, for collinear x, y, $z \in D$, the following affine invariant Lipschitz condition holds:*

$$\left\| F'(z)^{-1}\big(F'(y) - F'(x)\big)v \right\| \le \omega \|y - x\| \, \|v\| \ . \tag{2}$$

For the initial guess $x^0 \in D$ assume that

$$h_0 = \omega\|\Delta x^0\| < 2$$

and that $\bar{S}(x^0,\rho) \subset D$ for $\rho = \dfrac{\|\Delta x^0\|}{1-h_0/2}$.

Then the sequence $\{x^k\}$ of ordinary Newton iterates remains in $S(x^0,\rho)$ and converges to a unique solution $x^* \in \bar{S}(x^0,\rho)$. Its convergence speed can be estimated as

$$\|x^{k+1} - x^k\| \leq \tfrac{1}{2}\omega\|x^k - x^{k-1}\|^2 \ .$$

In actual computation, we can only solve discretized nonlinear equations of finite dimension, at best on a sequence of successively finer mesh levels, say

$$F_j(x_j) = 0 \ , \quad j = 0,1,\dots \ , \tag{3}$$

where $F_j : D_j \to Y_j$ denotes a nonlinear mapping defined on a convex domain $D_j \subset X_j$ of a finite-dimensional subspace $X_j \subset X$ with values in a finite dimensional space Y_j. The corresponding finite dimensional ordinary Newton method reads

$$F_j'(x_j^k)\Delta x_j^k = -F_j(x_j^k) \ , \quad x_j^{k+1} = x_j^k + \Delta x_j^k \ , \quad k = 0,1,\dots \ .$$

In each Newton step, a system of linear equations must be solved. This system can equally well be interpreted either as a discretization of the linearized operator equation (1) or as a linearization of the discrete nonlinear system (3). Again we assume that Theorem 1.1 holds, this time for the finite dimensional mapping F_j. Let ω_j denote the corresponding affine invariant Lipschitz constant. Then the quadratic convergence of this Newton method is governed by the relation

$$\|x_j^{k+1} - x_j^k\| \leq \tfrac{1}{2}\omega_j\|x_j^k - x_j^{k-1}\|^2 \ .$$

Under the assumptions of Theorem 1.1 there exist unique discrete solutions x_j^* on each level j. Of course, we want to choose appropriate discretization schemes such that

$$\lim_{j\to\infty} x_j^* = x^* \ . \tag{4}$$

From the synopsis of discrete and continuous Newton method, we immediately see that any comparison of the convergence behavior on different discretization levels j will direct us toward a comparison of the affine covariant Lipschitz constants ω_j. Of particular interest is the connection with the Lipschitz constant ω of the underlying operator equation.

In the earlier papers [1, 2] on mesh independence two assumptions of the kind

$$\|F_j'(x_j)^{-1}\| \leq \beta_j \ , \quad \|F_j'(x_j + v_j) - F_j'(x_j)\| \leq \gamma_j\|v_j\|$$

have been made in combination with the *uniformity* requirements

$$\beta_j \leq \beta \ , \quad \gamma_j \leq \gamma \ . \tag{5}$$

Obviously, these assumptions lack affine invariance. More important, however, and as a consequence of the noninvariance, these conditions are phrased in terms of *operator norms*, which, in turn, depend on the relation of norms in the domain and the image space of the mappings F_j and F, respectively. For typical PDEs we would obtain

$$\lim_{j\to\infty} \beta_j \to \infty \ ,$$

which clearly contradicts the uniformity assumption (5). Consequently, an analysis in terms of β_j and γ_j would not be applicable to this important case.

The situation is different with the affine invariant Lipschitz constants ω_j: they only depend on the choice of *norms in the domain space*. It is easy to verify that

$$\omega_j \leq \beta_j \gamma_j \ .$$

In Section 2 below we will show that the ω_j remain bounded in the limit $j \to \infty$, as long as ω is bounded – even if either β_j or γ_j blow up. Moreover, even when the product $\beta_j\gamma_j$ remains bounded, the Lipschitz constant ω_j may be considerably lower, i.e.

$$\omega_j \ll \beta_j \gamma_j \ .$$

A prerequisite for the asymptotic property (4) to hold is that the elements of the infinite dimensional space X can be well approximated by elements of the finite dimensional subspaces X_j. In general, however, the solution x^* has "better smoothness properties" than the generic elements of the space X. For this reason, the earlier papers [2, 9] had restricted their analysis to some smoother subset $W^* \subset X$ and explicitly assumed that

$$x^*, x^k, \Delta x^k, x^k - x^* \in W^* \ , \quad k = 0, 1, \dots \ .$$

However, such an assumption is hard to confirm in the concrete case. That is why we will drop it for our analysis to be presented.

Next, we revisit the paper [9] in some necessary detail. In that paper a family of linear projections

$$\pi_j : X \to X_j \ , \quad j = 0, 1, \dots$$

had been introduced, assumed to satisfy the *stability condition*

$$q_j = \sup_{x \in W^*, x \neq 0} \frac{\|\pi_j x\|}{\|x\|} \leq \overline{q} < \infty \ , \quad j = 0, 1, \dots \ . \tag{6}$$

The projection property $\pi_j^2 = \pi_j$ immediately gives rise to the lower bound

$$q_j \geq 1 \ . \tag{7}$$

As a measure of the *approximation quality* that paper had defined

$$\delta_j = \sup_{x \in W^*, x \neq 0} \frac{\|x - \pi_j x\|}{\|x\|} \ , \quad j = 0, 1, \dots \ . \tag{8}$$

The rather natural idea that a refinement of the discretization improves the approximation quality had been expressed by the asymptotic assumption

$$\lim_{j\to\infty} \delta_j = 0 \ . \tag{9}$$

The triangle inequality and (6) had supplied the upper bound

$$q_j \leq 1 + \delta_j \ . \tag{10}$$

By combination of (7), (9), and (10), asymptotic stability had arisen as

$$\lim_{j\to\infty} q_j = 1 \, . \tag{11}$$

However, as has been pointed out by Braess [5], the above theory has some weak point. In fact, from (6) we conclude that $x = 0$ implies $\pi_j x = 0$. The reverse, however, will not be true in general. Hence, one must be aware of pathological elements $x \neq 0$ with corresponding approximations $\pi_j x = 0$. On a uniform one-dimensional grid, such a pathological element might look just as $x(t)$ represented graphically in Fig. 1. Insertion of such elements into (8) would yield

$$\delta_j \geq 1$$

on each level j, on which such pathological elements exist. If one were to accept such an occurrence on *all* levels, then this would be in clear contradiction to the desired asymptotic property (9) and its consequence (11).

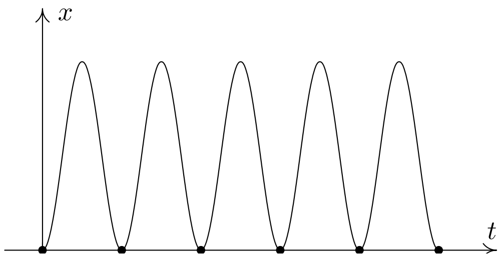

Figure 1: Pathological element $x \neq 0$ with $\pi_j x = 0$ ($\bullet$: mesh nodes).

In order to close this gap of that theory, one would have to relate the subset W^* and the projections π_j such that the occurrence of pathological elements would be asymptotically excluded. As an example, assume we have *nested* subspaces X_j, e.g. constructed by uniform mesh refinement. Suppose we begin with a 'sufficiently good' initial projection π_0 on a 'sufficiently' fine mesh, which already captures the main qualitative behavior of the solution x^* correctly. Then 'pathological' elements would no longer be expected to occur on finer meshes in actual computation. Thus, upon carefully choosing appropriate subsets of W^*, the theory from [9] could, in principle, be repaired. However, the technicalities of such a theory tend to obscure the underlying simple idea.

For this reason, we here abandon that approach and turn to a different one, which seems to us both simpler and more intuitive from the algorithmic point of view: we will avoid the (anyway computationally unavailable) projections π_j and define the approximation quality δ_j differently, just exploiting usual approximation results for discretization schemes.

2 Discrete versus Continuous Newton Sequences

In this section, we study the comparative behavior of discrete versus continuous Newton sequences. If not explicitly stated otherwise, the notation is taken from the previous section.

We will consider the phenomenon of mesh independence of Newton's method in two steps. First, we will show that the discrete Newton sequence tracks the continuous Newton sequence closely, with a maximal distance bounded in terms of the mesh size; both of the Newton sequences behave nearly identically until, eventually, a small neighborhood of the solution is reached. Second, we prove the existence of affine invariant Lipschitz constants ω_j for the discretized problems, which approach the Lipschitz constant ω of the continuous problem in the limit $j \to \infty$; again, the distance can be bounded in terms of the mesh size. Upon combining these two lines, we finally establish the existence of locally unique discrete solutions x_j^* in a vicinity of the continuous solution x^*.

To begin with, we prove the following nonlinear perturbation lemma.

Lemma 2.1. *Consider two Newton sequences* $\{x^k\}$, $\{y^k\}$ *starting at initial guesses* x^0, y^0 *and continuing as*

$$x^{k+1} = x^k + \Delta x^k \ , \quad y^{k+1} = y^k + \Delta y^k \ ,$$

where $\Delta x^k, \Delta y^k$ *are the corresponding ordinary Newton corrections. Assume the affine invariant Lipschitz condition* (2) *is satisfied. Then the following contraction result holds:*

$$\|x^{k+1} - y^{k+1}\| \le \omega \left(\tfrac{1}{2}\|x^k - y^k\| + \|\Delta x^k\| \right) \|x^k - y^k\| \tag{12}$$

Proof. Dropping the iteration index k we start with

$$\begin{aligned}
&x + \Delta x - y - \Delta y \\
&\quad = x - F'(x)^{-1}F(x) - y + F'(y)^{-1}F(y) \\
&\quad = x - F'(x)^{-1}F(x) + F'(x)^{-1}F(y) - F'(x)^{-1}F(y) - y + F'(y)^{-1}F(y) \\
&\quad = x - y - F'(x)^{-1}\big(F(x) - F(y)\big) + F'(x)^{-1}\big(F'(y) - F'(x)\big)F'(y)^{-1}F(y) \\
&\quad = F'(x)^{-1}\Big(F'(x)(x-y) - \int_{t=0}^{1} F'(y + t(x-y))(x-y)\,dt\Big) \\
&\qquad + F'(x)^{-1}(F'(y) - F'(x))\Delta y.
\end{aligned}$$

Upon using assumption (2), we conclude that

$$\begin{aligned}
\|x^{k+1} - y^{k+1}\| &\le \int_{t=0}^{1} \|F'(x^k)^{-1}\big(F'(x^k) - F'(y^k + t(x^k - y^k))\big)(x^k - y^k)\|\,dt \\
&\quad + \|F'(x^k)^{-1}(F'(y^k) - F'(x^k))\Delta y^k\| \\
&\le \frac{\omega}{2}\|x^k - y^k\|^2 + \omega\|x^k - y^k\|\,\|\Delta y^k\|,
\end{aligned}$$

which confirms (12). □

With the above auxiliary result, we are now ready to study the relative behavior of discrete versus continuous Newton sequences.

Theorem 2.2. *In addition to the notation as already introduced, let* $x^0 = x_j^0 \in X_j$ *denote a given starting value such that the assumptions of Theorem 1.1 hold for the continuous Newton iteration, including*

$$h_0 = \omega\|\Delta x^0\| < 2 \ .$$

For the discrete mapping F_j and all arguments $x_j \in D_j = S(x^0, \rho + 2/\omega) \cap X_j$ define

$$F_j'(x_j)\Delta x_j = -F_j(x_j) \ , \quad F'(x_j)\Delta x = -F(x_j) \ . \tag{13}$$

Assume that the discretization is fine enough such that

$$\|\Delta x_j - \Delta x\| \le \delta_j \le \frac{1}{2\omega} \tag{14}$$

uniformly for $x_j \in D_j$. Then the following cases occur:

I. *If $h_0 \le 1 - \sqrt{1 - 2\omega\delta_j}$, then*

$$\|x_j^k - x^k\| < 2\delta_j \le \frac{1}{\omega} \ , \quad k = 0, 1, \dots \ .$$

II. *If $1 - \sqrt{1 - 2\omega\delta_j} < h_0 < 1 + \sqrt{1 - 2\omega\delta_j}$, then*

$$\|x_j^k - x^k\| \le \frac{1}{\omega}\big(1 + \sqrt{1 - 2\omega\delta_j}\,\big) < \frac{2}{\omega} \ , \quad k = 0, 1, \dots \ .$$

In both cases I *and* II*, the asymptotic result*

$$\limsup_{k \to \infty} \|x_j^k - x^k\| \le \frac{1}{\omega}\big(1 - \sqrt{1 - 2\omega\delta_j}\,\big) < 2\delta_j \le \frac{1}{\omega}$$

holds.

Proof. In [13, pp. 99, 160], Wanner and Hairer introduced "Lady Windermere's fan" as a tool to prove discretization error results for evolution problems based on some linear perturbation lemma. We may copy this idea and exploit our nonlinear perturbation Lemma 2.1 in the present case. The situation is represented graphically in Figure 2.

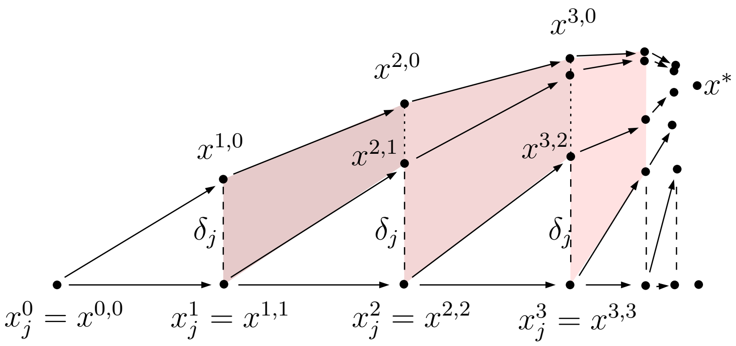

Figure 2: "Lady Windermere's fan" for continuous and discrete Newton method.

The discrete Newton sequence starting at the given initial point $x_j^0 = x^{0,0}$ is written as $\{x^{k,k}\}$. The continuous Newton sequence, written as $\{x^{k,0}\}$, starts at the same initial point $x^0 = x^{0,0}$ and runs toward the solution point x^*. In between we define further continuous Newton sequences, written as $\{x^{i,k}\}, k = i, i+1, \dots$, which start at the discrete Newton iterates $x_j^i = x^{i,i}$ and also run toward x^*. Note that the existence or even uniqueness of a discrete solution point x_j^* is not implied by the assumptions of the theorem.

For the purpose of repeated induction, we assume that

$$\|x_j^{k-1} - x^0\| < \rho + \frac{2}{\omega},$$

which certainly holds for $k = 1$. In order to characterize the deviation between discrete and continuous Newton sequences, we introduce the two majorants

$$\omega\|\Delta x^k\| \leq h_k \;, \quad \|x_j^k - x^k\| \leq \epsilon_k \;.$$

Recall from Theorem 1.1 that

$$h_{k+1} = \tfrac{1}{2}h_k^2 \;. \tag{15}$$

For the derivation of a second majorant recursion, we apply the triangle inequality in the form

$$\|x^{k+1,k+1} - x^{k+1,0}\| \leq \|x^{k+1,k+1} - x^{k+1,k}\| + \|x^{k+1,k} - x^{k+1,0}\|.$$

The first term can be treated using assumption (14) so that

$$\begin{aligned}\|x^{k+1,k+1} - x^{k+1,k}\| = \|x_j^k + \Delta x_j^k - \left(x^{k,k} + \Delta x^{k,k}\right)\| &= \|\Delta x_j^k - \Delta x^{k,k}\| \\ &\leq \delta_j \;.\end{aligned} \tag{16}$$

For the second term, we may apply our nonlinear perturbation Lemma 2.1 (see the shaded regions in Fig. 2) to obtain

$$\|x^{k+1,k} - x^{k+1,0}\| \leq \omega\Big(\frac{1}{2}\|x^{k,k} - x^{k,0}\| + \|\Delta x^{k,0}\|\Big)\|x^{k,k} - x^{k,0}\|$$

Combining these results then leads to

$$\|x^{k+1,k+1} - x^{k+1,0}\| \leq \delta_j + \frac{\omega}{2}\epsilon_k^2 + h_k\epsilon_k \;.$$

The above right side may be defined to be ϵ_{k+1}. Hence, together with (15), we arrive at the following set of majorant equations

$$h_{k+1} = \tfrac{1}{2}h_k^2 \;, \quad \epsilon_{k+1} = \delta_j + \tfrac{1}{2}\omega\epsilon_k^2 + h_k\epsilon_k \;.$$

If we introduce the quantities $\alpha_k = \omega\epsilon_k + h_k$ and $\delta = \omega\delta_j$, we may obtain the decoupled recursion

$$\alpha_{k+1} = \delta + \tfrac{1}{2}\alpha_k^2 \;, \tag{17}$$

which can be started with $\alpha_0 = h_0$, since $\epsilon_0 = 0$. Upon solving (17), we get the two equilibrium points

$$\hat{\alpha}_1 = 1 - \sqrt{1 - 2\delta} < 1 \;, \quad \hat{\alpha}_2 = 1 + \sqrt{1 - 2\delta} > 1 \;.$$

Insertion into the recursion (17) then leads to the form

$$\alpha_{k+1} - \hat{\alpha} = \tfrac{1}{2}(\alpha_k - \hat{\alpha})(\alpha_k + \hat{\alpha}) \;. \tag{18}$$

For $\alpha_k < \hat{\alpha}_2$ we see that

$$\tfrac{1}{2}(\alpha_k + \hat{\alpha}_1) < \tfrac{1}{2}(\hat{\alpha}_2 + \hat{\alpha}_1) = 1 \ ,$$

which implies that

$$|\alpha_{k+1} - \hat{\alpha}_1| < |\alpha_k - \hat{\alpha}_1| \ .$$

Hence, the fixed point $\hat{\alpha}_1$ is attractive, whereas $\hat{\alpha}_2$ is repelling. Moreover, since $\alpha_k + \hat{\alpha}_{1,2} > 0$, we immediately obtain the result

$$\mathrm{sign}(\alpha_{k+1} - \hat{\alpha}) = \mathrm{sign}(\alpha_k - \hat{\alpha}) \ .$$

Therefore, we have the following cases:

I. $\alpha_0 \leq \hat{\alpha}_1 \quad \Longrightarrow \quad \alpha_k \leq \hat{\alpha}_1$,

II. $\hat{\alpha}_1 < \alpha_0 < \hat{\alpha}_2 \quad \Longrightarrow \quad \hat{\alpha}_1 \leq \alpha_k < \hat{\alpha}_2$.

Insertion of the expressions for the used quantities then shows that cases I,II directly correspond to cases I,II of the theorem. Its last asymptotic result is now an immediate consequence of (18). Finally, with application of the triangle inequality

$$\|x_j^{k+1} - x^0\| \leq \epsilon_{k+1} + \|x^{k+1} - x^0\| < \frac{2}{\omega} + \rho \ ,$$

the induction and therefore the whole proof is completed. □

We are interested in the question whether a discrete solution point x_j^* exists. The above tracking theorem, however, only supplies the following result.

Corollary 2.3. *Under the assumptions of Theorem 2.2, there exists at least one accumulation point*

$$\hat{x}_j \in \bar{S}\,(x^*, 2\delta_j) \cap X_j \ \subset \ S\left(x^*, \frac{1}{\omega}\right) \cap X_j \ ,$$

which need not be a solution point of the discrete equations $F_j(x_j) = 0$.

In order to prove more, Theorem 1.1 directs us to study whether a Lipschitz condition of the kind (2) additionally holds.

Lemma 2.4. *Let Theorem 1.1 hold for the mapping $F : X \to Y$. For collinear $x_j, y_j, y_j + v_j \in X_j$, define quantitites $w_j \in X_j$ and $w \in X$ according to*

$$F'(x_j)w = (F'(y_j + v_j) - F'(y_j))\, v_j \ , \tag{19}$$

$$F_j'(x_j)w_j = \big(F_j'(y_j + v_j) - F_j'(y_j)\big)\, v_j \ . \tag{20}$$

Assume that the discretization method satisfies

$$\|w - w_j\| \leq \sigma_j \|v_j\|^2 \,. \tag{21}$$

Then there exist constants

$$\omega_j \leq \omega + \sigma_j \ , \tag{22}$$

such that the affine invariant Lipschitz condition

$$\|w_j\| \leq \omega_j \|v_j\|^2$$

holds for the discrete Newton process.

Proof. The proof is a simple application of the triangle inequality

$$\|w_j\| \leq \|w\| + \|w_j - w\| \leq \omega \|v_j\|^2 + \sigma_j \|v_j\|^2 = (\omega + \sigma_j) \|v_j\|^2.$$

□

Finally, the existence of a unique solution x_j^* is a direct consequence.

Corollary 2.5. *Under the assumptions of Theorem 2.2 and Lemma 2.4 the discrete Newton sequence* $\{x_j^k\}, k = 0, 1, \ldots$ *converges q-quadratically to a unique discrete solution point*

$$x_j^* \in \bar{S}(x^*, 2\delta_j) \cap X_j \ \subset \ S\left(x^*, \frac{1}{\omega}\right) \cap X_j \ .$$

Proof. We just need to apply Theorem 1.1 to the finite dimensional mapping F_j with the starting value $x_j^0 = x^0$, and the affine invariant Lipschitz constant ω_j from (22). □

Summarizing, we come to the following conclusion, at least in terms of the analyzed upper bounds: If the asymptotic properties

$$\lim_{j \to \infty} \delta_j = 0 \ , \quad \lim_{j \to \infty} \sigma_j = 0 \ ,$$

can be shown to hold, then the convergence speed of the discrete ordinary Newton method is asymptotically just the one for the continuous ordinary Newton method. Moreover, if related initial guesses x^0 and x_j^0 and a common termination criterion are chosen, then even the number of iterations will be nearly the same.

3 Application to discretization schemes

In order to apply the abstract mesh independence principles of Section 2 to discretization schemes for differential equations, we have to show two features. First,

$$\|\Delta x - \Delta x_j\| \leq \delta_j, \qquad \lim_{j \to \infty} \delta_j = 0, \tag{23}$$

where Δx is the exact and Δx_j is the approximate solution of the Newton equations (13).

Second,

$$\|w - w_j\| \leq \sigma_j \|v_j\|^2, \qquad \lim_{j \to \infty} \sigma_j = 0, \tag{24}$$

where w and w_j are the solutions of the Lipschitz equations (19) and (20) respectively.

The structure of the argumentation will be straightforward. The first step is to apply classical error estimates for the numerical method under consideration. These estimates usually depend on the regularity of the exact solution y of the linear equations. The second step is then to show appropriate regularity results for y.

ODE collocation methods. First we turn to nonlinear boundary value problems for ordinary differential equations. Assume $f : \mathbb{R}^m \to \mathbb{R}^m$ is s times continuously differentiable and $A \in \mathbb{R}^{l-m,m}, B \in \mathbb{R}^{l,m}$ are such that the BVP

$$\begin{aligned} \dot{x}(t) - f(x(t)) = 0 \quad & \text{for } t \in]a, b[\\ Ax(a) + Bx(b) - r = 0 & \end{aligned}$$

is well-defined.

On meshes $\Delta_j = \{a = t_{j,0} < t_{j,1} < \ldots < t_{j,n_j} = b\}$ with mesh size $\tau_j = \max \tau_{j,i}$ the discretizations F_j are defined by Gauss and Gauss-Lobatto collocation of order s, such that the finite dimensional spaces X_j are given by the corresponding spline spaces, i.e. spaces of piecewise polynomials of order s, together with a continuity requirement at the mesh-points.

The spaces are defined as

$$X_j := (\mathbb{P}_s[t_0, t_1] \times \ldots \times \mathbb{P}_s[t_{n_j-1}, t_{n_j}]) \cap C^0[a, b] \subset W^{1,\infty}[a, b],$$

for Gauss collocation and

$$X_j := (\mathbb{P}_s[t_0, t_1] \times \ldots \times \mathbb{P}_s[t_{n_j-1}, t_{n_j}]) \cap C^1[a, b] \subset W^{1,\infty}[a, b],$$

for Gauss-Lobatto collocation.

It turns out, that $W^{1,\infty}$ is the appropriate space to study the convergence of Newton's method applied to Gauss and Gauss-Lobatto collocation for first order systems. Additionally, in the following we will also use the piecewise L_∞-norm:

$$\|v\| := \max_{0 \le i \le n_j} \left\{ \|v\|_{L_\infty(t_i, t_{i+1})} \right\}$$

for piecewise smooth functions and their piecewise defined derivatives. These may not be defined at the gridpoints, but the norm $\|\cdot\|$ is then still well defined.

To derive (23) and (24) for collocation methods, we use classical error estimates for linear, non-autonomous problems, as established in Russell and Shampine [16] for Gauss-Lobatto collocation and extended in de Boor and Swartz [6] for Gauss collocation. The estimates we make use of here are not sharp, but sufficient for our purpose.

Lemma 3.1. *Let the linear boundary value problem*

$$\dot{u}(t) - G(t)u(t) = g(t) \tag{25}$$
$$Au(a) + Bu(b) = 0 \tag{26}$$

be uniquely solvable with condition number $\bar{\rho}[a, b] < \infty$ (cf. [7]). Let w be the exact solution of (25),(26) *and w_j the approximate solution obtained by Gauss or Gauss-Lobatto collocation of order s. Then for $p \le s$ the following error estimates hold for sufficiently small τ_j:*

$$\|u - u_j\| \le C(\bar{\rho}[a, b])\tau_j^p \|u^{(p+1)}\|, \tag{27}$$
$$\|\dot{u} - \dot{u}_j\| \le C(\bar{\rho}[a, b])\tau_j^p \|u^{(p+1)}\|. \tag{28}$$

Proof. The error bounds for Gauss-Lobatto collocation are presented in Theorem 2 in [16] which states that $\dot{u}_j - \dot{u}$ and $u_j - u$ are bounded by a multiple of the error of the best polynomial approximation to $\dot{u}$ with respect to the norm $\|\cdot\|_\infty$. A careful inspection of the proof shows that for sufficiently small τ_j only the condition number $\bar{\rho}[a,b]$ of the problem and the stability constant of the interpolation formula determine the corresponding constant $C(\bar{\rho})$. In particular, $C(\bar{\rho})$ is independent of $\|u^{(p+1)}\|$, τ_j, and g. The error bounds (27) and (28) are now a consequence of Jackson's Theorem (see e.g. [15]) on the best uniform approximation of smooth functions by polynomials.

For Gauss collocation this result can be obtained by careful analysis of the proof of Theorem 3.1 in [6]. This theorem states in (d) that for a fixed $u \in C^{p+1}$ the errors $\dot{u_j} - \dot{u}$ and $u_j - u$ are bounded by $C\tau_j^p$, which is not sufficient for our purpose, as C is not specified accurately enough. However, Theorem 3.1 is proven via the abstract Lemma 3.1 in [6], which again relates the collocation error to the best polynomial approximation to $\dot{u}$ (cf. part (d) of the conclusion). The corresponding constant is specified at the end of the proof of this lemma and obviously does not depend on $\|u^{(p+1)}\|$, τ_j, and g by the assumptions of the lemma, verified in the proof of Theorem 3.1. Now Jackson's Theorem again yields (27) and (28). $\square$

Lemma 3.1 provides us with a whole spectrum of error estimates. In classical convergence considerations, the strongest possible regularity assumption $p = s$ is chosen to obtain the highest possible order of convergence for a fixed, smooth solution u. A refined analysis based on these results yields even higher orders of uniform convergence $u_j \to u$ together with superconvergence at the coarse grid points.

Here, without restricting the Newton iterates a priori to some smoother subset W^* as has been done in [2, 9], we need to establish upper bounds for the approximation errors uniformly for all right hand sides in a bounded set in $W^{1,\infty}$ the low regularity of which impedes higher order approximation results. Therefore we will use the weakest possible regularity assumption $p = 1$ in the following and obtain estimates of order $O(\tau)$ for δ_j and σ_j.

Theorem 3.2. *Assume there is a bounded set $D \subset W^{1,\infty}$ and a twice continously differentiable function f, such that the linear boundary value problem*

$$\begin{aligned} \dot{u}(t) - f'(x(t))u(t) &= g(t) \\ Au(a) + Bu(b) &= 0 \end{aligned}$$

is uniquely solvable and uniformly well conditioned in $x \in D$. Then the following holds:

I. *There is a constant $M_1 < \infty$ such that for Gauss and Gauss-Lobatto collocation* (23) *holds with*
$$\delta_j = M_1 \tau_j$$
for all $x_j \in D \cap X_j$.

II. *If f'' is also Lipschitz continuous and* (2) *holds for $x_j, y_j, y_j + v_j \in D \cap X_j$, there is an $M_2 < \infty$ such that* (24) *holds with*
$$\sigma_j = M_2 \tau_j.$$

As will be made clear in the proof, these estimates cannot be improved substantially in a straightforward way.

Proof of Theorem 3.2. In the following argumentation the notation f, f', f'' will be used both for the functions and the corresponding superposition operators. In [17] Section 2.4 it is shown that this identification is allowed in the context of our norm $\|\cdot\|$, as boundedness and Lipschitz continuity are inherited from the function to the corresponding superposition operator.

First we derive (14) for δ_j. Let Δx satisfy $F'(x_j)\Delta x = -F(x_j)$. Then $w := x_j + \Delta x$ satisfies

$$\dot{w} - f'(x_j)w = -f'(x_j)x_j + f(x_j). \tag{29}$$

The right hand side is uniformly bounded in $x_j \in D$ due to the uniform boundedness of D and the continuity of f and f'. Consequently $\|w\|_{W^{1,\infty}}$ is uniformly bounded in $x_j \in D$, since the condition number of the BVP is bounded.

For the approximation error for the Newton correction we obtain

$$\|\Delta x - \Delta x_j\|_{W^{1,\infty}} = \|(x_j + \Delta x) - (x_j + \Delta x_j)\|_{W^{1,\infty}} = \|w - w_j\|_{W^{1,\infty}},$$

with w_j as the approximate solution of (29) obtained by collocation. To estimate $\|w - w_j\|_{W^{1,\infty}}$ by application of Lemma 3.1 for $p = 1$ we calculate

$$\begin{aligned}
\|\ddot{w}\| &= \left\| \tfrac{d}{dt}\left(f'(x_j)w - f'(x_j)x_j + f(x_j)\right) \right\| \\
&= \left\| \tfrac{d}{dt}\left(f'(x_j)\Delta x + f(x_j)\right) \right\| \\
&= \|f''(x_j)[\dot{x}_j, \Delta x] + f'(x_j)\Delta\dot{x} + f'(x_j)\dot{x}_j\| \\
&\le \|f''(x_j)\|\,\|\dot{x}_j\|\,\|\Delta x\| + \|f'(x_j)\|\,\|\dot{w}\|,
\end{aligned}$$

which is uniformly bounded in $W^{1,\infty}$ by a constant $C(D)$, hence

$$\delta_j = \|\Delta x - \Delta x_j\|_{W^{1,\infty}} \le C(\bar{\rho})\tau_j\|\ddot{w}\| \le C(\bar{\rho})C(D)\tau_j.$$

In the second step we derive (21) for σ_j. Let now w be defined as the exact solution of

$$\dot{w} - f'(x_j)w = \left(f'(y_j) - f'(y_j + v_j)\right)v_j$$

and w_j its approximation. Then we compute:

$$\begin{aligned}
\|\ddot{w}\| &= \left\| \tfrac{d}{dt}\big(\left(f'(y_j) - f'(y_j + v_j)\right)v_j + f'(x_j)w\big) \right\| \\
&\le \|\left(f'(y_j) - f'(y_j + v_j)\right)\dot{v}_j + f''(y_j)[\dot{y}_j, v_j] - f''(y_j + v_j)[\dot{y}_j + \dot{v}_j, v_j]\| \\
&\quad + \|f'(x_j)\dot{w} + f''(x_j)[\dot{x}_j, w]\| \\
&\le \|(f''(y_j) - f''(y_j + v_j))\dot{y}_j\|\,\|v_j\| + \|f''(y_j + v_j)\dot{v}_j\|\,\|v_j\| \\
&\quad + \|f'(y_j) - f'(y_j + v_j)\|\,\|\dot{v}_j\| + \|f'(x_j)\|\,\|w\|_{W^{1,\infty}} + \|f''(x_j)\dot{x}_j\|\,\|w\| \\
&\le (L_{f'} + L_{f''}\|\dot{y}_j\| + \|f''(y_j + v_j)\|)\|v_j\|^2_{W^{1,\infty}} + \|f''(x_j)\|\,\|\dot{x}_j\|)\|w\|_{W^{1,\infty}} \\
&\le \big(C_1 + \omega C_2\big)\|v_j\|^2_{W^{1,\infty}}.
\end{aligned}$$

In the last step we used (2): $\|w\|_{W^{1,\infty}} \le \omega\|v_j\|^2_{W^{1,\infty}}$. With the same argumentation as above Lemma 3.1 now yields (21) with $\sigma_j \le M_2\tau_j$.

Once Theorem 3.2 has been proved, we discuss briefly, why the estimates for δ_j and σ_j cannot be improved by application of Lemma 3.1 for $p > 1$. For this purpose, we would have to estimate $\|w^{(p+1)}\|$ (for both cases), which is possible by computations similar to the ones performed above with stronger assumptions on the smoothness of the right hand side. However, these estimates contain higher piecewise derivatives of elements of $D \subset X_j$. These higher derivatives can only be bounded by using inverse inequalities, which read

$$\|x_j^{(k)}\| \leq C(\min_{1\leq i\leq n_j} \tau_{j,i})^{-(k-1)}\|\dot{x_j}\|, \quad k = 1, \ldots, p.$$

Due to these inverse inequalities we would lose $p-1$ powers of τ and end up with $O(\tau)$ again. Moreover, this would force us to impose a quasi-uniformity assumption on the sequence of meshes. $\square$

FEM for semilinear elliptic PDEs. Assume $f : \mathbb{R} \to \mathbb{R}$ is locally Lipschitz continuously differentiable with

$$|f'(x) - f'(y)| \leq L(1 + \max(|x|, |y|))|x - y|.$$

This leads to the growth condition $f = \mathcal{O}(|x|^3)$, which in turn implies that the nonlinear superposition operator $\mathbf{f}$ generated by f maps $H_0^1(\Omega)$ continuously into $L_2(\Omega)$ on some convex polygonal domain $\Omega \subset \mathbb{R}^d$, $d \leq 3$, via the embedding $H_0^1(\Omega) \hookrightarrow L_6(\Omega)$ (cf. [3, 12]). We define the continuous problem F as the boundary value problem

$$F(x) = -\operatorname{div}(\kappa\nabla x) + \mathbf{f}(x) = 0, \quad x \in H_0^1(\Omega).$$

The discretizations F_j are provided by finite element approximations on shape-regular triangulations $\mathcal{T}_j$ with mesh size $\tau_j = \max_{T\in\mathcal{T}_j} \operatorname{diam} T$. We consider piecewise linear finite element spaces $X_j \subset H_0^1(\Omega)$ on the triangulations $\mathcal{T}_j$.

Theorem 3.3. *Assume there is some bounded set $D \subset H_0^1(\Omega)$ such that $F'(x)$ is uniformly elliptic for all $x \in D$. Then there exist constants $M_1, M_2 < \infty$ depending only on D and the problem setting $P = (\Omega, \kappa, f)$, such that the Newton-FEM discretizations F_j satisfy the Newton approximation condition* (23) *with*

$$\delta_j = M_1\tau_j$$

and the Lipschitz approximation condition (24) *with*

$$\sigma_j = M_2\tau_j$$

uniformly for all $x_j \in D \cap X_j$.

Proof. To begin with, we prove the approximation condition (23). Let Δx satisfy $F'(x_j)\Delta x = -F(x_j)$ and let Δx_j be its FEM approximation. Returning to equation (16) we notice that $x^{k+1,k}$ is more regular than $\Delta x^{k,k}$. Thus we introduce $w = x_j + \Delta x$, which satisfies

$$-\operatorname{div}(\kappa\nabla w) - f'(x_j)w = f(x_j) - f'(x_j)x_j \in L_2(\Omega)$$

and is therefore H^2-regular (cf. [12]). Consequently,

$$\|w_j - w\|_{H^1} \leq c\tau_j\|w\|_{H^2} \leq c\tau_j\|f(x_j) - f'(x_j)x_j\|_{L_2}$$

holds for its FEM approximation $w_j = x_j + \Delta x_j$ (cf. [4]). For the approximation error $\Delta x_j - \Delta x$ we now obtain

$$\begin{aligned}\|\Delta x_j - \Delta x\|_{H^1} &= \|(w_j - x_j) - \Delta x\|_{H^1}\\ &= c\|w_j - w\|_{H^1}\\ &\leq c\tau_j\|f(x_j) - f'(x_j)x_j\|_{L_2}.\end{aligned} \tag{30}$$

Exploiting the continuous imbedding $H^1(\Omega) \hookrightarrow L_6(\Omega)$ (cf. [12]) we estimate

$$\begin{aligned}
\|f(x_j) - f'(x_j)x_j\|_{L_2} &= \Big\| \int_{t=0}^{1} (f'(tx_j) - f'(x_j))x_j \, dt \Big\|_{L_2} \\
&\le \int_{t=0}^{1} L(1-t)\|(1+|x_j|)x_j^2\|_{L_2} \, dt \\
&\le \frac{L}{2}(\|x_j^2\|_{L_2} + \|x_j^3\|_{L_2}) \\
&= \frac{L}{2}(\|x_j\|_{L_4}^2 + \|x_j\|_{L_6}^3) \\
&\le Lc(\|x_j\|_{H^1}^2 + \|x_j\|_{H^1}^3) \\
&\le c
\end{aligned}$$

which, together with (30), confirms (14).

In the second step, we prove the Lipschitz approximation result (24). Define w now by

$$F'(x_j)w = (F'(y_j + v_j) - F'(y_j))v_j = (f'(y_j + v_j) - f'(y_j))v_j \in L_2(\Omega).$$

Again, w is H^2-regular, such that we obtain

$$\|w_j - w\|_{H^1} \le c\tau_j \|(f'(y_j + v_j) - f'(y_j))v_j\|_{L_2}.$$

Upon using Hölder's inequality we conclude

$$\begin{aligned}
\|(f'(y_j + v_j) - f'(y_j))v_j\|_{L_2} &\le L\|(1 + \max(|y_j|, |y_j + v_j|)^2 v_j^4\|_{L_1}^{1/2} \\
&\le L\|(1 + \max(|y_j|, |y_j + v_j|))^2\|_{L_3}^{1/2} \|v_j^4\|_{L_{3/2}}^{1/2} \\
&= L\|1 + \max(|y_j|, |y_j + v_j|)\|_{L_6} \|v_j\|_{L_6}^2 \\
&= Lc\|v_j\|_{H^1}^2,
\end{aligned}$$

which proves (21). □

Combining Theorem 2.2 and Lemma 2.4 with Theorem 3.3 we obtain asymptotic mesh independence for FEM approximations of semilinear elliptic equations.

FEM for strongly nonlinear elliptic PDEs. For strongly nonlinear PDEs with a second order differential operator depending on the solution, the analytic treatment of the approximation conditions (23) and (24) is considerably more difficult. The global regularity of the right hand side is, in general, only H^{-1}, which results in sharp edges in the Newton correction. These bucklings, however, coincide geometrically with the edges of the triangulation, such that the finite element approximation quality does not deteriorate. This is indeed observed in actual computation.

The regularity theory necessary for addressing such problems is beyond the scope of the present paper. As a substitute, we give a numerical example from [11], where the phenomenon of asymptotic mesh independence may be studied.

Example: Parametric minimal surface. Consider the variational problem

$$\min \int_\Omega \sqrt{1+|\nabla u|^2}\, dx$$

subject to the boundary conditions

$$\begin{aligned} u &= \cos(x)\cos(y) && \text{on } \Gamma_D = \partial\Omega\backslash\Gamma_N, \\ \frac{\partial u}{\partial n} &= 0 && \text{on } \Gamma_N \end{aligned}$$

on $\Omega = [-\pi/2, 0]^2$. The functional gives rise to the first and second order expressions

$$\begin{aligned} \langle F(u), v\rangle &= \int_\Omega \left(1+|\nabla u|^2\right)^{-1/2} \nabla u^T \nabla v\, dx, \\ \langle F'(u)v, w\rangle &= \int_\Omega \Big(- \left(1+|\nabla u|^2\right)^{-3/2} \nabla w^T (\nabla u \nabla u^T) \nabla v \\ &\qquad + \left(1+|\nabla u|^2\right)^{-1/2} \nabla w^T \nabla v \Big)\, dx. \end{aligned}$$

We define two different problem settings by choosing

(a) $\Gamma_N = [-\pi/2, 0] \times \{0\}$,

(b) $\Gamma_N = [-\pi/2, 0] \times \{0\} \cup \{0\} \times [-\pi/4, 0]$.

Note that by symmetry, problem (a) represents a Dirichlet problem on a convex domain, whereas the deliberate choice of boundary conditions (b) leads to a Dirichlet problem on a highly nonconvex slit domain, on which no physically meaningful solution exists.

The adaptive Newton-multilevel code Newton-KASKADE [10, 11] has been run on both problems, providing affine invariant computational estimates $[\omega_j] \le \omega_j$ on each mesh refinement level j. On each level, a few Newton steps have been computed using the approximation from the level before, and the maximum estimate encountered in these steps has been selected as $[\omega_j]$. As can be seen from Table 1, the Lipschitz constants for the well-defined problem (a) remain bounded and rather independent of the refinement level, apart from some fluctuation due to the finite sampling of ω_j. In contrast to that, the estimates for the Lipschitz constant of problem (b) are dramatically increasing by five orders of magnitude. This indicates that the problem has finite dimensional solutions on each of the successive meshes, each unique within the corresponding finite dimensional Kantorovich ball with radius $\rho_j \sim 1/\omega_j$; however, these balls shrink from radius $\rho_0 \approx 1$ to $\rho_{12} \approx 10^{-5}$. Frank extrapolation of this effect insinuates the conjecture that there exists no continuous unique solution of the underlying minimization problem.

	problem (a)		problem (b)	
j	♯nodes	$[\omega_j]$	♯nodes	$[\omega_j]$
0	4	1.32	5	7.5
1	7	1.17	10	4.2
2	18	4.55	17	7.3
3	50	6.11	26	9.6
4	123	5.25	51	22.5
5	158	20.19	87	50.3
6	278	19.97	105	1486.2
7	356	9.69	139	2715.6
8	487	8.47	196	5178.6
9	632	11.73	241	6837.2
10	787	44.21	421	12040.2
11	981	49.24	523	167636.0
12	1239	20.10	635	1405910.0
13	1610	32.93		
14	2054	37.22		

Table 1: Estimated Lipschitz constants $[\omega_j]$ on different refinement levels j.

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