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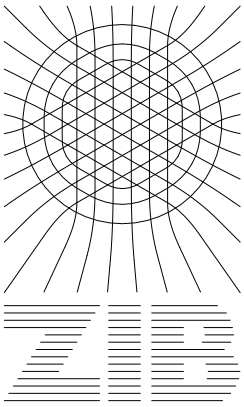

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Global Inexact Newton Multilevel FEM for Nonlinear Elliptic Problems

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Abstract

The paper deals with the multilevel solution of *elliptic* partial differential equations (PDEs) in a *finite element* setting: *uniform ellipticity* of the PDE then goes with *strict monotonicity* of the derivative of a nonlinear convex functional. A *Newton multigrid method* is advocated, wherein *linear residuals* are evaluated within the multigrid method for the computation of the Newton corrections. The globalization is performed by some *damping* of the ordinary Newton corrections. The convergence results and the algorithm may be regarded as an extension of those for *local* Newton methods presented recently by the authors. An *affine conjugate* global convergence theory is given, which covers both the *exact* Newton method (neglecting the occurrence of approximation errors) and *inexact* Newton–Galerkin methods addressing the crucial issue of accuracy matching between discretization and iteration errors. The obtained theoretical results are directly applied for the construction of adaptive algorithms. Finally, illustrative numerical experiments with a NEWTON–KASKADE code are documented.

Key words. nonlinear PDEs, elliptic PDEs, multilevel methods, multigrid methods, inexact Newton methods, large scale convex optimization, finite element methods

AMS subject classification. 35J20, 35J60, 49M15, 65N30, 65N55

1 Introduction

The present paper deals with the multilevel solution of *elliptic* partial differential equations (PDEs), which come up in a variety of scientific and engineering applications such as continuum mechanics. In a *finite element* setting (see e.g. the recent textbook of BRAESS [4]), such problems arise as *convex* minimization problems: *uniform ellipticity* of the PDE then goes with *strict monotonicity* of the derivative of the nonlinear functional. As for the numerical solution by multilevel methods, there are two basic algorithmic lines (cf. the textbooks [9, 11]): a) the *nonlinear multigrid method* or the *full approximation scheme* (FAS) , wherein *nonlinear residuals* are evaluated within multigrid cycles, and b) the *Newton multigrid method*, wherein *linear residuals* are evaluated within the multigrid method for the computation of the Newton corrections. The present paper follows the second line. It may be regarded as an extension of convergence results and algorithms presented recently by the authors in [8] for *local* Newton methods. The globalization herein is performed by some *damping* of the ordinary Newton corrections — in the spirit of earlier suggestions by BANK AND ROSE [1] or by HACKBUSCH AND REUSKEN [10], but rather different both in the presented theoretical results and in the suggested algorithms.

In Section 2 below, an *affine conjugate* global convergence theory of the Newton method with damping is given — based on the observation that affine conjugacy is a natural requirement for optimization problems in general. The analysis covers both the *exact* Newton method, which neglects the occurrence of approximation errors, and *inexact* Newton–Galerkin methods, which include the crucial issue of *accuracy matching* between inner and outer iteration. In Section 3, the obtained theoretical results are transferred into adaptive algorithms, essentially by means of replacing certain theoretical Kantorovitch quantities by computationally available estimates – following ideas presented in a different context in [6]. In this way, an adaptive damping strategy can be derived. Moreover, an accuracy matching strategy for inner versus outer iteration is suggested on the basis of a simplified computational complexity model. Finally, in Section 4, the obtained theoretical results and algorithm suggestions are illustrated by numerical experiments with a NEWTON–KASKADE code.

2 Affine Conjugate Global Convergence Results

Consider the *minimization problem*

$$f(x) = \min ,$$

wherein $f : D \subset X \to \mathbb{R}$ is assumed to be a *strictly convex* C^2- functional defined on an open convex set D. In order to assert the *existence* of a minimum point $x^* \in D$, we assume that the Banach space X is *reflexive* and that for some $x^0 \in D$, $x^0 \neq x^*$, the level set $\mathcal{L}_0 := \{x \in D \,|\, f(x) \leq f(x^0)\}$ is closed and bounded. *Uniqueness* of the minimum point x^* follows from the strict convexity of f and the convexity of D.

The nonlinear minimization problem is equiavalent to the nonlinear operator equation

$$F(x) := f'(x) = 0 \,, \quad x \in D \,. \tag{2.1}$$

In order to guarantee the feasibility of Newton's method, we further assume that (2.1) is a strictly elliptic problem, i.e. the symmetric Frechét–derivative $F'(x) = f''(x)$ is strictly positive.

Let X be endowed with a norm $\|\cdot\|$. In addition, we will also be interested in *local energy products* defined for each $x \in D$ to be symmetric bilinear forms of the kind $\langle \cdot \,, F'(x) \cdot \rangle$,

that also induce *local energy norms* of the kind $\langle \cdot\,,\, F'(x)\cdot\rangle^{1/2}$. Motivated by the notation in Hilbert spaces, where we can actually define the operator $F'(x)^{1/2}$, we also introduce here the shorthand notation $\|F'(x)^{1/2}\cdot\| \equiv \langle\cdot,\, F'(x)\cdot\rangle^{1/2}$ in connection with the local norm only.

Following [8], we want to carefully observe the associated *affine conjugacy* property, which means that we *simultaneously* treat the whole class of transformed convex minimization problems

$$g(y) = f(By) = \min\,,\quad x = By\,,$$

wherein B is understood to be an arbitrary *bounded linear bijective operator*. By transformation, we arrive at the gradient mappings

$$G(y) = B^*F(By) = 0\,,$$

and the Fréchet–derivatives

$$G'(y) = B^*F'(x)B\,,\quad x = By\,.$$

By construction, all $G'(\cdot)$ are selfadjoint strictly positive operators. The associated linear system for the full ordinary Newton correction reads

$$G'(y^k)\Delta y^k = -G(y^k) \quad\Longleftrightarrow\quad B^*F'(x^k)B\Delta y^k = -B^*F(x^k)\,,$$

which implies that $\Delta x^k = B\Delta y^k$. It is therefore only natural to require affine conjugacy also for any damped Newton iteration both in the theoretical convergence analysis and in the algorithmic realization. As a strict consequence of such a requirement, any convergence theorems should only use affine conjugate theoretical quantities like iterative *functional values* $f(x^k)$ or *local energy products* of iterative *corrections* Δx^k.

As for a globalization of the ordinary Newton method, we may either use continuation methods (cf. [6]) or some damping strategy, which is the option taken here. It is well–known that the geometrical concept behind any damping of Newton's method is the so–called *Newton path*. Under the assumptions of the implicit function theorem, the associated Newton path $\overline{x}(\lambda)$ for $0 \le \lambda \le 1$ connects the starting point $\overline{x}(0) = x^k$ with the solution point $\overline{x}(1) = x^*$. It is characterized in the image space of the mapping F by the homotopy

$$F\big(\overline{x}(\lambda)\big) = (1-\lambda)F(x^k) \tag{2.2}$$

and in the domain space of F by the initial value problem for the implicit differential equation

$$\frac{d\overline{x}}{d\lambda} = -F'(\overline{x})^{-1}F(x^k)\,,\qquad \overline{x}(0) = x^k\,. \tag{2.3}$$

From this, we observe that the Newton correction is just the local tangent of the Newton path in x^k, since

$$\left.\frac{d\overline{x}}{d\lambda}\right|_{\lambda=0} = -F'(x^k)^{-1}F(x^k) \equiv \Delta x^k, \tag{2.4}$$

which motivates the name. Moreover, on the basis of (2.2), any *level function* of the special form

$$T(x|B) := \tfrac{1}{2}\|B^*F(x)\|^2$$

will show a *monotonic decrease along the Newton path* according to

$$T\big(\overline{x}(\lambda)|B\big) = (1-\lambda)^2 T(x^k|B). \tag{2.5}$$

It is, however, not at all clear a–priori, whether our problem dependent nonlinear functional f also decreases monotonically. For this reason, we first study the behavior of f along the Newton path $\overline{x}(\lambda)$ as a function of λ.

Lemma 2.1 *Let $f \in C^2(D)$ denote some strictly convex functional to be minimized over some convex domain $D \in X$. Let $F'(x) = f''(x)$ be symmetric strictly positive in D and let $\overline{x} : [0,1] \to D$ denote the Newton path starting at some iterate $\overline{x}(0) = x^k$ and ending at the solution point $\overline{x}(1) = x^*$ with $F(x^*) = 0$. Then $f(\overline{x}(\lambda))$ is a strictly monotone decreasing function of λ.*

Proof. By means of the abstract mean value theorem in Banach space we may verify that

$$f(\overline{x}(\lambda)) - f(x^k) = \int_{\sigma=0}^{\lambda} \langle F(\overline{x}(\sigma)), \dot{\overline{x}}(\sigma) \rangle \, d\sigma.$$

Insertion of (2.2) and (2.3) then leads to

$$f(\overline{x}(\lambda)) - f(x^k) = -\int_{\sigma=0}^{\lambda} (1-\sigma) \|F'(\overline{x}(\sigma))^{-1/2} F(x^k)\|^2 \, d\sigma,$$

with a strictly positive definite integrand. Therefore, for $0 \le \lambda_2 < \lambda_1 \le 1$:

$$f(\overline{x}(\lambda_1)) - f(\overline{x}(\lambda_2)) = -\int_{\sigma=\lambda_2}^{\lambda_1} (1-\sigma) \|F'(\overline{x}(\sigma))^{-1/2} F(x^k)\|^2 \, d\sigma < 0 \, .$$

■

Obviously, this result is the desired generalization of the monotone level function decrease (2.5). On this firm geometrical basis we are now ready to consider the *exact Newton iteration with damping* ($k = 0, 1, ...$)

$$F'(x^k)\Delta x^k = -F(x^k), \qquad x^{k+1} = x^k + \lambda_k \Delta x^k, \qquad \lambda_k \in]0,1] \tag{2.6}$$

under the tentative requirement of iterative *functional decrease*

$$f(x^{k+1}) < f(x^k)$$

As a first step, we study the local behavior of the functional f along the Newton direction Δx^k starting at x^k as a function of λ.

Theorem 2.2 *Let $f : D \to \mathbb{R}^1$ be a strictly convex C^2–functional to be minimized over some open convex domain $D \subset X$. Let $F(x) = f'(x)$ with $F'(x) = f''(x)$ symmetric strictly positive. Assume the special affine conjugate Lipschitz condition*

$$\|F'(x)^{-1/2}(F'(y) - F'(x))(y-x)\| \le \omega \|F'(x)^{1/2}(y-x)\|^2 \quad \text{for} \quad x, y \in D \tag{2.7}$$

with $0 \le \omega < \infty$. For some iterate $x^k \in D$, define the quantities

$$\epsilon_k := \|F'(x^k)^{1/2} \Delta x^k\|^2 \, , \quad h_k := \omega \|F'(x^k)^{1/2} \Delta x^k\| \, .$$

Moreover, let $x^k + \lambda \Delta x^k \in D$ for $0 \le \lambda \le \lambda^k_{\max}$ with

$$\lambda^k_{\max} := \frac{4}{1 + \sqrt{1 + 8h_k/3}} \le 2 \, .$$

Then

$$f(x^k + \lambda \Delta x^k) \le f(x^k) - t_k(\lambda)\epsilon_k \tag{2.8}$$

where

$$t_k(\lambda) = \lambda - \frac{\lambda^2}{2} - \frac{\lambda^3}{6} h_k \; . \tag{2.9}$$

The optimal choice of damping factor is

$$\overline{\lambda}_k = \frac{2}{1 + \sqrt{1 + 2h_k}} \leq 1 \; . \tag{2.10}$$

Proof. Dropping the iteration index k, we apply the mean value theorem to obtain

$$\begin{aligned} f(x + \lambda \Delta x) - f(x) &= -\lambda \epsilon + \frac{\lambda^2}{2} \epsilon \\ &+ \lambda^2 \int_{s=0}^{1} \int_{t=0}^{1} s \left\langle \Delta x, \left(F'(x + st\lambda \Delta x) - F'(x) \right) \Delta x \right\rangle dt ds \; . \end{aligned}$$

Upon recalling the Lipschitz condition (2.7), the Cauchy–Schwarz inequality yields

$$\begin{aligned} &f(x + \lambda \Delta x) - f(x) + \left(\lambda - \frac{\lambda^2}{2} \right) \epsilon \\ &\quad \leq \omega \lambda^3 \int_{s=0}^{1} \int_{t=0}^{1} s^2 t \| F'(x)^{1/2} \Delta x \|^3 dt ds = \frac{\lambda^3}{6} h \cdot \epsilon \; , \end{aligned} \tag{2.11}$$

which confirms (2.8) and the cubic parabola (2.9). Maximization of t_k by solving the quadratic equation $t_k' = 0$ yields $\overline{\lambda}_k$ as in (2.10). Moreover, by observing that

$$t_k = \lambda \left(1 - \frac{\lambda}{2} - \frac{\lambda^2}{6} h_k \right) = 0$$

has only one *positive* root $\lambda_{\max}^k$, the remaining statements are readily verified. ∎

From this theorem for the exact Newton iteration, we may directly proceed to obtain the comparable results for the *inexact Newton iteration with damping* ($k = 0, 1, ...$)

$$F'(x^k) \delta x^k = -F(x^k) + r^k, \qquad x^{k+1} = x^k + \lambda_k \delta x^k, \qquad \lambda_k \in]0, 1]. \tag{2.12}$$

The inner iteration, which is formally represented by the introduction of the inner residual r^k, will be further specified to satisfy a *Galerkin condition* of the kind

$$\langle \delta x^k, F'(x^k)(\delta x^k - \Delta x^k) \rangle = \langle \delta x^k, r^k \rangle = 0 \tag{2.13}$$

and to have a relative error denoted by

$$\delta_k := \frac{\| F'(x^k)^{1/2} (\Delta x^k - \delta x^k) \|}{\| F'(x^k)^{1/2} \delta x^k \|} \; .$$

For this specification, we immediately verify the following corollary:

Corollary 2.3 *The statements of Theorem 2.2 hold for inexact Newton – Galerkin methods as well, if only the exact Newton corrections Δx^k are replaced by the inexact Newton corrections δx^k and ϵ_k, h_k are replaced by*

$$\epsilon_k^\delta := \| F'(x^k)^{1/2} \delta x^k \|^2 = \frac{\epsilon_k}{1 + \delta_k^2} \; , h_k^\delta := \omega \| F'(x^k)^{1/2} \delta x^k \| = \frac{h_k}{\sqrt{1 + \delta_k^2}} \; . \tag{2.14}$$

Proof. Dropping the iteration index k, the first line of the proof of Theorem 2.2 may be rewritten as

$$f(x+\lambda\delta x) - f(x) = -\lambda\epsilon^\delta + \frac{\lambda^2}{2}\epsilon^\delta$$

$$+\lambda^2 \int_{s=0}^{1}\int_{t=0}^{1} s\left\langle \delta x, \big(F'(x+st\lambda\delta x) - F'(x)\big)\delta x\right\rangle dtds + \langle \delta x, r\rangle \ ,$$

wherein the last right hand term vanishes due to the Galerkin condition (2.13) so that merely the replacement of Δx by δx needs to be performed. ■

With these local results established, we are now ready to formulate the associated global convergence theorem.

Theorem 2.4 *General assumptions as Theorem 2.2 or Corollary 2.3, respectively (in the latter case δ_k bounded). Let the level set $\mathcal{L}_0 := \{x \in D \mid f(x) \le f(x^0)\}$ be closed and bounded. Let $F'(x) = f''(x)$ be symmetric uniformly positive for all $x \in \mathcal{L}_0$. Then the damped (inexact) Newton iteration (for $k = 0, 1, \ldots$) with damping factors in the range*

$$\lambda_k \in [\varepsilon \ , \ \ \min(1, \lambda^k_{\max} - \varepsilon)]$$

and sufficiently small $\varepsilon > 0$ depending on $\mathcal{L}_0$ converges to the solution point x^*.

Proof. The proof just applies the local reduction results of the preceding Theorem 2.2 or Corollary 2.3. The essential remaining task to show is that there is a common minimal reduction factor for all possible arguments $x^k \in \mathcal{L}_0$. For this purpose, we simply construct a polygonal upper bound for $t_k(\lambda)$ such that (omitting technical details)

$$f(x^k + \lambda\Delta x^k) \le f(x^k) - \frac{\varepsilon\epsilon_k}{2}$$

for λ in the above indicated range and all possible iterates x^k with some

$$\varepsilon < \min(\overline{\lambda}_k, \lambda^k_{\max} - \overline{\lambda}_k) \ .$$

This implies a strict reduction of the functional in each iterative step as long as $\epsilon_k > 0$ and therefore global convergence in the compact level set $\mathcal{L}_0$ towards the minimum point x^* with $\epsilon_* = 0$. ■

Remark 1. It may be worth noting that the above analysis is nicely connected with the analysis for the *local* Newton methods ($\lambda = 1$) as discussed in [8]. If we require that

$$\lambda^k_{\max} = \frac{4}{1 + \sqrt{1 + 8h_k/3}} \ge 1,$$

then we arrive at the local contraction condition

$$h_k \le 3.$$

This is exactly the condition that would have been obtained in the proof of Theorem 2.1 or 3.1 in [8], if the requirement $f(x^{k+1}) \le f(x^k)$ had been made. However, the condition $h_{k+1} \le h_k$ cannot be guaranteed, so that $\lambda^{k+1}_{\max} \ge 1$ is not assured. In order to assure such a condition, the more stringent assumption $h_k \le 2$ is required as in [8].

Remark 2. Similar results can be obtained without assuming a Galerkin condition like (2.13). In particular we get

$$t_k(\lambda) = (1-\delta_k)\lambda - \frac{\lambda^2}{2} - \frac{\lambda^3}{6}h_k^\delta \ ,$$

such that $\delta_k < 1$ is required to assert functional decrease, which is optimal for

$$\overline{\lambda}_k = \frac{2(1-\delta_k)}{1+\sqrt{1+2(1-\delta_k)h_k^\delta}} \le 1 \ .$$

The global convergence theorem would be the proper analog of Theorem 2.4.

Summarizing, we have thus established the *theoretical optimal damping strategy* (2.10) in terms of the computationally unavailable Kantorovitch quantities h_k for the exact Newton method or h_k^δ for the inexact Newton–Galerkin methods.

3 Adaptive Newton–Galerkin Algorithms

In this section, we want to use the above theoretical results for the construction of Newton–Galerkin algorithms. Examples of inner iterations that satisfy the Galerkin condition (2.13) are:

- for $X = \mathbb{R}^n$ any *preconditioned conjugate gradient* (PCG) method,
- for $X = W^{1,p}$, $1 < p < \infty$ any *finite element* method (FEM).

Adaptivity issues to be treated are the number of inner PCG iterations in the Newton – PCG method or the iterative meshes to be generated within a Newton – FEM. In both cases, an adaptive damping strategy needs to be worked out.

3.1 Adaptive damping strategy

We first want to construct a *computational* damping strategy on the basis of the *theoretically optimal* damping strategy as derived in the preceding Section 2. In order to construct such a strategy, we will apply a recipe that has been suggested in [6] in a different context: we replace the computationally unavailable (affine conjugate) Kantorovitch quantities h_k by certain (also affine conjugate) computational *local* estimates $[h_k] \le h_k$ and the damping factors $\overline{\lambda}_k$ due to (2.10) by the computational estimates

$$[\overline{\lambda}_k] := \frac{2}{1+\sqrt{1+2[h_k]}} \le 1 \ . \tag{3.1}$$

Since $[h_k] \le h_k$, we have

$$[\overline{\lambda}_k] \ge \overline{\lambda}_k$$

so that both a *prediction strategy* and a *correction strategy* need to be worked out. The efficiency of such a strategy will depend on the required accuracy of the computational estimate, which is analyzed in the following lemma.

Lemma 3.1 *Standard assumptions and notation as just introduced. Let*

$$0 \le h_k - [h_k] \le \sigma[h_k] \quad \text{for some} \quad \sigma < 1 \ . \tag{3.2}$$

Then, for $\lambda = [\overline{\lambda}_k]$, the following functional decrease is guaranteed:

$$f(x^k + \lambda \Delta x^k) \le f(x^k) - \frac{\lambda}{6}(\lambda+2)\epsilon_k \ . \tag{3.3}$$

Proof. With $h_k \leq (1+\sigma)[h_k]$ and (2.11) we have

$$f(x^k + \lambda \Delta x^k) - f(x^k) \leq -t_k(\lambda)\epsilon_k = \left(-\lambda + \frac{\lambda^2}{2} + \frac{\lambda^3}{6} h_k\right) \epsilon_k$$
$$\leq \left(-\lambda + \frac{\lambda^2}{2} + \frac{\lambda^3}{6}(1+\sigma)[h_k]\right) \epsilon_k \, .$$

At this point, recall that $\overline{\lambda}_k$ is a root of $t_k' = 0$ so that $[\overline{\lambda}_k]$ is a root of

$$1 - \lambda - \frac{\lambda^2}{2}[h_k] = 0 \, .$$

Insertion of the above quadratic term into the estimate then yields

$$f(x + \lambda \Delta x) - f(x) \leq \left(-\lambda + \frac{\lambda^2}{2} + \frac{\lambda}{3}(1+\sigma)(1-\lambda)\right) \epsilon_k \, . \tag{3.4}$$

Upon using $\sigma < 1$, we arrive at the upper bound (3.3). ∎

The above *functional monotonicity test* (3.3) is suggested for use in actual computation. If we further impose $\sigma = \frac{1}{2}$ in (3.2), i.e. if we require at least one exact binary digit in the Kantorovitch quantity estimate, then (3.4) leads to the *restricted functional monotonicity test*

$$f(x^k + \lambda \Delta x^k) - f(x^k) \leq -\frac{\lambda}{2} \epsilon_k \, . \tag{3.5}$$

We are now ready to discuss specific computational estimates $[h_k]$. Some careful examination shows that we have three basic cheap ways of computational estimation.

From (2.11) we have the *third* order bound

$$E_3(\lambda) := f(x^k + \lambda \Delta x^k) - f(x^k) + \lambda \left(1 - \frac{\lambda}{2}\right) \epsilon_k \leq \frac{\lambda^3}{6} h_k \epsilon_k \, , \tag{3.6}$$

which, in turn, naturally inspires the computational estimate

$$[h_k] := \frac{6|E_3(\lambda)|}{\lambda^3 \epsilon_k} \leq h_k \, . \tag{3.7}$$

If $E_3(\lambda) < 0$, this means that the Newton method performs locally better than for the mere quadratic model of f (equivalent to $h_k = 0$). Therefore, we decide to set

$$[\overline{\lambda}_k] = 1 \, , \quad \text{if } E_3(\lambda) < 0 \, . \tag{3.8}$$

On the level of the gradient mapping we have the *second* order bound

$$E_2(\lambda) := \langle \Delta x^k \, , \, F(x^k + \lambda \Delta x^k) - (1-\lambda) F(x^k) \rangle \leq \tfrac{1}{2} \lambda^2 h_k \epsilon_k \tag{3.9}$$

which inspires the associated estimate

$$[h_k] := \frac{2|E_2(\lambda)|}{\lambda^2 \epsilon_k} \leq h_k \, . \tag{3.10}$$

On the Frechet derivative level we may derive the *first* order bound

$$E_1(\lambda) := \left\langle \Delta x^k \, , \, \left(F'(x^k + \lambda \Delta x^k) - F'(x^k)\right) \Delta x^k \right\rangle \leq \lambda h_k \epsilon_k \tag{3.11}$$

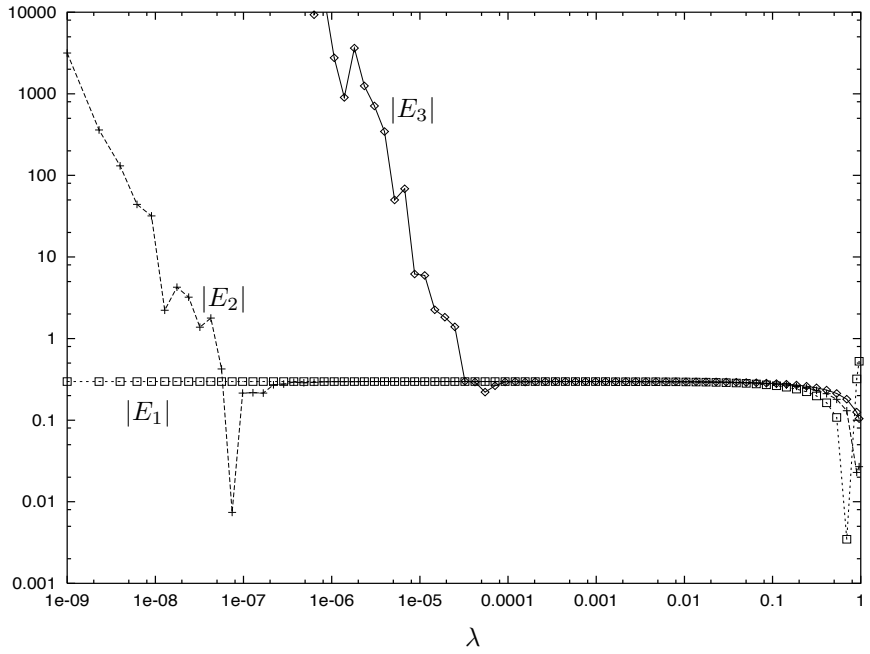


Figure 1: Cancellation of leading digits in estimators $[h_k]$ based on formulas for $|E_3|$, $|E_2|$, $|E_1|$, respectively.

which leads to the associated estimate

$$[h_k] := \frac{|E_1(\lambda)|}{\lambda \epsilon_k} \leq h_k \; . \tag{3.12}$$

Again, due to the Galerkin condition (2.13), we get the same results for inexact Newton-Galerkin methods, if we replace Δx^k by δx^k, ϵ_k by ϵ_k^δ, and h_k by h_k^δ. In actual computation the theoretical orthogonality condition (2.13) may be perturbed, e.g. by numerical quadrature errors in FEM or by rounding errors from scalar products in PCG. For this reason, the terms E_3 and E_2 must be evaluated in the special form

$$E_3(\lambda) := f(x^k + \lambda \delta x^k) - f(x^k) - \lambda \langle F(x^k), \delta x^k \rangle - \frac{\lambda^2}{2} \epsilon_k^\delta$$

and

$$E_2(\lambda) := \langle \delta x^k, F(x^k + \lambda \delta x^k) - F(x^k) \rangle - \lambda \epsilon_k^\delta$$

with the local energy computed as $\epsilon_k^\delta = \langle \delta x^k, F'(x^k) \delta x^k \rangle$. In this form, the *discrete* approximations are *differentiable with respect to* λ just as the associated continuous terms. In addition, cancellation of leading digits in the terms $E_i, i = 1, 2, 3$ should be carefully monitored — see Fig. 1, where a snapshot at some iterate in the illustrative example in Section 4 below is taken. The third order expression is the most sensitive one in this respect, but also preferable from the point of view of simplicity.

In principle, any of the above three estimates can be inserted into the expression (3.1) for $[\overline{\lambda}_k]$ requiring at least one trial value of λ (or, respectively, x^{k+1}). We have therefore only designed a possible *correction strategy*

$$\lambda_k^{i+1} := \frac{2}{1 + \sqrt{1 + 2[h_k](\lambda)}} \Big|_{\lambda = \lambda_k^i} \tag{3.13}$$

In order to construct a theoretically backed initial estimate λ_k^0, we may recall that $h_{k+1} = \Theta_k h_k$, where

$$\Theta_k := \frac{\|F'(x^{k+1})^{-1/2} F(x^{k+1})\|}{\|F'(x^k)^{-1/2} F(x^k)\|} \ .$$

Under the tacit assumption that any "local" Lipschitz constants do not change "too much" from one iterate to the next, this inspires the definition

$$[h_{k+1}]_0 := \Theta_k [h_k]_{i^*} \ ,$$

wherein i^* denotes the index of the last computed estimate within the previous iterative step k. For $k \geq 0$, we are thus led to the *prediction strategy*:

$$\lambda_{k+1}^0 := \frac{2}{1 + \sqrt{1 + 2[h_{k+1}]_0}} \leq 1 \ . \tag{3.14}$$

Still, the starting value λ_0^0 needs to be set ad hoc, taking into account the expected difficulty of the problem to be solved.

3.2 Accuracy matching

With computational estimates for h_k^δ at hand, we now want to develop a suitable accuracy matching between the outer iteration (characterized by h_k) and the inner iteration (characterized by δ_k). For h_k small, local strategies based on the contraction of correction energies have already been described in [8]. We therefore restrict out attention to the case of h_k large. For actual computation, we are interested in the first bit of the damping factors $[\overline{\lambda}_k^\delta]$ rather than in the accuracy of the quantities $[h_k^\delta]$, which come out of the inexact Newton iteration. In view of (2.10) and (2.14), we obtain for $h \gg 1$ the rough estimate

$$\overline{\lambda}_k^\delta \approx \sqrt{\frac{2}{h_k^\delta}} \ll 1$$

In order to catch the first binary digit in $\overline{\lambda}_k^\delta$ (see Lemma 3.1), we arrive at the requirement

$$\sqrt[4]{1 + \delta_k^2} \leq 1 + \tfrac{1}{2} \ ,$$

which is nearly equivalent to

$$\delta_k \leq 2 \ .$$

Within this mildly restricted range, we are free to use the overall *computational complexity* as the only criterion for choosing δ_k.

As a slight modification of the concept presented in [8], the *information gain* at iteration step k can be defined as

$$I_k := f(x^k) - f(x^{k+1}) = -t_k(\overline{\lambda_k})\epsilon_k^\delta \ ,$$

which is roughly estimated as

$$I_k \approx \frac{2}{3}\sqrt{\frac{2}{h_k^\delta}}\ \epsilon_k^\delta \sim (1 + \delta_k^2)^{-\frac{3}{4}} \ .$$

Following [8], we aim at maximizing the *information gain per unit work*

$$i_k = \frac{I_k}{A_k}$$

within each step k, wherein the *amount of work* A_k depends highly on the inner iteration. We examine two different cases (compare [8]):

Finite dimensional problems: Newton–PCG. Consider a nonlinear elliptic problem in *fixed* finite dimension N (possibly large). Such a problem may arise as a discretized nonlinear elliptic PDE, which has been treated by a grid generator before starting the solution process. For the inner iteration we assume that some *preconditioned conjugate gradient* (PCG) method has been selected without further specification of the preconditioner. At iteration step k, the computational work involved is

- evaluation of the Jacobian matrix $F'(x^k)$ and the right hand side $F(x^k)$, where the computational amount is typically independent of δ_k,
- some PCG iterations, where the computational amount of one iteration again is independent of δ_k, and the number of iterations can be estimated as $\log(1+\delta_k^{-2})$.

The total amount of work roughly scales as

$$A_k \sim \text{const} + \log(1+\delta_k^{-2}) \; .$$

From this, the information gain per unit work arises as

$$i_k \sim \big(\text{const} + \log(1+\delta_k^{-2})\big)^{-1} (1+\delta_k^2)^{3/4} \; .$$

Obviously, the optimal choice of δ_k depends on the involved constant, which, in turn, depends on the preconditioner used and the computational costs of evaluating $F'(x_k)$, $F(x^k)$, respectively, within the PCG iteration. In the absence of knowledge about the above constant, we suggest a fixed default value, say $\delta_k = 1$.

Infinite dimensional problems: adaptive Newton–FEM. Consider a nonlinear elliptic PDE problem in *finite element* formulation, which is a strictly convex minimization problem over some infinite dimensional space X. Recall that the above theory covers the case of X being a reflexive Banach space. For the inner iteration we assume an *adaptive* multilevel FEM such as KASKADE [7, 3, 2]. Let d denote the underlying spatial dimension. At iteration step k on discretization level j let N_k^j be the number of nodes and ϵ_k^j the local energy. With $l = l_k$ we mean that discretization level, at which we achieve the prescribed tolerance δ_k. The important difference to the fixed dimension case now is that within an *adaptive* multilevel method the approximating dimension of the problem depends on the required accuracy. In the linear elliptic case we have the rough relation for the relative discretization error (on energy equilibrated meshes)

$$\left(\frac{N_k^0}{N_k^l}\right)^{\frac{2}{d}} \sim \frac{\epsilon_k^\infty - \epsilon_k^i}{\epsilon_k^\infty} \le \delta_k^2 \; .$$

With a suitable preconditioner such as BPX, the number of PCG iterations *inside* KASKADE is essentially independent of the number of nodes. Therefore the amount of work involved within one linear FEM call can be estimated as

$$A_k \sim N_k^l \sim \frac{N_k^0}{\delta_k^d} \; .$$

From this we end up with

$$i_k \sim \frac{\delta_k^d}{(1+\delta_k^2)^{3/4}} \; .$$

For $d = 1$, this function has its maximum at $\delta_{\text{opt}} = \sqrt{2}$. For $d = 2, 3$, the function is monotonically increasing, so that the optimal choice of δ_k is as large as possible within $\delta_k \le$

2. On the other hand, the FEM error estimators are typically less reliable when the error is "too" large, and our applied complexity model is anyway only useful asymptotically for δ_k small. Thus we suggest to choose δ_k moderately large for any d to obtain a more robust algorithm. For all the numerical experiments in Section 4 below, we took the default value $\delta_k = 1$, unless stated differently. This setting defines our *standard* option of adaptive mesh refinement within NEWTON–KASKADE.

4 Numerical Experiments with NEWTON – KASKADE

In this section, we want to demonstrate properties of the above derived global adaptive Newton–multilevel FEM. For convenience, we pick the linear elliptic FEM code KASKADE [2] with linear finite elements for the inner iteration. Of course, any other *adaptive* linear multigrid method could equally well be selected.

Illustrative example (see also [13, 8]). Consider the functional to be minimized

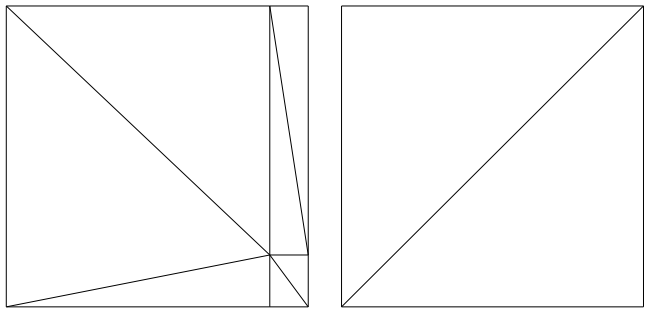
$$f(u) = \int_\Omega \Big(\big(1 + |\nabla u|^2\big)^p - gu \Big) dx \ , \ \ p > \frac{1}{2} \ , \ \ x \in \Omega \subset \mathbb{R}^d \ , \ \ u \in W^{1,2p}(\Omega) \ .$$

The functional gives rise to the derived expressions

$$\begin{aligned} \Big\langle F(u), v \Big\rangle &= \int_\Omega \big(2p(1 + |\nabla u|^2)^{p-1} \langle \nabla u, \nabla v \rangle - gv \big) dx \ , \\ \Big\langle w, F'(u)v \Big\rangle &= \int_\Omega 2p \big(2(p-1)(1 + |\nabla u|^2)^{p-2} \langle \nabla w, \nabla u \rangle \langle \nabla u, \nabla v \rangle + (1 + |\nabla u|^2)^{p-1} \langle \nabla w, \nabla v \rangle \big) dx \end{aligned}$$

With $\langle \cdot, \cdot \rangle$ the Euclidean inner product in $\mathbb{R}^d$, the term $\Big\langle v, F'(u)v \Big\rangle$ is strictly positive for $p \geq \frac{1}{2}$. The computational costs roughly line up as

$$\mathrm{cost}(f) < \mathrm{cost}(F) \approx \mathrm{cost}(F') \ .$$



Good coarse grid Bad coarse grid

Figure 2: Good and bad coarse grid.

For $p = \frac{1}{2}$, which characterizes the (parametric) *minimal surface* problem, the Banach space $W^{1,1}$ is no longer *reflexive*. Nevertheless, for special boundary conditions and

inhomogeneities g, a solution *exists* even in $C^{0,1}$ (see [15]). In order to test our algorithm in the extreme critical case, we select just this value and

$$\Omega = \left[-\frac{\pi}{2}, 0\right] \times \left[-\frac{\pi}{2}, \frac{\pi}{2}\right] \ , \quad u|_{\partial\Omega} = s \cos x \cos y \ , \quad g \equiv 0 \ .$$

Taking the Z_2–symmetry along the x–axis into account, we halve Ω and impose homogeneous Neumann boundary conditions at $y = 0$. The parameter s is set to $s = 3.5$. As the initial guess we take the values on the boundary as prescribed and inside just zero. The initial grid is selected to take care of the expected boundary layer at $x = 0$ — see "good" coarse grid in Fig. 2.

In a *first* numerical experiment, we compared three options of the mesh refinement strategy within the inner iteration:

(I) *standard* mesh option ($\delta_k = 1$ for all k) as advocated in Section 3.2 above,

(II) *sequential* mesh option as used in several Newton–multigrid implementations (cf. [12]): in this option, each mesh refinement level is kept fixed until the associated discrete nonlinear system on that level has been solved to sufficient prescribed accuracy,

(III) *finer* mesh option ($\delta_k = 0.25$ for all k) to illustrate the effect of finer than necessary grids in the inexact Newton process.

In Fig. 3, the automatically obtained damping factors $[\overline{\lambda}_k]$ are repesented.

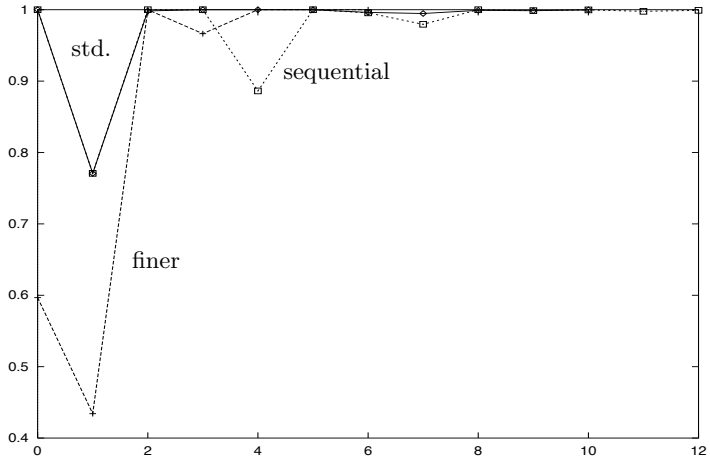


Figure 3: Iterative damping factors $[\overline{\lambda}_k]$ for three mesh refinement options.

In Fig. 4, the estimated iterative energy norms of the (exact) corrections Δx^k are arranged using

$$\|F'(x^k)^{1/2} \Delta x^k\| = \frac{\|F'(x^k)^{1/2} \delta x^k\|}{\sqrt{1 + \delta_k^2}} \ .$$

The number N_k of nodes varies from about 10 up to 10^5, when the iterates approach the solution point. Clearly, the *finer* mesh option just requires more work to achieve comparable accuracies. Our *standard* option ($k_{\rm fin} = 11$) essentially envelopes the more traditional *sequential* option ($k_{\rm fin} = 13$), which performs few unnecessary Newton iterations. Asymptotically, only one Newton iteration per refinement level appears — which dominates the computational work.

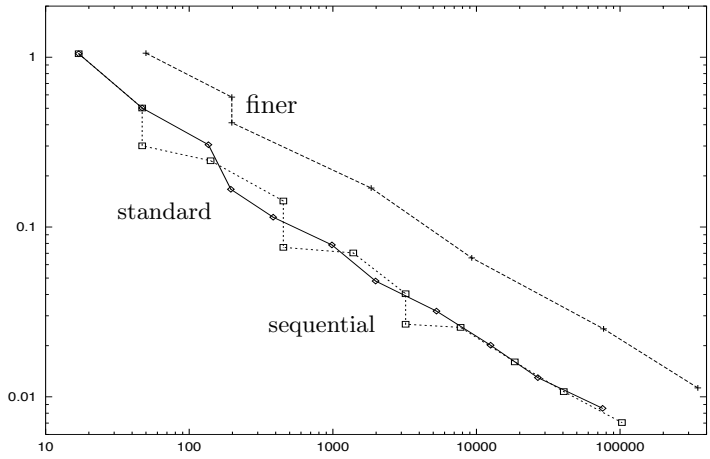


Figure 4: Iterative (exact) energy error norms $\epsilon_k^{1/2}$ versus number of nodes N_k for three mesh refinement options.

In a *second* numerical experiment we tested our quite sophisticated coarse grid versus some "unaware" coarse grid (see, once again, Fig. 2). The results are shown in Fig. 5. Obviously the bad coarse grid requires many more iterations to catch the nonlinearity — an effect that is well–known from experience reported in the engineering literature.

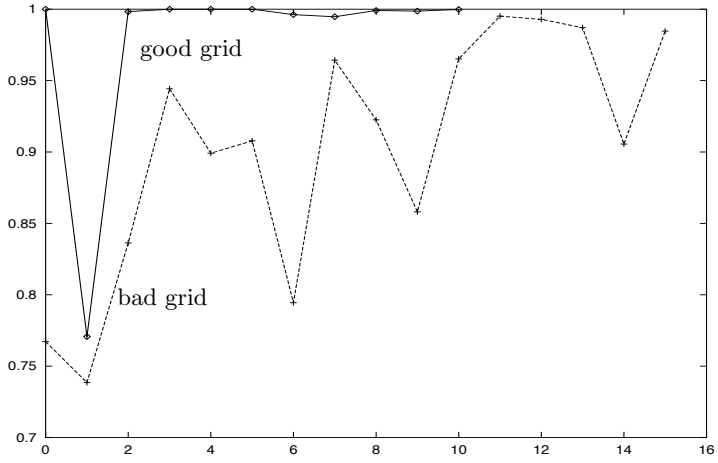


Figure 5: Iterative damping factors $[\overline{\lambda}_k]$ for "good" and "bad" initial coarse grids (*standard* mesh refinement option).

In a *third* numerical experiment, we deliberately chose a domain Ω such that for $p = 1/2$ *no* solution *exists*. For this problem, we compared the performance of our *standard* option with the *sequential* option that has been traditionally implemented in Newton–multigrid methods. The results are shown in Fig. 6 in terms of the automatically obtained damping factors. As can be seen, the *sequential* option repeatedly produces factors λ approaching 1 — thus wrongly indicating solvability of the problem (though only on a finite grid). The *standard* option, however, which is closer related to our convergence theory, gives a much clearer overall indication that a solution cannot be found ($\lambda < 0.01$) — after 20 Newton iterations as opposed to more than 60 iterations in the *sequential* option, where the algorithm has been stopped.

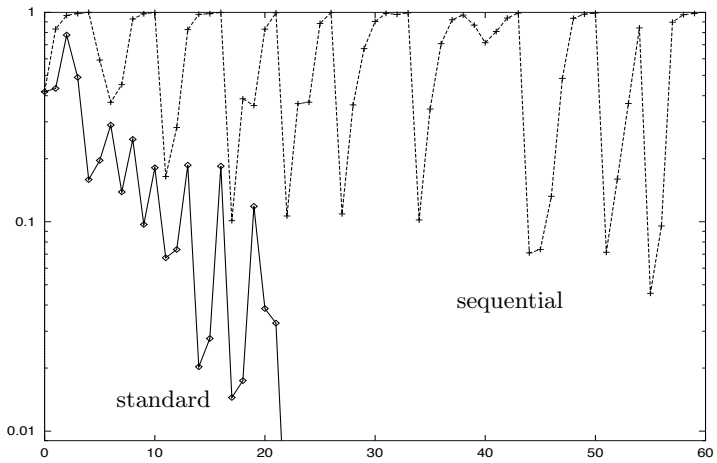


Figure 6: Standard versus sequential mesh refinement option in terms of damping factors λ.

Conclusion

The paper presents a rather simple affine conjugate global convergence theory for adaptive Newton–multilevel methods applied to the solution of nonlinear elliptic PDEs. The characterizing theoretical quantities can be cheaply estimated in the course of the computation — thus leading to a theoretically backed damping strategy and an easily implementable accuracy matching.

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