Quasi-Newton iterative solution of non-orthotropic elliptic problems in 3D with boundary nonlinearity

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Abstract

We consider the numerical solution of elliptic problems in 3D with boundary nonlinearity, such as arising in stationary heat conduction models. We allow general non-orthotropic materials where the matrix of heat conductivities is a non-diagonal full matrix. The solution approach involves the finite element method (FEM) and Newton type iterations. We develop a quasi-Newton method for this problem, using spectral equivalence to approximate the derivatives. We derive the convergence of the method, and numerical experiments illustrate the robustness and the reduced computational cost.

1 Introduction

In this paper we consider the numerical solution of elliptic problems in bounded domains in $\mathbb{R}^3$ involving boundary nonlinearity. Such problems can describe stationary heat conduction with radiation boundary conditions. The studied problems have the form

$$-\mathrm{div}\big(A\nabla u\big) = f \quad \text{in } \Omega, \tag{1.1}$$

$$u_{|\partial\Omega} = \overline{u} \quad \text{on } \Gamma_D, \tag{1.2}$$

$$\nu^\top A\nabla u + s(x,u) = g \quad \text{on } \Gamma_N, \tag{1.3}$$

where Ω is a bounded domain in $\mathbb{R}^3$ with Lipschitz continuous boundary $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$, where Γ_D and Γ_N have positive 2-dimensional (surface) measure, and ν is the outward unit normal to Γ_N. The 3×3 matrix A is symmetric and uniformly positive definite, further, f, $\bar{u}$ and s are given functions with properties specified later. A central issue is the growth rate of s, since its treatment requires a careful choice of function space.

An important problem of the form (1.1)–(1.3), arising in heat radiation, involves a 4th power in the nonlinearity, detailed in Section 2. Nonlinear heat radiation problems have been widely studied in several situations owing to their importance, see, e.g., [1, 2, 5, 9, 11, 12, 13, 14], including problem (2.1)–(2.2) on 2D domains and axially symmetric 3D domains. The general 3D case was then mathematically clarified in the motivating paper [10], where the proper function space was set up, and the convergence of the finite element approximation and of Newton's method was derived. However, their results only cover the case of diagonal matrix A (orthotropic materials), further, they only consider the exact Newton method. On the other hand, most often it is much useful from practical aspect to involve quasi-Newton type methods where the Jacobians are approximated, and hence one can spare a significant computational work.

In this paper we first discuss the background of the problem. The nonnegativity of the solution enables one to use a rewritten form of the problem, which allows the use of a proper

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operator formulation. Then we develop a quasi-Newton method for this problem in the form of variable preconditioning using spectral equivalence, based on our earlier results on other elliptic problems [3, 6, 7]. We prove the convergence of the quasi-Newton method using proper preconditioning operators allowing very simple updating, and finally, numerical experiments illustrate the theoretical results. We observe robustness of the methods, that is, a convergence speed bounded independently of the mesh size, and a reduced computational cost thanks to the quasi-Newton method.

2 The heat radiation problem

2.1 The problem and its properties

As mentioned before, an important problem with the structure (1.1)–(1.3) arises in heat radiation with 4th power boundary nonlinearity. We are motivated by the paper [10], where this problem was treated carefully. The problem consists of the elliptic heat conduction equation with mixed Stefan-Boltzmann radiation boundary conditions:

$$-\text{div}\big(A\nabla u\big) = f \quad \text{in } \Omega\,, \tag{2.1}$$

$$u_{|\partial\Omega} = \overline{u} \quad \text{on } \Gamma_D, \qquad \alpha u + \nu^\top A\nabla u + \beta u^4 = g \quad \text{on } \Gamma_N, \tag{2.2}$$

with the conditions given for (1.1)–(1.3). In particular, A is the matrix of heat conductivities, $f \geq 0$ is the density of body heat sources, $\bar{u} \geq 0$ is the prescribed temperature. The heat transfer coefficient is denoted by $\alpha \geq 0$, and $\beta = \sigma f_{em}$ with the Stefan-Boltzmann constant $\sigma = 5.669 \cdot 10^{-8}$ Wm^{-2}K^{-4} and the relative emissivity function $0 \leq f_{em} \leq 1$. We look for the absolute temperature $u \geq 0$.

2.2 Formulation and nonnegativity of the solution

A proper approach to study a nonlinear elliptic problem is to write its weak form as an operator equation in a Banach or Hilbert space [6, 15], often related to the minimization of a potential. This approach is taken in [10] as well. However, problem (2.1)–(2.2) in its original form does not allow to involve a convex potential, since the term $u \mapsto u^4$ is not monotone. Consider now the problem where this term is replaced with $|u|^3u$. If the solution of the modified form of the problem is nonnegative, then $|u|^3u$ and u^4 coincide, hence the original and the modified BVPs are equivalent. The paper [10] proves the desired nonnegativity under the restriction that A is a diagonal matrix.

We give a simple proof for nonnegativity for the full matrix case, adapting the idea of the proof of [8, Theorem 5]. See [1, 14] for related investigations. Some generalizations, allowed by our proof, are mentioned in Subsection 2.4 and Remark 3.7.

The modified form of BVP (2.1)–(2.2) is the following:

$$-\text{div}\big(A\nabla u\big) = f \quad \text{in } \Omega, \tag{2.3}$$

$$u_{|\Gamma_D} = \overline{u} \quad \text{on } \Gamma_D, \qquad \alpha u + \nu^\top A\nabla u + \beta|u|^3 u = g \quad \text{on } \Gamma_N. \tag{2.4}$$

For the proper formulation of the problem, besides the sign conditions posed for (2.1)–(2.2), we assume that the entries a_{ij} of the function-valued matrix A are in $L^\infty(\Omega)$, further, $f \in L^2(\Omega)$, $g \in L^2(\Gamma_2)$, $\bar{u} \in H^1(\Omega)$, $\bar{u}|_{\Gamma_N} \in L^5(\Gamma_N)$, $\alpha,\ \beta \in L^\infty(\Gamma_N)$, and there exists $\beta_0 > 0$ such that $\beta \ge \beta_0$ a. e. Furthermore, $A(x)$ is not only symmetric and positive definite for any $x \in \Omega$, but we assume that there exists constants $\mu_0,\ \mu_1 > 0$ such that, for all $x \in \Omega$ and vector $v \in \mathbb{R}^3$,

$$\mu_0 |v|^2 \le A(x)v \cdot v \le \mu_1 |v|^2 \,. \tag{2.5}$$

The weak solution is looked for within the space $H^1(\Omega)$, and the test functions within the space

$$H^1_D(\Omega) := \{v \in H^1(\Omega) :\ v_{|\Gamma_D} = 0 \ \text{ in trace sense}\}\,,$$

which has the natural norm

$$\|v\|_{H^1_D} := \|\nabla v\|_{L^2(\Omega)}.$$

However, as pointed out in [10], the traces of the variational solution should belong to the Lebesgue space $L^5(\Gamma_N)$, which is true in 2D but no longer true in 3D for a general function in $H^1(\Omega)$. (The need for 5th power integrals on Γ_N will be seen in (2.8).) Hence, the proper function space for problem (2.3)–(2.4) in 3D is

$$V := \left\{v \in H^1(\Omega) :\ v|_{\Gamma_N} \in L^5(\Gamma_N)\right\}, \tag{2.6}$$

which is a Banach space equipped with the norm

$$\|v\|_V := \|v\|_{H^1(\Omega)} + \|v\|_{L^5(\Gamma_N)}.$$

Moreover, we will use the Banach space

$$V_D := V \cap H^1_D(\Omega)$$

with the norm

$$\|v\|_{V_D} := \|v\|_{H^1_D(\Omega)} + \|v\|_{L^5(\Gamma_N)}, \tag{2.7}$$

to serve as the proper space for the test functions and the solution of the homogenized problem, which vanish on Γ_D.

Then the weak form of problem (2.3)–(2.4) can be written as follows: we look for $u \in V$, satisfying $u - \bar{u} \in V_D$, such that

$$\int_\Omega A\nabla u \cdot \nabla v + \int_{\Gamma_N} (\alpha + \beta |u|^3) uv = \int_\Omega fv + \int_{\Gamma_N} gv \qquad (\forall v \in V_D). \tag{2.8}$$

Theorem 2.1. *If u is the weak solution of (2.3)–(2.4), then u is a.e. nonnegative.*

Proof. Let u satisfy (2.8), and let us use the specific test function

$$v := \min\{u,\ 0\}. \tag{2.9}$$

We must check that $v \in V_D$. Indeed, $u \in H^1(\Omega)$ implies $v \in H^1(\Omega)$, see [10], and obviously $u|_{\Gamma_N} \in L^5(\Gamma_N)$ implies $v|_{\Gamma_N} \in L^5(\Gamma_N)$; finally, $v|_{\Gamma_D} = \min\{\bar{u},\ 0\} = 0$. Throughout the proof, (in)equalities are understood almost everywhere (a.e.).

By definition, we have $v \le 0$. In order to prove that $u \ge 0$, we must show that $v = 0$ on Ω.

Let us substitute this v in (2.8), and rewrite the latter with the following decomposition of Ω:

$$\Omega_+ := \{x \in \Omega : \quad u(x) > 0\} \quad \text{and} \quad \Omega_- := \{x \in \Omega : \quad u(x) \le 0\}.$$

Since $v = 0$ and $\nabla v = 0$ in Ω_+, thus the integrals used in (2.8) are zero on the subdomain Ω_+, that is, it suffices to integrate on Ω_-, and, similarly, on $\Gamma_{N^-} := \{x \in \Gamma_N : \quad u(x) \le 0\}$, respectively. In turn, $u = v$ on $\Omega_- \cup \Gamma_{N^-}$ and $\nabla u = \nabla v$ in Ω_-, hence we obtain

$$\int_{\Omega_-} A\nabla v \cdot \nabla v + \int_{\Gamma_{N^-}} (\alpha + \beta|v|^3)v^2 = \int_{\Omega_-} fv + \int_{\Gamma_{N^-}} gv\,. \tag{2.10}$$

Now we can add zero (the integrals on Ω_+ and on Γ_+) to both sides, thus we again integrate on the whole domain Ω and Γ_N:

$$\int_{\Omega} A\nabla v \cdot \nabla v + \int_{\Gamma_N} (\alpha + \beta|v|^3)v^2 = \int_{\Omega} fv + \int_{\Gamma_N} gv. \tag{2.11}$$

Here, owing to the positive definiteness of A and the sign conditions $\alpha, \beta \ge 0$, we have

$$\int_{\Omega} A\nabla v \cdot \nabla v \ge 0, \qquad \int_{\Gamma_N} (\alpha + \beta|v|^3)v^2 \ge 0, \tag{2.12}$$

which implies that the l. h. s. of (2.11) is nonnegative. On the other hand, the r. h. s. of (2.11) is nonpositive due to $v \le 0$ and the sign conditions $f, g \ge 0$. Therefore, both sides of (2.11) are zero, and in particular,

$$\int_{\Omega} A\nabla v \cdot \nabla v = 0.$$

Then the positive definiteness of A yields that $\nabla v = 0$, so $v = c$ is constant. Moreover, we know that $v|_{\Gamma_D} = 0$, hence $c = 0$, that is, $v = 0$, which we wanted to prove. ∎

2.3 Well-posedness, finite element approximation and Newton iteration

In this section we collect those results of [10] which are directly applicable here to (2.3)–(2.4), and, knowing now the nonnegativity property, to the original problem (2.1)–(2.2) as well. The main point is that [10] does not explicitly exploit the diagonality assumption, the latter is only used therein to obtain the nonnegativity property. The following theorems of [10] only use the property

$$a(v, v) := \int_{\Omega} A\nabla v \cdot \nabla v + \int_{\Gamma_N} \alpha v^2 \ge c\|v\|^2_{H^1(\Omega)} \qquad (\forall v \in V_D)$$

for some constant $c > 0$. This ellipticity property remains naturally valid in our full matrix case, owing to the uniformly positivity condition (2.5):

$$a(v, v) \ge \mu_0 \int_{\Omega} |\nabla v|^2 = \mu_0\|v\|^2_{H^1_D(\Omega)} \ge \mu_0 c_D\|v\|^2_{H^1(\Omega)}\,, \tag{2.13}$$

where $c_D > 0$ is a suitable constant, using that $\|v\|_{H^1_D(\Omega)}$ and $\|v\|_{H^1(\Omega)}$ are equivalent norms, thanks to the property that Γ_D has positive surface measure.

Altogether, the four theorems below follow from (2.13) and [10, Theorems 2.1, 3.1, 3.2, 3.3], respectively.

Theorem 2.2. *Problem (2.3)–(2.4) has a unique weak solution.*

The family of finite element spaces $V_h \subset V_D$ $(h > 0)$ is chosen to satisfy the standard approximation property:

$$\text{for any } v \in V_D, \quad \operatorname{dist}(v, V_h) \to 0 \quad \text{as } h \to 0. \tag{2.14}$$

Theorem 2.3. *Assume that subspaces $\{V_h\}_{h\to 0}$ satisfy hypothesis* (2.14)*. Let u and u_h be the exact and the FEM solutions, respectively. Then*

$$\|u - u_h\|_V \to 0 \quad \text{as } h \to 0.$$

The convergence order can be estimated under the following condition on the interpolant $I_h u$:

$$\text{for some } s \in [1,\, 7/6],\ c > 0 \text{ and integer } k \geq 2, \qquad \|u - I_h u\|_s \leq c h^{k-s}. \tag{2.15}$$

Theorem 2.4. *Assume that $\bar{u} \in H^1(\Omega)$ and $\bar{u}|_{\Gamma_N} \in L^6(\Gamma_N)$. Let u and u_h be the exact and the FEM solutions, respectively. If $u \in H^k(\Omega)$, and* (2.15) *holds, then there exists a positive constant c independent of h such that*

$$\|u - u_h\|_V \leq c h^{2(k-1)/5} \quad \text{as } h \to 0. \tag{2.16}$$

Finally, the convergence of the Newton iteration $(u_{h,n})_{n\in\mathbf{N}^+} \subset V_h$ to the FEM solution u_h is formulated with the error $e_n := \|u_{h,n} - u_h\|_V$:

Theorem 2.5. *The Newton iteration is well-defined, and there exist positive constants δ and c independent of n such that for every $e_0 < \delta$, we have*

$$e_{n+1} \leq c e_n^2.$$

2.4 Some possible generalizations

The above-mentioned results can be extended to some more general equations, the main point being the nonnegativity in Theorem 2.1.

Firstly, we can consider problem (1.1)–(1.3) with a continuous boundary nonlinearity s, satisfying the following properties: there exist constants $c_1, c_2 \geq 0$ and $q > 1$ such that

$$s(x,\xi)\xi \geq 0, \qquad |s(x,\xi)| \leq c_1 + c_2|\xi|^{q-1} \qquad (\forall x \in \Gamma_N,\ \xi \in \mathbf{R}). \tag{2.17}$$

Then the problem can be posed in the Banach space with modified exponent w.r.t. (2.6):

$$V := \left\{ v \in H^1(\Omega) :\ v|_{\Gamma_N} \in L^q(\Gamma_N) \right\},$$

since the corresponding integral on Γ_N in the weak form remains finite:

$$\int_{\Gamma_N} |s(x,u)v| \leq \int_{\Gamma_N} \left(c_1 + c_2|u|^{q-1}\right)|v| \leq c_1\|v\|_{L^1(\Gamma_N)} + c_2\|u\|^{q-1}_{L^q(\Gamma_N)}\|v\|_{L^q(\Gamma_N)}\,.$$

Furthermore, one can repeat the proof of Theorem 2.1 such that the integral on Γ_N is modified, but in (2.12) we obtain

$$\int_{\Gamma_N} s(x,v)v \geq 0$$

due to the assumption, hence the nonnegativity result remains true.

The consequences mentioned in Subsection 2.3 also remain true in the above case, since the used ellipticity (2.13) is not modified.

Secondly, one may also involve convection in the equation, replacing (1.1) by

$$-\mathrm{div}\big(A\nabla u\big) + \mathbf{w}\cdot\nabla u = f \quad \text{in } \Omega$$

for a given vector field $\mathbf{w} \in C^1(\overline{\Omega}, \mathbf{R}^3)$. Following the usual assumptions, the field is assumed to be divergence-free and the inflow boundary is part of the Dirichlet boundary:

$$\mathrm{div}\,\mathbf{w} = 0 \ \text{ on } \ \Omega, \qquad \mathbf{w}\cdot\nu \geq 0 \ \text{ on } \ \Gamma_N\,.$$

Then for any $v \in V_D$

$$\int_\Omega (\mathbf{w}\cdot\nabla v)\,v = \frac{1}{2}\int_\Omega \mathrm{div}\,(\mathbf{w}\,v^2) = \frac{1}{2}\int_{\Gamma_N} (\mathbf{w}\cdot\nu)\,v^2 \geq 0\,,$$

hence the modified integral on Ω in (2.12) satisfies

$$\int_\Omega \big(A\nabla v\cdot\nabla v + (\mathbf{w}\cdot\nabla v)\,v\big) \geq 0$$

and thus the nonnegativity proof of Theorem 2.1 can be repeated again.

3 The quasi-Newton method (variable preconditioning)

In this section we formulate our quasi-Newton method where the Jacobians are approximated based on spectral equivalence in the function space, that is, we define a kind of variable preconditioning using proper preconditioning operators. Such an approach has been used in our earlier papers [3, 4, 7] in other situations, now we adapt it to the case of boundary nonlinearity in the given function space. The quasi-Newton method allows to spare computational cost, and the setting of spectral equivalence in the function space enables a straightforward definition of the approximate Jacobians.

3.1 Background in Banach space

We will use an abstract result based on our papers [3, 4]. The theorem is presented in a form that will fit the situation of the studied radiation problem. The formulation involves the "energy $*$-norm" $\|v\|_* := \langle v,\, F'(z^*)^{-1}v\rangle^{1/2}$, which is equivalent to the original one.

Theorem 3.1. *Let X be a real Banach space, $F : X \to X'$ a nonlinear operator, and let us consider the operator equation*

$$F(z) = 0. \tag{3.1}$$

Let F have a bihemicontinuous Gâteaux derivative that satisfies the following properties:

(i) For any $z \in X$ the operator $F'(z)$ is symmetric.

(ii) There exists a constant $\lambda > 0$ such that

$$\lambda \|h\|^2 \leq \langle F'(z)h, h\rangle \qquad (\forall z, h \in X). \tag{3.2}$$

(iii) There exists a continuous nondecreasing function $\Lambda : \mathbb{R}_0^+ \to \mathbb{R}^+$ such that

$$\langle F'(z)h, h\rangle \leq \Lambda(\|z\|)\|h\|^2 \qquad (\forall z, h \in X). \tag{3.3}$$

(iv) There exists a continuous nondecreasing function $L : \mathbb{R}_0^+ \to \mathbb{R}^+$ such that

$$\|F'(z) - F'(w)\| \leq L(\max\{\|z\|, \|w\|\})\, \|z - w\| \qquad (\forall z,\, w \in X). \tag{3.4}$$

Denote by $z^* \in X$ the unique solution of (3.1). Let z_0 be in a sufficiently small neighbourhood of z^*, and let the sequence (z_n) be defined by

$$z_{n+1} := z_n - \frac{2}{M_n + m_n} B_n^{-1} F(z_n) \qquad (n \in \mathbb{N}), \tag{3.5}$$

where $0 < m_n \leq M_n$ and for any $n \in \mathbb{N}$ the bounded symmetric linear operator $B_n : X \to X'$ is chosen such that

$$m_n \langle B_n h, h\rangle \leq \langle F'(z_n)h, h\rangle \leq M_n \langle B_n h, h\rangle \qquad (\forall h \in X). \tag{3.6}$$

We require (m_n) to be positively bounded from below and (M_n) bounded from above. Then (z_n) converges to z^*, that is,

$$\|z_n - z^*\| \leq \frac{1}{\lambda}\|F(z_n)\| \to 0,$$

moreover,

$$\limsup \frac{\|F(z_{n+1})\|_*}{\|F(z_n)\|_*} \leq \limsup \frac{M_n - m_n}{M_n + m_n} < 1. \tag{3.7}$$

This theorem is a special case of [3, Theorem 2.5], where a non-uniform lower bound was allowed and damping was used to extend the convergence domain. The latter might be applied here as well, but is not included in the theorem for simplicity. Some more remarks:

- The Hilbert space predecessor of Theorem 3.1 in just the same form is found in [4, Theorem 2.3].
- Condition *(iii)* is redundant since the existence of Λ is actually a consequence of condition *(iv)*, however, in practice a direct estimation will give sharper values of Λ.
- The convergence is linear if the lim sup in (3.7) is positive and superlinear if this lim sup is 0. The arising estimates are inherited by the original norm since it is equivalent to the energy $*$-norm. The superlinear estimates can be refined up to second order by assuming stricter bounds on M_n/m_n, see also [3, Theorem 2.5].

3.2 Convergence of the quasi-Newton method for the radiation problem

The application of Theorem 3.1 to our elliptic problem will require the solution and the test functions to be in the same Banach space, hence we homogenize BVP (2.3)–(2.4) by letting $z := u - \bar{u}$. This yields the following problem:

$$-\mathrm{div}\big(A\nabla z\big) = \tilde{f} \quad \text{in } \Omega, \tag{3.8}$$

$$z_{|\partial\Omega} = 0 \quad \text{on } \Gamma_D, \tag{3.9}$$

$$\alpha(z+\bar{u}) + \nu^\top A\nabla z + \beta|z+\bar{u}|^3(z+\bar{u}) = \tilde{g} \quad \text{on } \Gamma_N, \tag{3.10}$$

where formally $\tilde{f} := f + \mathrm{div}\,\big(A\nabla\bar{u}\big)$, $\tilde{g} := g - \nu^\top A\nabla\bar{u}$. In weak form, we then look for $z \in V_D$ such that

$$\int_\Omega A\nabla z\cdot\nabla v + \int_{\Gamma_N}(\alpha+\beta|z+\bar{u}|^3)(z+\bar{u})v = \int_\Omega\big(fv - A\nabla\bar{u}\cdot\nabla v\big) + \int_{\Gamma_N} gv \qquad (\forall v \in V_D). \tag{3.11}$$

In what follows, we apply the finite element method (FEM) for (3.11) in some FEM subspace $V_h \subset V_D$, endowed with the same norm $\|.\|_{V_D}$ as in (2.7). (The sole restriction is that, when refining the mesh, property (2.14) should hold for the family, then Theorem 2.3 ensures the convergence of the FEM.) In a given FEM subspace $V_h \subset V_D$, the problem to solve is obtained by replacing V_D by V_h in (3.11).

Our goal is to solve the FEM problem with a quasi-Newton iteration, that is, we must show the applicability of Theorem 3.1 where $X = V_h$ and the corresponding operator $F : V_h \to V_h'$ is defined via the weak form:

$$\langle F(z),\ v\rangle = \int_\Omega A\nabla z\cdot\nabla v + \int_{\Gamma_N}(\alpha+\beta|z+\bar{u}|^3)(z+\bar{u})v - \int_\Omega \tilde{f}v - \int_{\Gamma_N}\tilde{g}v \quad (\forall z, v \in V_h). \tag{3.12}$$

We note that elements of V_h might be denoted in a usual way by z_h, v_h etc., but we can omit such subscripts for simplicity, since from now on we only work in V_h.

Theorem 3.2. *Assumptions (i)-(iv) of Theorem 3.1 hold for the operator defined by* (3.12).

Proof. The derivative of the real function $t \mapsto (\alpha+\beta|t+\bar{u}|^3)(t+\bar{u})$ is $t \mapsto \alpha + 4\beta|t+\bar{u}|^3$. Then, following standard techniques (see [6]), we can differentiate in the integral and obtain

$$\langle F'(z)h,\ v\rangle = \int_\Omega A\nabla h\cdot\nabla v + \int_{\Gamma_N}(\alpha+4\beta|z+\bar{u}|^3)hv \qquad (\forall z, h, v \in V_h). \tag{3.13}$$

This shows that condition *(i)* holds trivially. To check conditions *(ii)-(iii)*, set $v = h$:

$$\langle F'(z)h,\ h\rangle = \int_\Omega A\nabla h\cdot\nabla h + \int_{\Gamma_N}(\alpha+4\beta|z+\bar{u}|^3)h^2. \tag{3.14}$$

Owing to (2.5) and $\alpha, \beta \geq 0$, we have

$$\langle F'(z)h,\ h\rangle \geq \int_\Omega A\nabla h\cdot\nabla h \geq \mu_0\|\nabla h\|^2_{L^2(\Omega)} = \mu_0\|h\|^2_{H^1_D}\,.$$

Since $V_h \subset H^1(\Omega)$ is a finite dimensional subspace, we have $\|h\|_{H^1_D} \geq c_1 \|h\|_{V_D}$ for some constant $c_1 > 0$, which yields

$$\langle F'(z)h,\ h\rangle \geq \mu_0 c_1^2 \|h\|_{V_D}^2, \tag{3.15}$$

this yields condition *(ii)*. Now let

$$\alpha_\infty := \|\alpha\|_{L^\infty(\Gamma_N)} (\mathrm{meas}(\Gamma_N))^{3/5}, \quad \beta_\infty := 4\|\beta\|_{L^\infty(\Gamma_N)}.$$

We will use the following form of Hölder's inequality: with $\frac{3}{5} + \frac{2}{5} = 1$,

$$\int_{\Gamma_N} |v|^3 h^2 \leq \|v^3\|_{L^{5/3}(\Gamma_N)} \|h^2\|_{L^{5/2}(\Gamma_N)} = \|v\|^3_{L^5(\Gamma_N)} \|h\|^2_{L^5(\Gamma_N)} \qquad (\forall v, h \in L^5(\Gamma_N)).$$

Applying this to the second term of (3.14) yields

$$\int_{\Gamma_N} (\alpha + 4\beta|z+\bar{u}|^3)h^2 \leq \|\alpha\|_{L^\infty(\Gamma_N)} \int_{\Gamma_N} 1^3 h^2 + 4\|\beta\|_{L^\infty(\Gamma_N)} \int_{\Gamma_N} |z+\bar{u}|^3 h^2$$
$$\leq \left(\alpha_\infty + \beta_\infty \|z+\bar{u}\|^3_{L^5(\Gamma_N)}\right) \|h\|^2_{L^5(\Gamma_N)} \leq \left(\alpha_\infty + \beta_\infty \left(\|z\|_{L^5(\Gamma_N)} + \|\bar{u}\|_{L^5(\Gamma_N)}\right)^3\right) \|h\|^2_{L^5(\Gamma_N)}.$$

Using this together with (2.5) and (2.7), we can estimate (3.14) as

$$\langle F'(z)h,\ h\rangle \leq \mu_1 \|h\|^2_{H^1_D(\Omega)} + \left(\alpha_\infty + \beta_\infty \left(\|z\|_{L^5(\Gamma_N)} + \|\bar{u}\|_{L^5(\Gamma_N)}\right)^3\right) \|h\|^2_{L^5(\Gamma_N)} \leq \Lambda(\|z\|_{V_D}) \|h\|^2_{V_D},$$

where

$$\Lambda(t) := \max\left\{\mu_1,\ \alpha_\infty + \beta_\infty \left(t + \|\bar{u}\|_{L^5(\Gamma_N)}\right)^3\right\} \qquad (t \geq 0). \tag{3.16}$$

This establishes condition *(iii)*. Finally, to obtain condition *(iv)*, first observe that for each $z,\ w \in H^1(\Omega)$ the symmetry of $F'(z) - F'(w)$ makes it possible to obtain its norm using the quadratic form:

$$\|F'(z) - F'(w)\| = \sup_{\|h\|_{V_D}=1} |\langle (F'(z) - F'(w))h, h\rangle|.$$

Applying (3.14) yields

$$\|F'(z) - F'(w)\| = 4 \sup_{\|h\|_{V_D}=1} \left| \int_{\Gamma_N} \beta(|z+\bar{u}|^3 - |w+\bar{u}|^3)h^2 \right| \leq \beta_\infty \sup_{\|h\|_{V_D}=1} \int_{\Gamma_N} \left| |z+\bar{u}|^3 - |w+\bar{u}|^3 \right| h^2 .$$

Here we have

$$\left| |z+\bar{u}|^3 - |w+\bar{u}|^3 \right| = \left| |(z+\bar{u})^3| - |(w+\bar{u})^3| \right| \leq |(z+\bar{u})^3 - (w+\bar{u})^3|,$$

therefore,

$$\|F'(z) - F'(w)\| \leq \beta_\infty \sup_{\|h\|_{V_D}=1} \int_{\Gamma_N} |z-w| \left| (z+\bar{u})^2 + (z+\bar{u})(w+\bar{u}) + (w+\bar{u})^2 \right| h^2.$$

Using the same form of general Hölder inequality as above implies

$$\|F'(z) - F'(w)\| \le \beta_\infty \|z-w\|_{L^5(\Gamma_N)} \Big(\|z+\bar u\|^2_{L^5(\Gamma_N)}$$
$$+\|z+\bar u\|_{L^5(\Gamma_N)} \|w+\bar u\|_{L^5(\Gamma_N)} + \|w+\bar u\|^2_{L^5(\Gamma_N)} \Big) \sup_{\|h\|_{V_D}=1} \|h\|^2_{L^5(\Gamma_N)}.$$

Using $\|\cdot\|_{L^5(\Gamma_N)} \le \|\cdot\|_{V_D}$, this yields

$$\|F'(z) - F'(w)\| \le L(\max\{\|z\|_{V_D}, \|w\|_{V_D}\}) \|z-w\|_{V_D},$$

where

$$L(t) := 3\beta_\infty (t + \|\bar u\|_{L^5(\Gamma_N)})^2 \qquad (t \ge 0), \tag{3.17}$$

hence *(iv)* is satisfied. ∎

From the obtained properties we can draw the general conclusion:

Corollary 3.3. *If bounded symmetric linear operators $B_n : V_h \to V_h'$ satisfy condition* (3.6)*, then the quasi-Newton iteration* (3.5) *for the weak nonlinear elliptic operator* (3.12) *converges according to* (3.7)*.*

Clearly, the application of the result needs a suitable definition of the operators B_n. We give a reasonable choice in the next section.

3.3 Preconditioning operators

In this section we propose choices for the auxiliary operators B_n. We must fulfil a double goal: B_n should be a good approximation of $F'(z_n)$, but essentially simpler to realize.

The general idea is to compose B_n from precomputed parts, so that the stepwise updating needs a minimal computational task. In general, we can approximate the principal part using an arbitrary but spectrally equivalent matrix coefficient: let G be a function-valued matrix with entries $g_{ij} \in L^\infty(\Omega)$, such that there exists constants $\lambda_0,\ \lambda_1 > 0$ for which

$$\lambda_0\ G(x)v \cdot v \le A(x)v \cdot v \le \lambda_1\ G(x)v \cdot v \tag{3.18}$$

for all $x \in \Omega$ and vector $v \in \mathbb{R}^3$. For given $n \in \mathbb{N}$, using the already computed iterate z_n, let B_n be defined via the weak form

$$\langle B_n h,\ v\rangle := \int_\Omega G(x)\ \nabla h \cdot \nabla v\ + (\alpha_0 + w_n) \int_{\Gamma_N} hv \qquad (\forall v, h \in V_h), \tag{3.19}$$

where, for some fixed $0 < \varrho, \tau \le 1$, using that $z_n \in V_h$,

$$\alpha_0 := \varrho \max \alpha, \qquad w_n := 4\tau \max\{\beta |z_n + \bar u|^3\}.$$

Then the discretization matrix corresponding to B_n has the form

$$\mathbf{B}_n = \mathbf{G} + (\alpha_0 + w_n)\mathbf{M},$$

where $\mathbf{G}$ is the stiffness matrix weighted with G and $\mathbf{M}$ is the boundary mass matrix on Γ_N, both precomputable.

We will make use of the following Sobolev embedding estimate: there exists a constant $C_2 > 0$ such that

$$\|v\|_{L^2(\Gamma_N)} \leq C_2 \|\nabla v\|_{L^2(\Omega)} \qquad (\forall v \in H^1_D(\Omega)). \tag{3.20}$$

This is due to the property $v_{|\Gamma_D} = 0$. Since $V_h \subset V_D \subset H^1_D(\Omega)$, we can apply (3.20) in our FEM subspace.

Now we verify that the B_n satisfy the corresponding condition in Theorem 3.1.

Theorem 3.4. *The spectral equivalence (3.6) holds for operators (3.13) and (3.19) with constants*

$$m_n = 1 \Big/ \Big(\frac{1}{\lambda_0} + \frac{(\alpha_0 + w_n) C_2^2}{\mu_0} \Big) \quad \textit{and} \quad M_n \equiv M := \max\Big\{ \lambda_1,\ \frac{1}{\varrho},\ \frac{1}{\tau} \Big\} \qquad (n \in \mathbb{N})$$

(that is, M_n has a fixed value independently of n).

Proof. We have

$$\langle B_n h,\ h \rangle := \int_\Omega G(x)\ \nabla h \cdot \nabla h\ + (\alpha_0 + w_n) \int_{\Gamma_N} h^2 \qquad (\forall h \in V_h). \tag{3.21}$$

We can use (2.5) with (3.14) and get

$$\begin{aligned} \langle F'(z) h,\ h \rangle &= \int_\Omega A \nabla h \cdot \nabla h + \int_{\Gamma_N} (\alpha + 4\beta |z + \bar{u}|^3) h^2 \\ &\leq \lambda_1 \int_\Omega G(x)\ \nabla h \cdot \nabla h + \big(\max \alpha + 4 \max\{\beta |z_n + \bar{u}|^3\} \big) \int_{\Gamma_N} h^2 \\ \leq \max\Big\{ \lambda_1,\ \frac{1}{\varrho},\ \frac{1}{\tau} \Big\} &\Big(\int_\Omega G(x)\ \nabla h \cdot \nabla h\ + (\alpha_0 + w_n) \int_{\Gamma_N} h^2 \Big) = M \langle B_n h,\ h \rangle, \end{aligned} \tag{3.22}$$

where

$$M := \max\Big\{ \lambda_1,\ \frac{1}{\varrho},\ \frac{1}{\tau} \Big\}.$$

Note that now $M_n \equiv M$ is independent of n.

For the other direction, we first note that from (3.18),

$$\int_\Omega G(x)\ \nabla h \cdot \nabla h \leq \frac{1}{\lambda_0} \int_\Omega A(x)\ \nabla h \cdot \nabla h\,, \tag{3.23}$$

further, the Sobolev estimate (3.20) and (2.5) yield

$$(\alpha_0 + w_n) \int_{\Gamma_N} h^2 = (\alpha_0 + w_n)\, \|h\|^2_{L^2(\Gamma_N)} \leq (\alpha_0 + w_n) C_2^2\, \|\nabla h\|^2_{L^2(\Omega)} \leq \frac{(\alpha_0 + w_n) C_2^2}{\mu_0} \int_\Omega A(x)\ \nabla h \cdot \nabla h\,. \tag{3.24}$$

Adding these up, we obtain

$$\langle B_n h,\ h \rangle \leq \Big(\frac{1}{\lambda_0} + \frac{(\alpha_0 + w_n) C_2^2}{\mu_0} \Big) \int_\Omega A(x)\ \nabla h \cdot \nabla h \tag{3.25}$$

$$\leq \Big(\frac{1}{\lambda_0}+\frac{(\alpha_0+w_n)C_2^2}{\mu_0}\Big)\Big(\int_\Omega A\nabla h\cdot\nabla h+\int_{\Gamma_N}(\alpha+4\beta|z+\bar u|^3)h^2\Big) = \Big(\frac{1}{\lambda_0}+\frac{(\alpha_0+w_n)C_2^2}{\mu_0}\Big)\langle F'(z)h,\ h\rangle$$

since, from $\alpha,\beta\geq 0$, the integral on Γ_N is nonnegative. That is, we have

$$m_n\langle B_n h,\ h\rangle \leq \langle F'(z)h,\ h\rangle,$$

where

$$m_n := 1\Big/\Big(\frac{1}{\lambda_0}+\frac{(\alpha_0+w_n)C_2^2}{\mu_0}\Big).$$

■

Theorem 3.5. *Using the operators (3.19), the quasi-Newton iteration* (3.5) *for the weak nonlinear elliptic operator* (3.12) *converges according to* (3.7).

PROOF. The linear operators B_n in (3.19) are bounded and symmetric, and they satisfy condition (3.6) by Theorem 3.4. Hence, Corollary 3.3 yields that the iteration (3.5) converges according to (3.7). ■

Remark 3.6. (Special cases.)

(i) If the matrix A has a simple structure, then there is no need to replace it, hence we can let $G := A$. In this case

$$\lambda_0 = \lambda_1 = 1\ .$$

(ii) If the matrix A has a large variation, and/or the domain has symmetries, then one may approximate the operator with a constant times Laplacian. In this case we can let $G := \tilde\mu\, I$, where, using (2.5), $\tilde\mu := \frac{\mu_0+\mu_1}{2}$, and I is the identity matrix. This suggestion replaces the coefficients in $F'(z_n)$ by constant scalars. Then B_n corresponds to the FEM discretization of linear elliptic Poisson problems with mixed boundary conditions:

$$\begin{aligned} -\tilde\mu\,\Delta h = r \qquad &\text{in } \Omega \\ h_{|\partial\Omega} = 0 \quad \text{on } \Gamma_D, \qquad &\tfrac{\partial h}{\partial\nu} + (\alpha_0+w_n)h = \gamma \quad \text{on } \Gamma_N\,. \end{aligned} \tag{3.26}$$

Remark 3.7. (Generalizations.) The above results can be extended to problem (1.1)–(1.3) for some $s\in C^1$ if, besides conditions (2.17), the function $\xi\mapsto\partial_\xi s(x,\xi)$ is nonnegative and satisfies proper local Lipschitz continuity. The boundary integrals in (3.13) and (3.19) are replaced by

$$\int_{\Gamma_N}\partial_\xi s(x,z+\bar u)hv \qquad \text{and} \qquad \tau\,\max\partial_\xi s(x,z_n+\bar u)\int_{\Gamma_N} hv\,,$$

respectively.

Remark 3.8. (2D analogues.) In this paper we focus on the practically realistic 3D situation. The 2D case may also be of interest, e.g. on thin domains or on cross-sections. We note that our proposed method and Theorem 3.5 is valid in 2D as well, moreover, then the situation is simpler, since we can just use $H^1_D(\Omega)$ as underlying function space.

4 Numerical experiments

In this section we present the results of numerical experiments. Our goal is to reinforce the robust convergence provided by the theoretical results, and to compare the performance of the quasi-Newton method with the exact Newton method.

Following [10], we solve BVP (2.1)-(2.2) on the unit cube $\Omega = (0,\, 1)^3$ with boundary portions

$$\Gamma_N := \{(x,\, y,\, z) \in \overline{\Omega}: \quad z = 1\}, \quad \Gamma_D = \partial\Omega \setminus \Gamma_N$$

and using the data of [10, Section 4]. However, to address the setting of the present paper, we include nondiagonal coefficients in the heat conductivity matrix, and let

$$A := 60 \cdot \begin{pmatrix} 1 & \mu & 0 \\ \mu & 1 & \mu \\ 0 & \mu & 1 \end{pmatrix},$$

where $0 < \mu < 1/\sqrt{2}$ (the upper bound is required for uniform positivity). The parameters are $\alpha = 90,\ \beta = 0.75 \cdot 5.669 \cdot 10^{-8}$. The heat sources in Ω and on Γ_N are

$$f(x, y, z) = 36000\pi^2 z \sin \pi x \sin \pi y$$

and

$$g(x, y, z) = 27000 + 45000 \sin \pi x \sin \pi y + 344.39175(1 + \sin \pi x \sin \pi y)^4,$$

respectively, while $\bar{u}(x, y, z) = \bar{u}$ constant on Γ_D. (These data in [10] give rise to an exact solution, which we reproduced for $\mu = 0$ and $\bar{u} = 300$. However, we are now interested in the more general case.) We wish to study the numerical behaviour with varying μ and $\bar{u}$, that is, how sensitive the method is to the measure of non-diagonality and to the prescribed temperature. The latter is important since higher temperatures yield an overall greater role of the nonlinear term, due to the used fourth power.

We applied trilinear finite elements. Matlab 2021a was used for the simulation. To obtain the mesh, we defined values k_i and then applied a uniform mesh with mesh parameters $h_i = \frac{1}{k_i+1}$, thus the number of degrees of freedom (DOF) can be calculated as $k_i^2(k_i + 1)$. We chose four different meshes, corresponding to k_i values 14, 20, 30 and 40, resulting in DOF 2940, 8400, 27900 and, 65600, respectively. The integration was done with the midpoint rule, and the auxiliary equation was solved by a direct solver. The stopping criterion was the standard Sobolev norm going below 10^{-6}. The initial condition was the constant 0 function.

For each iteration step n, the preconditioner used for the quasi-Newton method is the following:

$$\langle B_n h,\ v\rangle = \int_\Omega A\,\nabla h \cdot \nabla v + \alpha \int_{\Gamma_N} hv + \max\{3\beta |z_n + \bar{u}|^3\} \int_{\Gamma_N} hv \tag{4.1}$$

(that is, $G = A$, $\varrho = 1$ and $\tau = 3/4$). Here the first two terms and the integral in the third term do not depend on n. Thus, for every n, the stiffness matrix can be assembled from 2 precomputed matrices just using a linear combination.

The iteration numbers of (the exact) Newton method and the quasi-Newton method can be seen in Tables 1 and 2, respectively, for certain values of μ and $\bar{u}$ and for different mesh sizes. Apparently both methods are robust w.r.t. the mesh size, and slightly sensitive to the other parameters.

	$\mu = 0.2$			$\mu = 0.4$		
DOF	$\bar{u} = 300$	$\bar{u} = 600$	$\bar{u} = 1500$	$\bar{u} = 300$	$\bar{u} = 600$	$\bar{u} = 1500$
2940	3	3	4	3	3	4
8400	3	3	4	3	3	4
27900	3	3	4	3	3	4
65600	3	3	4	3	3	4

Table 1: Number of iterations using Newton's method.

	$\mu = 0.2$			$\mu = 0.4$		
DOF	$\bar{u} = 300$	$\bar{u} = 600$	$\bar{u} = 1500$	$\bar{u} = 300$	$\bar{u} = 600$	$\bar{u} = 1500$
2940	3	4	4	3	4	4
8400	3	3	4	3	3	4
27900	3	3	4	3	3	4
65600	3	3	4	3	3	4

Table 2: Number of iterations using the quasi-Newton method.

The ratios of the total runtimes (that is, not for just an individual iteration step but for the whole iteration) can be seen in Table 3. In particular, ratios of runtimes of assembling the stiffness matrix are shown in Table 4. We may observe that in most cases the quasi-Newton method consumed less overall runtime, and this is mostly due to the significantly cheaper assembly of stiffness matrices, thanks to their simplified structure.

	$\mu = 0.2$			$\mu = 0.4$		
DOF	$\bar{u} = 300$	$\bar{u} = 600$	$\bar{u} = 1500$	$\bar{u} = 300$	$\bar{u} = 600$	$\bar{u} = 1500$
2940	0.9009	1.1895	0.8843	0.8884	1.1850	0.8881
8400	0.8863	0.8819	0.8855	0.8923	0.8728	0.8830
27900	0.9095	0.9082	0.9056	0.9048	0.9199	0.9029
65600	0.9086	0.9083	0.9103	0.9068	0.9126	0.9108

Table 3: Ratio of total runtimes: $t_{\mathrm{qN}}/t_{\mathrm{N}}$.

Finally, the obtained numerical solutions allow us to examine the effects of some features of the problem. First, Table 5 reflects the effect of the nonlinearity in the Stefan–Boltzmann condition. Here (for the same parameters μ and $\bar{u}$ as above) we give the maximal and minimal values of the homogenized solution z_n for the "linear" problem, in which the 4th power term is neglected (that is, we set $\beta = 0$) and for the "nonlinear" problem, which is the same as throughout this section (that is, we set $\beta = 0.75 \cdot 5.669 \cdot 10^{-8}$). The function z_n here corresponds to our finest mesh with DOF 65600.

Further, Figures 1 and 2 show colourmaps of the numerical solution. On Figure 1 we visualize the solution obtained for some specific parameters, whereas Figure 2 illustrates how the solution varies on the radiating upper subsurface as we modify the non-orthotropic parameter μ.

	$\mu = 0.2$			$\mu = 0.4$		
DOF	$\bar{u} = 300$	$\bar{u} = 600$	$\bar{u} = 1500$	$\bar{u} = 300$	$\bar{u} = 600$	$\bar{u} = 1500$
2940	0.0272	0.0268	0.0268	0.0273	0.0272	0.0295
8400	0.0126	0.0123	0.0127	0.0131	0.0127	0.0129
27900	0.0049	0.0048	0.0047	0.0045	0.0045	0.0046
65600	0.0023	0.0022	0.0024	0.0023	0.0023	0.0024

Table 4: Ratio of average runtimes of assembling the stiffness matrix for an individual iteration step: $t_{\text{as,qN}}/t_{\text{as,N}}$.

	$\mu = 0.2$			$\mu = 0.4$		
	$\bar{u} = 300$	$\bar{u} = 600$	$\bar{u} = 1500$	$\bar{u} = 300$	$\bar{u} = 600$	$\bar{u} = 1500$
$nonlin \max z_n$	253.57	147.89	58.94	196.44	107.85	49.83
$lin \max z_n$	262.38	178.61	82.25	201.35	130.32	61.83
$nonlin \min z_n$	0	-24.38	-360.02	0	-25.02	-357.75
$lin \min z_n$	0	-19.13	-152.66	0	-19.98	-158.26

Table 5: Maximal and minimal values of the homogenized solution z_n for linear/nonlinear problems for DoF = 65600.

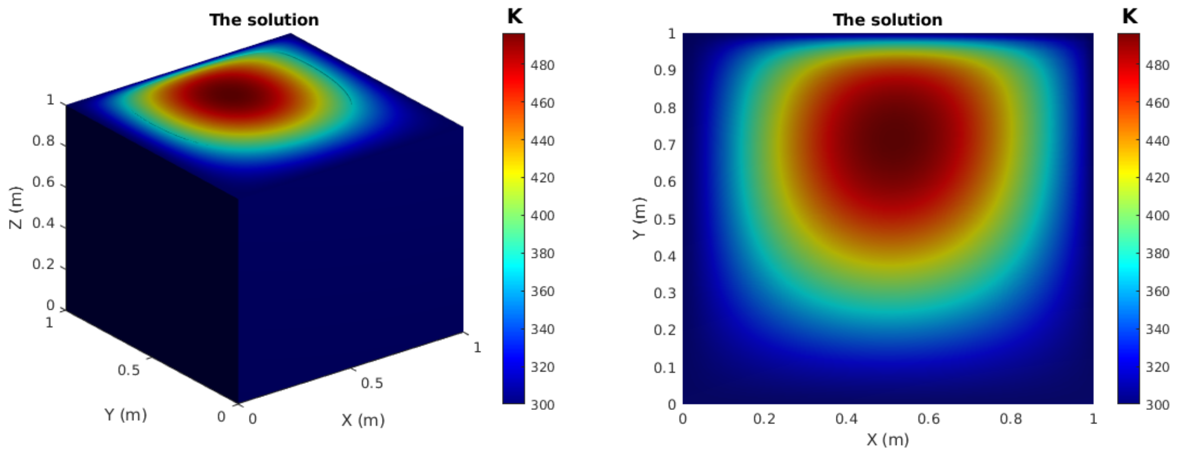

Figure 1: Heat colourmap of the numerical solution $u_n = z_n + \bar{u}$ on the whole cube and on the subsurface Γ_N, respectively, for DoF = 65600, $\bar{u} = 300$, and $\mu = 0.4$.

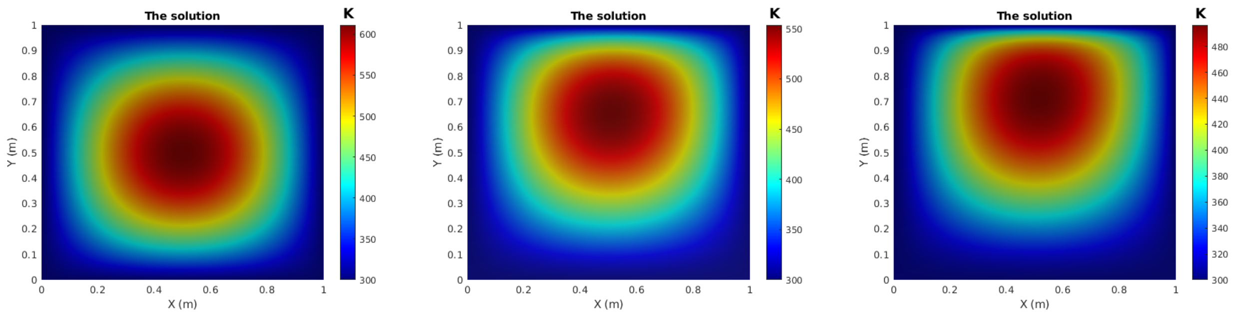

Figure 2: Heat colourmap of the numerical solution $u_n = z_n + \bar{u}$ on the subsurface Γ_N for DoF = 65600, $\bar{u} = 300$, for varied values of μ: respectively, $\mu = 0$, $\mu = 0.2$, $\mu = 0.4$.

Altogether, compared to the full Newton's method, we observe that (besides simpler coding) our quasi-Newton method leads to a reduced computational cost, which is a significant aspect for 3D problems. The main source of reducing the cost is that the stiffness matrices of the preconditioning operators can be assembled from two precomputed matrices just using a linear combination in each step of the quasi-Newton iteration. We also note that the gain in cost may be even higher for domains with irregular geometry, whose boundary (where the quasi-Newton provides the simplifications) contains a higher relative number of DOFs than for our test problem. The study of such models might be the subject of further research.

Acknowledgements. This research has been supported by the BME NC TKP2020 grant of NKFIH Hungary and also carried out in the ELTE Institutional Excellence Program (1783-3/2018/FEKUTSRAT) supported by the Hungarian Ministry of Human Capacities, and further, it was supported by the Hungarian Scientific Research Fund NKFIH grants SNN125119 and K 137699.

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