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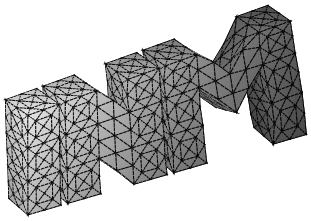

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Technische Universität Graz
Institut für Numerische Mathematik
Steyrergasse 30
A 8010 Graz

WWW: `http://www.numerik.math.tu-graz.at`

Fast evaluation of volume potentials in boundary element methods

G. Of, O. Steinbach, P. Urthaler

Institute of Computational Mathematics
Graz University of Technology
Steyrergasse 30, 8010 Graz, Austria

Abstract

The solution of inhomogeneous partial differential equations by boundary element methods requires the evaluation of volume potentials. A direct standard computation of the classical Newton potentials is possible, but expensive. Here, a fast evaluation of the Newton potentials by using the fast multipole method is described and analyzed. In particular, an approximation by the fast multipole method is investigated and related error estimates are given. Furthermore, an indirect evaluation of the normal derivative of the Newton potential is presented. A numerical analysis is presented for all approaches mentioned above. Numerical results are given for the Poisson equation, and for the system of linear elastostatics.

1 Introduction

Fast boundary element methods are well established when solving homogeneous partial differential equations, see, e.g., [15]. This is mainly due to the fact that only a boundary triangulation is needed. When dealing with inhomogeneous partial differential equations, volume potentials require an integration over the whole domain, and the advantage of the boundary element methods seems to be lost. Besides a direct evaluation of the volume potential, there are several approaches available to deal with those volume integrals. In engineering, the most common one seems to be the dual reciprocity method, see [1, 5] and the references given therein. The main idea of the dual reciprocity approach is to use integration by parts to rewrite the volume integrals as surface potentials. In fact, a particular solution of the partial differential equation is constructed. In particular, the right hand side of the partial differential equation is approximated by basis functions, e.g. radial basis functions, which allow a simple solution of the partial differential equation. On the other hand, particular solutions are computed by finite difference methods or by finite element methods [11] by embedding the domain into an auxiliary domain and solving the inhomogeneous equation on a uniform grid. Due to the uniform grid fast

Fourier transformation based solvers can be used [2]. A particular solution can also be obtained by evaluating the Newton potential of such an auxiliary domain by a fast multipole method, which was done for example in [4] for a two-dimensional Poisson problem. Given a particular solution one has to solve the homogeneous boundary value problem with modified boundary values. The inhomogeneity can also be incorporated directly into the formulation, which requires the evaluation of the Newton potential of the domain itself by the fast multipole method. In [10], the dual reciprocity method, the computation of a particular solution by finite element methods and the evaluation of the Newton potential of the domain by the fast multipole method are compared for 2D. In their comparison, the fast multipole method seems to be superior. In the literature, Dirichlet boundary value problems in 2D are treated mostly. Thus the normal derivative of the Newton potentials as in the hypersingular boundary integral equation is often neglected. Evaluation of volume potentials in 3D are studied for the solution of volume integral equations e.g. in [17, 26]. Here we will consider an acceleration of the direct evaluation of Newton potentials by using fast boundary element methods. In this paper, we propose and analyze the use of the fast multipole method [6, 7, 12] for an efficient evaluation of the Newton potentials in the symmetric formulation of boundary integral equations. Additionally, we investigate an indirect approach for the evaluation of the normal derivative of the Newton potential as used within the hypersingular boundary integral equation which is based on the knowledge of the first Newton potential only. It turns out, that the latter approach seems to be more efficient than the direct evaluation of both Newton potentials. This approach can be extended directly to handle non–linear and time dependent boundary value problems.
The paper is organized as follows: In Sect. 2 we describe the symmetric formulation of boundary integral equations and the use of a Galerkin boundary element method to solve mixed boundary value problems for the Poisson equation. In Sect. 3 we first discuss the standard evaluation of Newton potentials, before describing the use of fast multipole methods for their acceleration. In addition, we derive an alternative representation of the normal derivative of the Newton potential. Then we analyze the fast multipole approximation of both Newton potentials and derive related error estimates for the boundary element solutions of the related boundary value problems. Finally, some numerical experiments for the Poisson equation and for the system of linear elastostatics in Sect. 4 confirm the theoretical results.

2 Boundary integral equations

For a simply connected bounded domain $\Omega \subset \mathbb{R}^3$ with a Lipschitz boundary $\Gamma = \partial\Omega$, we consider the Poisson equation with mixed boundary conditions as a model problem

$$-\Delta u(x) = f(x) \text{ for } x \in \Omega,\ u(x) = g_D(x) \text{ for } x \in \Gamma_D,\ \frac{\partial}{\partial n_x} u(x) = g_N(x) \text{ for } x \in \Gamma_N \quad (2.1)$$

where $\Gamma = \overline{\Gamma}_D \cup \overline{\Gamma}_N$, and n_x is the exterior unit normal vector which is defined for almost all $x \in \Gamma$. The solution of the mixed boundary value problem (2.1) is given by the

representation formula for $x \in \Omega$

$$u(x) = \int_\Gamma U^*(x,y)t(y)ds_y - \int_\Gamma \frac{\partial}{\partial n_y} U^*(x,y)u(y)ds_y + \int_\Omega U^*(x,y)f(y)dy \qquad (2.2)$$

where

$$U^*(x,y) = \frac{1}{4\pi}\frac{1}{|x-y|}$$

is the fundamental solution of the Laplace operator, and $t = \frac{\partial}{\partial n}u$ is the related normal derivative of u. We will use the symmetric formulation of boundary integral equations to compute the remaining Cauchy data. When applying the Dirichlet and Neumann traces to the representation formula (2.2), we obtain a system of boundary integral equations,

$$\begin{pmatrix} u \\ t \end{pmatrix} = \begin{pmatrix} \frac{1}{2}I - K & V \\ D & \frac{1}{2}I + K' \end{pmatrix} \begin{pmatrix} u \\ t \end{pmatrix} + \begin{pmatrix} N_0 f \\ N_1 f \end{pmatrix}. \qquad (2.3)$$

In (2.3),

$$(Vw)(x) = \int_\Gamma U^*(x,y)w(y)ds_y \quad \text{for } x \in \Gamma$$

is the single layer potential $V : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$,

$$(Kv)(x) = \lim_{\varepsilon \to 0} \int_{y \in \Gamma : |y-x| > \varepsilon} \frac{\partial}{\partial n_y} U^*(x,y)v(y)ds_y \quad \text{for } x \in \Gamma$$

is the double layer potential $K : H^{1/2}(\Gamma) \to H^{1/2}(\Gamma)$,

$$(K'w)(x) = \lim_{\varepsilon \to 0} \int_{y \in \Gamma : |y-x| > \varepsilon} \frac{\partial}{\partial n_x} U^*(x,y)w(y)ds_y \quad \text{for } x \in \Gamma$$

is the adjoint double layer potential $K' : H^{-1/2}(\Gamma) \to H^{-1/2}(\Gamma)$, and

$$(Dv)(x) = -\frac{\partial}{\partial n_x} \int_\Gamma \frac{\partial}{\partial n_y} U^*(x,y)v(y)ds_y \quad \text{for } x \in \Gamma$$

is the hypersingular boundary integral operator $D : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$. Note that the mapping properties of all boundary integral operators are well known, see, e.g. [3, 9, 16, 20]. In particular, the single layer potential V is $H^{-1/2}(\Gamma)$–elliptic, and the hypersingular boundary integral operator D is $H^{1/2}(\Gamma)$–semi–elliptic.

Due to the inhomogeneous partial differential equation, we have to introduce in addition the Newton potentials

$$(N_0 f)(x) = \int_\Omega U^*(x,y)f(y)dy \quad \text{for } x \in \Gamma \qquad (2.4)$$

and

$$(N_1 f)(x) = \frac{\partial}{\partial n_x} \int_\Omega U^*(x,y) f(y) dy \quad \text{for } x \in \Gamma. \tag{2.5}$$

When using the symmetric formulation of boundary integral equations to solve the mixed boundary value problem (2.1), the first equation in (2.3) is considered for $x \in \Gamma_D$, while the second equation in (2.3) is used for $x \in \Gamma_N$. In particular, let $\widetilde{g}_N \in H^{-1/2}(\Gamma)$ and $\widetilde{g}_D \in H^{1/2}(\Gamma)$ be arbitrary but fixed extensions of the given data $g_N \in H^{-1/2}(\Gamma_N)$ and $g_D \in H^{1/2}(\Gamma_D)$, respectively. Then we have to find

$$\widetilde{t} = t - \widetilde{g}_N \in \widetilde{H}^{-1/2}(\Gamma_D), \quad \widetilde{u} = u - \widetilde{g}_D \in \widetilde{H}^{1/2}(\Gamma_N)$$

as the unique solution of the system of boundary integral equations,

$$(V\widetilde{t})(x) - (K\widetilde{u})(x) = (\frac{1}{2}I + K)\widetilde{g}_D(x) - (V\widetilde{g}_N)(x) - (N_0 f)(x) \quad \text{for } x \in \Gamma_D, \tag{2.6}$$

$$(K'\widetilde{t})(x) + (D\widetilde{u})(x) = (\frac{1}{2}I - K')\widetilde{g}_N(x) - (D\widetilde{g}_D)(x) - (N_1 f)(x) \quad \text{for } x \in \Gamma_N. \tag{2.7}$$

Let

$$S_h^0(\Gamma_D) = \operatorname{span}\{\psi_k\}_{k=1}^{N_D} \subset \widetilde{H}^{-1/2}(\Gamma_D), \quad S_h^1(\Gamma_N) = \operatorname{span}\{\varphi_i\}_{i=1}^{M_N} \subset \widetilde{H}^{1/2}(\Gamma_N)$$

be some boundary element spaces, e.g. of piecewise constant basis functions ψ_k and piecewise linear basis functions φ_i, which are defined with respect to an admissible boundary element mesh of mesh size h. N_D denotes the number of elements of Γ_D, while M_N is the number of nodes without Dirichlet boundary conditions. The Galerkin variational problem of the system of boundary integral equations (2.6) and (2.7) reads: Find $(\widetilde{t}_h, \widetilde{u}_h) \in S_h^0(\Gamma_D) \times S_h^1(\Gamma_N)$ such that

$$\langle V\widetilde{t}_h, \tau_h\rangle_{\Gamma_D} - \langle K\widetilde{u}_h, \tau_h\rangle_{\Gamma_D} = \langle(\frac{1}{2}I + K)\widetilde{g}_D - V\widetilde{g}_N - N_0 f, \tau_h\rangle_{\Gamma_D} \tag{2.8}$$

for all $\tau_h \in S_h^0(\Gamma_D)$ and

$$\langle K'\widetilde{t}_h, v_h\rangle_{\Gamma_N} + \langle D\widetilde{u}_h, v_h\rangle_{\Gamma_N} = \langle(\frac{1}{2}I - K')\widetilde{g}_N - D\widetilde{g}_D - N_1 f, v_h\rangle_{\Gamma_N} \tag{2.9}$$

for all $v_h \in S_h^1(\Gamma_N)$. The Galerkin formulation (2.8) and (2.9) is equivalent to a linear system of algebraic equations,

$$\begin{pmatrix} V_h & -K_h \\ K_h^\top & D_h \end{pmatrix} \begin{pmatrix} \underline{\widetilde{t}} \\ \underline{\widetilde{u}} \end{pmatrix} = \begin{pmatrix} \underline{f}_1 \\ \underline{f}_2 \end{pmatrix} - \begin{pmatrix} \underline{N}_0 \\ \underline{N}_1 \end{pmatrix}, \tag{2.10}$$

where the blocks of the stiffness matrix are

$$V_h[\ell, k] = \langle V\psi_k, \psi_\ell\rangle_{\Gamma_D}, \quad K_h[\ell, i] = \langle K\varphi_i, \psi_\ell\rangle_{\Gamma_D}, \quad D_h[j, i] = \langle D\varphi_i, \varphi_j\rangle_{\Gamma_N}$$

for $k, \ell = 1, \ldots, N_D$, $i, j = 1, \ldots, M_N$. Moreover, for $\ell = 1, \ldots, N_D$ and for $j = 1, \ldots, M_N$ we have

$$f_{1,\ell} = \langle (\frac{1}{2} I + K) \widetilde{g}_D - V \widetilde{g}_N, \psi_\ell \rangle_{\Gamma_D}, \quad f_{2,j} = \langle (\frac{1}{2} I - K') \widetilde{g}_N - D \widetilde{g}_D, \varphi_j \rangle_{\Gamma_N}.$$

In the case of an inhomogeneous partial differential equation, the right hand side of the linear system (2.10) involves contributions due to the Newton potentials $N_0 f$ and $N_1 f$. In particular, we need to compute, for $\ell = 1, \ldots, N_D$ and $j = 1, \ldots, M_N$,

$$N_{0,\ell} = \int_{\Gamma_D} \psi_\ell(x) \int_\Omega U^*(x,y) f(y) dy \, ds_x, \tag{2.11}$$

$$N_{1,j} = \int_{\Gamma_N} \varphi_j(x) \frac{\partial}{\partial n_x} \int_\Omega U^*(x,y) f(y) dy \, ds_x \, . \tag{2.12}$$

Note that the bilinear form

$$a(t,u;\tau,v) = \langle Vt, \tau \rangle_{\Gamma_D} - \langle Ku, \tau \rangle_{\Gamma_D} + \langle K't, v \rangle_{\Gamma_N} + \langle Du, v \rangle_{\Gamma_N}$$

which is related to the variational problem (2.8) and (2.9) is bounded, i.e.

$$a(t,u;\tau,v) \leq c_2^A \, \|(t,u)\|_{H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)} \|(\tau,v)\|_{H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)} \tag{2.13}$$

for all $(t,u), (\tau,v) \in \widetilde{H}^{-1/2}(\Gamma_D) \times \widetilde{H}^{1/2}(\Gamma_N)$, and $\widetilde{H}^{-1/2}(\Gamma_D) \times \widetilde{H}^{1/2}(\Gamma_N)$–elliptic, i.e.

$$a(\tau,v;\tau,v) \geq c_1^A \, \|(\tau,v)\|^2_{H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)} \tag{2.14}$$

for all $(\tau,v) \in \widetilde{H}^{-1/2}(\Gamma_D) \times \widetilde{H}^{1/2}(\Gamma_N)$, where

$$\|(\tau,v)\|^2_{H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)} = \|\tau\|^2_{H^{-1/2}(\Gamma)} + \|v\|^2_{H^{1/2}(\Gamma)} \, .$$

Hence we conclude the unique solvability of the Galerkin variational problem (2.8) and (2.9), and of the linear system (2.10). Moreover, there holds the error estimate, see, e.g., [20, Sect. 12.3],

$$\begin{aligned} \|(\widetilde{t} - \widetilde{t}_h, \widetilde{u} - \widetilde{u}_h)\|^2_{H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)} &= \|\widetilde{t} - \widetilde{t}_h\|^2_{H^{-1/2}(\Gamma)} + \|\widetilde{u} - \widetilde{u}_h\|^2_{H^{1/2}(\Gamma)} \\ &\leq c \, h^3 \left[|\widetilde{t}|^2_{H^1_{\rm pw}(\Gamma)} + |\widetilde{u}|^2_{H^2(\Gamma)} \right] \end{aligned} \tag{2.15}$$

when assuming $\widetilde{g}_N \in H^1_{\rm pw}(\Gamma)$ and $\widetilde{g}_D \in H^2(\Gamma)$. Note that the error estimate (2.15) remains valid when a fast boundary element method is used to accelerate the application of the discrete boundary integral operators which are involved in the linear system (2.10), see, e.g., [14, Theorem 4.1, Remark 4.3] for the use of a fast multipole method in the case of a homogeneous partial differential equation. Note that an appropriate choice of all involved fast multipole parameters is required in this case.

3 Evaluation of Newton potentials

3.1 Direct evaluation

To compute the discrete Newton potential $\underline{N}_0$ as given in (2.11), the order of integration is interchanged first. In particular, for a piecewise constant basis function ψ_ℓ we have

$$N_{0,\ell} \;=\; \int_\Omega f(y) \int_{\tau_\ell} U^*(x,y) ds_x dy \;=\; \sum_{k=1}^{N_\Omega} \int_{T_k} f(y) \int_{\tau_\ell} U^*(x,y) ds_x dy$$

where $\overline{\Omega} = \bigcup_{i=1}^{N_\Omega} T_i$ is some volume mesh with suitable chosen elements T_i, e.g. tetrahedra. Then, by using some numerical integration scheme, this gives

$$\widetilde{N}_{0,\ell} \;=\; \sum_{k=1}^{N_\Omega} \Delta_k \sum_{\iota=1}^{M_T} \omega_\iota f(y_\iota^k) \int_{\tau_\ell} U^*(x, y_\iota^k) ds_x \tag{3.1}$$

where Δ_k is the volume of the element T_k, and M_T is the number of local integration nodes. Note that the remaining surface integral corresponds to the discretization of the single layer potential via collocation which can be computed analytically, see, e.g., [15, Appendix C.2.1]. For the discrete Newton potential $\underline{N}_1$ as defined in (2.12) we get analogously

$$N_{1,j} \;=\; \sum_{k=1}^{N_\Omega} \int_{T_k} f(y) \int_\Gamma \varphi_j(x) \frac{\partial}{\partial n_x} U^*(x,y) ds_x \, dy \,.$$

Hence we compute the approximation

$$\widetilde{N}_{1,j} \;=\; \sum_{k=1}^{N_\Omega} \Delta_k \sum_{\iota=1}^{M_T} \omega_\iota f(y_\iota^k) \int_\Gamma \varphi_j(x) \frac{\partial}{\partial n_x} U^*(x, y_\iota^k) ds_x, \tag{3.2}$$

where the remaining surface integral corresponds to the discretization of the double layer potential via collocation which again can be computed analytically [15, Appendix C.2.2]. While the error of the numerical integration formulae (3.1) and (3.2) can be included in the resulting error estimates of the perturbed variational formulation via the Strang lemma, see e.g. [20], the numerical effort to compute (3.1) and (3.2) is not optimal. In particular, the complexity is at least of order $N_\Gamma N_\Omega$ where N_Ω is the number of volume elements, and N_Γ is the total number of boundary elements.

3.2 Fast multipole evaluation of Newton potentials

For an efficient evaluation of the Newton potential $N_0 f$ by using the Fast Multipole Method [6, 7, 12] the kernel of the volume integral is replaced by a series expansion, i.e. for $x \neq y$

$$k(x,y) = \frac{1}{|x-y|} = \sum_{n=0}^{\infty} \frac{|x|^n}{|y|^{n+1}} P_n(\hat{x} \cdot \hat{y}), \quad \hat{x} = \frac{x}{|x|}, \quad \hat{y} = \frac{y}{|y|},$$

where P_n are the Legendre polynomials. The truncation of the series expansion and the separation of the variables by an appropriate reformulation of the spherical harmonics, see e.g. [23, 25], lead to the approximation

$$k_p(x,y) = \sum_{n=0}^{p} \sum_{m=-n}^{n} \overline{S_n^m(y)} R_n^m(x) \tag{3.3}$$

where for $m \geq 0$

$$\begin{aligned} R_n^{\pm m}(x) &= \frac{1}{(n+m)!} \frac{d^m}{du^m} P_n(u)|_{u=\hat{x}_3} (\hat{x}_1 \pm i\hat{x}_2)^m |x|^n, \\ S_n^{\pm m}(y) &= (n-m)! \frac{d^m}{du^m} P_n(u)|_{u=\hat{y}_3} (\hat{y}_1 \pm i\hat{y}_2)^m \frac{1}{|y|^{n+1}}\,. \end{aligned}$$

The series expansion (3.3) approximates the kernel only well for volume elements T_k which are well separated from the boundary elements τ_ℓ. Therefore the domain Ω has to be divided into a farfield $\mathrm{FF}(\ell)$, where the approximation (3.3) is valid, and into a nearfield $\mathrm{NF}(\ell)$, where the approximation is not valid. Hence we obtain an approximation

$$\widetilde{N}_{0,\ell} = \sum_{k \in \mathrm{NF}(\ell)} \int_{T_k} f(y) \int_{\tau_\ell} U^*(x,y) ds_x dy + \frac{1}{4\pi} \int_{\tau_\ell} \sum_{k \in \mathrm{FF}(\ell)} \int_{T_k} k_p(x,y) f(y) dy ds_x\,.$$

The first sum over the nearfield $\mathrm{NF}(\ell)$ is evaluated directly as given in (3.1). In the farfield $\mathrm{FF}(\ell)$, the kernel is approximated by the series expansion (3.3),

$$\begin{aligned} \widetilde{N}_{0,\ell} &= \sum_{k \in \mathrm{NF}(\ell)} \Delta_k \sum_{\iota=1}^{M_T} \omega_\iota f(y_\iota^k) \int_{\tau_\ell} U^*(x, y_\iota^k) ds_x \\ &\qquad + \frac{1}{4\pi} \int_{\tau_\ell} \sum_{k \in \mathrm{FF}(\ell)} \int_{T_k} f(y) \sum_{n=0}^{p} \sum_{m=-n}^{n} \overline{S_n^m(y)} R_n^m(x) dy ds_x \\ &= \sum_{k \in \mathrm{NF}(\ell)} \Delta_k \sum_{\iota=1}^{M_T} \omega_\iota f(y_\iota^k) \int_{\tau_\ell} U^*(x, y_\iota^k) ds_x + \frac{1}{4\pi} \sum_{n=0}^{p} \sum_{m=-n}^{n} M_n^m(O,\ell) \widetilde{L}_n^m(FF(\ell)) \end{aligned}$$

where

$$M_n^m(O,\ell) = \int_{\tau_\ell} R_n^m(x) ds_x,\ L_n^m(O,k) = \int_{T_k} \overline{S_n^m(y)} f(y) dy,\ \widetilde{L}_n^m(FF(\ell)) = \sum_{k \in FF(\ell)} L_n^m(O,k).$$

Note that O describes the origin of a local coordinate system. The coefficients $\widetilde{L}_n^m(FF(\ell))$ still depend on the farfield of the boundary element τ_ℓ. Hence, the computation of the Newton potential $\underline{\widetilde{N}}_0$ still requires $N_\Gamma N_\Omega$ operations. To end up with a more efficient evaluation, an approximation of the coefficients $\widetilde{L}_n^m(FF(\ell))$ is computed by utilizing a hierarchical cluster structure to compute approximations of as large partial sums of $\widetilde{L}_n^m(FF(\ell))$ as possible.

The cluster structure is set up over the volume elements T_k and over the boundary elements τ_ℓ as follows. First, a cube is created which contains the computational domain Ω. All elements inside the cube define the coarse cluster ω_1^0 which is subdivided into eight clusters ω_j^1. Each element is then assigned to one son cluster ω_j^1 by its center point. Clusters which contain no elements are neglected. This process is continued recursively until a desired depth L of the cluster tree is reached, as long as the average number of elements per cluster does not fall below a suitable chosen minimum. For each cluster ω_j^λ of level λ, C_j^λ is the cluster center and $r_j^\lambda = \sup_{x\in\omega_j^\lambda} |x - C_j^\lambda|$ is the cluster radius. A cluster ω_i^λ is in the nearfield of a cluster ω_j^λ, if

$$\operatorname{dist}\{C_i^\lambda, C_j^\lambda\} \;\le\; (d+1)\max\{r_i^\lambda, r_j^\lambda\} \tag{3.4}$$

with the nearfield parameter $d > 1$. The nearfield of a son cluster is always contained in the nearfield of the father cluster. If ω_i^L is the cluster containing τ_ℓ, and ω_j^L is the cluster containing T_k, then the nearfield $\mathrm{NF}(\ell)$ and the farfield $\mathrm{FF}(\ell)$ of the boundary element τ_ℓ are defined as

$$\mathrm{NF}(\ell) := \{k, 1 \le k \le N_\Omega : (3.4) \text{ holds}\}, \quad \mathrm{FF}(\ell) := \{1, \ldots, N_\Omega\} \setminus \mathrm{NF}(\ell).$$

To compute approximations of the coefficients $\widetilde{L}_n^m(FF(\ell))$ efficiently, two kinds of series expansions with respect to different local coordinate systems are used. Let ω_j^L be a cluster in the farfield of the cluster ω_i^L which contains the boundary element τ_ℓ. The contribution of all elements of ω_j^L to the farfield part of $\widetilde{N}_{0,\ell}$ can be given by

$$\widetilde{N}_{0,\ell}^{\omega_j^L} = \frac{1}{4\pi} \sum_{n=0}^{p} \sum_{m=-n}^{n} M_n^m(C_i^L, \ell) \sum_{T_k \in \omega_j^L} L_n^m(C_i^L, k).$$

The origin of the local coordinate system is chosen as the center C_i^L of the cluster ω_i^L. This series expansion is called the local expansion. Alternatively, by interchanging the roles of x and y, one can use the so called multipole expansion

$$\widehat{N}_{0,\ell}^{\omega_j^L} = \frac{1}{4\pi} \sum_{n=0}^{p} \sum_{m=-n}^{n} \int_{\tau_\ell} \overline{S_n^m(y - C_j^L)} ds_y \sum_{T_k \in \omega_j^L} \int_{T_k} R_n^m(x - C_j^L) f(x) dx, \tag{3.5}$$

where the point of origin is chosen as the center C_j^L of the cluster ω_j^L. The sum of all local expansions contains the information of all elements outside the nearfield of the cluster ω_i^L, whereas the multipole expansion contains the information of all elements inside the cluster ω_j^L.

Next, a brief description of the fast multipole algorithm and the involved operators is presented. For a detailed description see e.g. [6, 7, 12]. According to the multipole expansion (3.5), the coefficients

$$\hat{M}_n^m(C_j^L, k) = \int_{T_k} R_n^m(x - C_j^L) f(x) dx \tag{3.6}$$

are calculated for each volume element T_k first, where C_j^L is the center of the cluster w_j^L associated to T_k. Then the coefficients of the multipole expansion (3.5) are calculated for all clusters ω_j^L on the finest level by

$$\tilde{M}_n^m(C_j^L, \omega_j^L) = \sum_{T_k \in \omega_j^L} \hat{M}_n^m(C_j^L, k).$$

By the translation

$$\tilde{M}_n^m(C_j^\lambda, \omega_j^\lambda) = \sum_{\omega_i^{\lambda+1} \in \mathrm{Sons}(\omega_j^\lambda)} \sum_{s=0}^{n} \sum_{t=-s}^{s} R_s^t(\overrightarrow{C_j^\lambda C_j^{\lambda+1}}) \tilde{M}_{n-s}^{m-t}(C_i^{\lambda+1}, \omega_i^{\lambda+1})$$

the coefficients of the multipole expansion are computed recursively for all father clusters ω_j^λ. Multipole expansions can be converted into local expansions by

$$L_n^m(C_i^\lambda, \omega_j^\lambda) = \sum_{s=0}^{\infty} \sum_{t=-s}^{s} (-s)^n \overline{S_{n+s}^{m+t}}(\overrightarrow{C_j^\lambda C_i^\lambda}) \tilde{M}_s^t(C_j^\lambda, \omega_j^\lambda)$$

to compute approximations of the coefficients $L_n^m(O, i)$, if ω_j^λ is in the farfield of ω_i^λ. This is done on the coarsest possible cluster level, i.e., the two clusters ω_i^λ and ω_j^λ are in their mutual farfield, whereas the father clusters are in the nearfield of each other. This procedure guarantees that the admissibility condition is always adhered and the single expansions can be used many times. The local coefficients are converted on several levels. Thus, their contributions have to be shifted to the clusters of finer levels. In detail, the coefficients of local expansion of each cluster ω_i^λ are translated to its son clusters $\omega_j^{\lambda+1}$ by

$$\tilde{L}_n^m(C_j^{\lambda+1}, \mathrm{FF}(\omega_i^\lambda)) = \sum_{s=n}^{p} \sum_{t=-s}^{s} R_{s-n}^{t-m}(\overrightarrow{C_i^\lambda C_j^{\lambda+1}}) \tilde{L}_s^t(C_i^\lambda, \mathrm{FF}(\omega_i^\lambda)).$$

The local coefficients $\tilde{L}_n^m(C_j^{\lambda+1}, \mathrm{FF}(\omega_i^{\lambda+1}))$ of a cluster $\omega_j^{\lambda+1}$ are defined by the sum of the translated coefficients of the father cluster and of all local coefficients converted from multipole expansions to the cluster $\omega_j^{\lambda+1}$ directly. Finally all $\tilde{L}_n^m(FF(\ell)) = \tilde{L}_n^m(C_i^L, \mathrm{FF}(\omega_i^L))$ are computed by the described algorithm, and the farfield part of the sum (3.5) can be evaluated efficiently.

For the Newton potential $N_1 f$, the fast multipole method can be used in almost the same way. Again the set of volume elements T_k is split into near- and farfield. The nearfield part is evaluated directly by (3.2), whereas in the farfield the kernel approximation is used. This leads to the approximation

$$\widetilde{N}_{1,\ell} = \sum_{k \in \mathrm{NF}(\ell)} \Delta_k \sum_{\iota=1}^{M_T} \omega_\iota f(y_\iota^k) \int_{\Gamma_N} \varphi_\ell(x) \frac{\partial}{\partial n_x} U^*(x, y_\iota^k) ds_x + \frac{1}{4\pi} \sum_{n=0}^{p} \sum_{m=-n}^{m} M_n^m(O, \ell) \tilde{L}_n^m(\mathrm{FF}(\ell))$$

Operations	Complexity
Computation of the multipole expansion for all N_Ω volume elements.	$N_\Omega \mathcal{O}(p^2)$
Translation of the multipole expansions of all clusters of the volume tree to its father clusters.	$2a_\Omega \mathcal{O}(p^4)$
Conversion of the multipole expansion into a local expansion. For each cluster of the boundary tree at most c_d conversion occur.	$c_d 2a_\Gamma \mathcal{O}(p^4)$
Translation of the local expansions to all son cluster of the boundary tree.	$2a_\Gamma \mathcal{O}(p^4)$
Evaluation of the local expansion for all N_Γ boundary elements.	$N_\Gamma \mathcal{O}(p^2)$
At most $\mathcal{O}(\log^2 N_\Omega)$ nearfield contributions are computed per boundary element.	$N_\Gamma \mathcal{O}(\log^2 N_\Omega)$

Table 1: Complexity estimation for the fast multipole method for Newton potentials.

with the coefficients

$$M_n^m(O,\ell) = \int_{\Gamma_N} \varphi_\ell(x) \frac{\partial}{\partial n_x} R_n^m(x) ds_x.$$

Approximations of the coefficients $\tilde{L}_n^m(\mathrm{FF}(\ell))$ can be calculated in the same way as for the Newton potential $N_0 f$. Thus, the only difference is the computation of the coefficients $M_n^m(O,\ell)$, where linear test functions φ_ℓ and normal derivatives of the coefficients $R_n^m(x)$ are involved.

For the direct evaluation (3.1) and (3.2) of the Newton potentials $N_0 f$ and $N_1 f$ one ends up with a complexity of $\mathcal{O}(N_\Gamma^{5/2})$ essential operations, where $N_\Omega \sim N_\Gamma^{3/2}$. Any expansion of the fast multipole method is described by $\mathcal{O}(p^2)$ coefficients. The number of clusters on the finest level is denoted by a_Γ for the cluster tree containing boundary elements and a_Ω for the cluster tree containing volume elements. The cluster trees can be built in such a way that

$$a_\Gamma = \mathcal{O}\left(\frac{N_\Gamma}{\log^2 N_\Gamma}\right), \qquad a_\Omega = \mathcal{O}\left(\frac{N_\Omega}{\log^2 N_\Omega}\right).$$

Due to the cluster tree, the total number of cluster is bounded by $2a_\Gamma$ and $2a_\Omega$, respectively. For a detailed description of the notation and an analysis of the effort of a fast multipole realization of the boundary integral operators of the Laplacian see [14]. For the fast multipole method of the volume potentials, the computational complexity of the individual operations is outlined in Table 1. The number of conversions of multipole expansions to the local expansion of a single cluster is bounded by a constant c_d, if the nearfield parameter d is fixed. The expansion degree p has to be chosen proportional to $\log N_\Gamma$ according to the error estimates in Lemma 3.2 and 3.3. Thus the computational complexity of the fast multipole method turns out to be $\mathcal{O}(N_\Gamma^{3/2} \log^2 N_\Gamma)$ essential operations.

Remark 3.1. *If less than $\mathcal{O}(N_\Gamma^{3/2})$ volume elements are sufficient to guarantee the optimal accuracy of the boundary element method, e.g. by a suitable choice of cubature rules, the fast multipole realization of the Newton potential will perform better as estimated here. Our implementation would be able to take advantage of such a modification.*

3.3 An alternative representation of $N_1 f$

The Newton potential $N_1 f$ allows an alternative representation which only requires the evaluation of the Newton potential $N_0 f$ in combination with some other boundary integral operators. In particular, the first boundary integral equation in (2.3) results in the Dirichlet to Neumann map

$$t = V^{-1}(\frac{1}{2}I + K)u - V^{-1}N_0 f\,. \tag{3.7}$$

Inserting (3.7) into the second equation in (2.3) we obtain

$$t \;=\; [D + (\frac{1}{2}I + K')V^{-1}(\frac{1}{2}I + K)]u + N_1 f - (\frac{1}{2}I + K')V^{-1}N_0 f\,. \tag{3.8}$$

A comparison of (3.8) with (3.7) gives

$$N_1 f - (\frac{1}{2}I + K')V^{-1}N_0 f \;=\; -V^{-1}N_0 f,$$

and therefore we conclude the alternative representation

$$(N_1 f)(x) = (-\frac{1}{2}I + K')V^{-1}(N_0 f)(x) \quad \text{for } x \in \Gamma. \tag{3.9}$$

For the evaluation of the discrete Newton potential $\underline{N}_1$ as defined in (2.12), we then obtain

$$N_{1,j} = \langle N_1 f, \varphi_j\rangle_\Gamma = \langle(-\frac{1}{2}I + K')V^{-1}N_0 f, \varphi_j\rangle_\Gamma = \langle(-\frac{1}{2}I + K')w, \varphi_j\rangle_\Gamma$$

where $w = V^{-1}N_0 f \in H^{-1/2}(\Gamma)$ is the unique solution of the variational problem

$$\langle Vw, z\rangle_\Gamma = \langle N_0 f, z\rangle_\Gamma \quad \text{for all } z \in H^{-1/2}(\Gamma). \tag{3.10}$$

The Galerkin discretization of the variational problem (3.10), e.g. by using piecewise constant basis functions ψ_ℓ, $\ell = 1, \ldots, N_\Gamma$ defines an approximation $\widetilde{w}_h \in S_h^0(\Gamma)$ as the unique solution of the Galerkin formulation

$$\langle V\widetilde{w}_h, \psi_\ell\rangle_\Gamma = \langle\widetilde{N}_0 f, \psi_\ell\rangle_\Gamma \quad \text{for all } \ell = 1, \ldots, N_\Gamma. \tag{3.11}$$

The Galerkin formulation (3.11) is equivalent to a linear system of algebraic equations, $\overline{V}_h\underline{\widetilde{w}} = \overline{N}_0$, where $\overline{V}_h$ is the Galerkin stiffness matrix of the single layer potential, and $\overline{N}_0$ is the discrete multipole approximation of the Newton potential $N_0 f$, both are defined

with respect to the complete boundary Γ. Inserting the approximate solution $\widetilde{w}_h$ into the definition of $N_{1,j}$ we further obtain

$$\widehat{N}_{1,j} = \langle (-\frac{1}{2}I + K')\widetilde{w}_h, \varphi_j \rangle_\Gamma,$$

and therefore we find the representation

$$\underline{\widehat{N}}_1 = (-\frac{1}{2}\overline{M}_h^\top + \overline{K}_h^\top)\underline{\widetilde{w}} = (-\frac{1}{2}\overline{M}_h^\top + \overline{K}_h^\top)\overline{V}_h^{-1}\underline{\overline{N}}_0 \tag{3.12}$$

where

$$\overline{K}_h[\ell, i] = \langle K\varphi_i, \psi_\ell \rangle_\Gamma, \quad \overline{M}_h[\ell, i] = \langle \varphi_i, \psi_\ell \rangle_\Gamma$$

for $i = 1, \ldots, M_N$, $\ell = 1, \ldots, N_\Gamma$.

3.4 Error estimates

Due to the evaluation of the Newton potentials by using the fast multipole method as described in Sect. 3.2, or by using the indirect evaluation of the Newton potential $N_1 f$ as described in Sect. 3.3, instead of (2.10) we have to consider a perturbed variational problem to find $(\widehat{t}_h, \widehat{u}_h) \in S_h^0(\Gamma_D) \times S_h^1(\Gamma_N)$ such that

$$\langle V\widehat{t}_h, \tau_h \rangle_{\Gamma_D} - \langle K\widehat{u}_h, \tau_h \rangle_{\Gamma_D} = \langle (\frac{1}{2}I + K)\widetilde{g}_D - V\widetilde{g}_N - \widetilde{N}_0 f, \tau_h \rangle_{\Gamma_D} \tag{3.13}$$

for all $\tau_h \in S_h^0(\Gamma_D)$ and

$$\langle K'\widehat{t}_h, v_h \rangle_{\Gamma_N} + \langle D\widehat{u}_h, v_h \rangle_{\Gamma_N} = \langle (\frac{1}{2}I - K')\widetilde{g}_N - D\widetilde{g}_D - \widetilde{N}_1 f, v_h \rangle_{\Gamma_N} \tag{3.14}$$

for all $v_h \in S_h^1(\Gamma_N)$, where $\tilde{N}_0$ and $\tilde{N}_1$ are the approximations of the Newton potentials. It remains to estimate the errors $\widetilde{t}_h - \widehat{t}_h$ and $\widetilde{u}_h - \widehat{u}_h$ due to the perturbation of the right hand side. Note that errors due to numerical integration or due to an approximation of the boundary data are neglected. In particular, the integration of the coefficients R_n^m and S_n^m and the integration in the nearfield are assumed to be exact. Moreover, a globally quasi–uniform mesh is assumed for simplicity in the representation.
The approximation error of the fast multipole method can be regulated by various parameters such as the expansion degree p, the nearfield parameter d, and the cluster radius r. In particular, the truncation error can be estimated as follows.

Proposition 3.1. [7, 14] *Let $d > 1$ and $r > 0$. For $x, y \in \mathbb{R}^3$ satisfying $|x| \le r$, and $|y| \ge dr$ the following error estimates for the kernel $k(x, y) = |x - y|^{-1}$ and for the local expansion* (3.3) *hold:*

$$|k(x, y) - k_p(x, y)| \le \frac{1}{(d-1)r} \left(\frac{1}{d}\right)^{p+1}, \tag{3.15}$$

$$\left|\frac{\partial}{\partial n_x}(k(x, y) - k_p(x, y))\right| \le \frac{1+\pi}{(d-1)r^2} \left(p + 1 + \frac{d}{d-1}\right) \left(\frac{1}{d}\right)^{p+1}. \tag{3.16}$$

Several parameters may depend on the boundary element mesh size h: The number N_Γ of boundary elements is of order $\mathcal{O}(h^{-2})$, and thus the number N_Ω of volume elements is of order $\mathcal{O}(h^{-3})$. The number of clusters on the finest level is supposed to be of order $\mathcal{O}(\log^2 h^{-2})$ which implies the inequality

$$r \geq ch\,. \tag{3.17}$$

Now we are in a position to bound the errors of the multipole approximations $\widetilde{N}_0 f$ and $\widetilde{N}_1 f$, respectively.

Lemma 3.2. *Let d be fixed, and let $p \sim \log N_\Gamma = \frac{3}{2}\log h^{-1}$ be appropriately chosen. For the multipole approximation $\widetilde{N}_0 f$ the error estimate holds*

$$\|N_0 f - \widetilde{N}_0 f\|_{L_2(\Gamma)} \leq ch^2 \|f\|_{L_2(\Omega)} \quad \textit{for all } f \in L_2(\Omega). \tag{3.18}$$

Proof. With the error estimate (3.15) and by using the Cauchy–Schwarz inequality we first obtain

$$\begin{aligned}
\|N_0 f - \widetilde{N}_0 f\|^2_{L_2(\Gamma)} &= \frac{1}{16\pi^2} \sum_{\ell=1}^{N} \int_{\tau_\ell} \left| \sum_{k \in \mathrm{FF}(\ell)} \int_{T_k} [k(x,y) - k_p(x,y)] f(y) dy \right|^2 ds_x \\
&\leq \frac{1}{16\pi^2} \sum_{\ell=1}^{N} \int_{\tau_\ell} \left(\sum_{k \in \mathrm{FF}(\ell)} \int_{T_k} |k(x,y) - k_p(x,y)|\, |f(y)| dy \right)^2 ds_x \\
&\leq \frac{1}{16\pi^2} \frac{1}{(d-1)^2 r^2} \left(\frac{1}{d}\right)^{2p+2} \int_\Gamma \left(\int_\Omega |f(y)| dy \right)^2 ds_x \\
&\leq \frac{1}{16\pi^2} \frac{1}{(d-1)^2 r^2} \left(\frac{1}{d}\right)^{2p+2} |\Gamma|\, |\Omega|\, \|f\|^2_{L_2(\Omega)}\,.
\end{aligned}$$

To get the proposed consistency estimate (3.18), we have to choose, for a fixed nearfield parameter d, the expansion degree p such that

$$\frac{1}{d-1} \left(\frac{1}{d}\right)^{p+1} \leq ch^3$$

is satisfied, with c independent of h. By using (3.17), i.e. $h \sim r$, the proposition follows. □

Lemma 3.3. *Let d be fixed, and let $p \sim \log N_\Gamma = \frac{3}{2}\log h^{-1}$ be appropriately chosen. For the multipole approximation $\widetilde{N}_1 f$ there holds the error estimate*

$$\|N_1 f - \widetilde{N}_1 f\|_{L_2(\Gamma)} \leq \widetilde{c} h^{3/2} \|f\|_{L_2(\Omega)} \quad \textit{for all } f \in L_2(\Omega). \tag{3.19}$$

Proof. We use the error estimate (3.16) and the Cauchy–Schwarz inequality to obtain in a similar way as in the proof of Lemma 3.2

$$\|N_1 f - \widetilde{N}_1 f\|^2_{L_2(\Gamma)} \leq \frac{1}{16\pi^2} \frac{1}{(d-1)^2 r^4} \left(p + 1 + \frac{d}{d-1}\right) \left(\frac{1}{d}\right)^{2p+2} |\Gamma|\, |\Omega|\, \|f\|^2_{L_2(\Omega)}\,.$$

This time we have to choose the expansion degree p such that

$$\left(p+1+\frac{1}{d-1}\right)\left(\frac{1}{d}\right)^{p+1} \leq ch^{7/2}$$

is satisfied for a fixed nearfield parameter d and $h \sim r$, with c independent of h, to get the proposed consistency estimate (3.19). □

Theorem 3.4. *Let $(\widehat{t}_h, \widehat{u}_h) \in S_h^0(\Gamma_D) \times S_h^1(\Gamma_N)$ be the unique solution of the perturbed variational problem (2.8) and (2.9). Assume $\widetilde{g}_N \in H^1_{pw}(\Gamma)$ and $\widetilde{g}_D \in H^2(\Gamma)$. Then there holds the error estimate*

$$\|\widetilde{t} - \widehat{t}_h\|^2_{H^{-1/2}(\Gamma)} + \|\widetilde{u} - \widehat{u}_h\|^2_{H^{1/2}(\Gamma)} \leq c\, h^3 \left[|\widetilde{t}|^2_{H^1_{pw}(\Gamma)} + |\widetilde{u}|^2_{H^2(\Gamma)} + \|f\|^2_{L_2(\Omega)}\right].$$

Proof. By the triangle inequality and by using the error estimate (2.15) we first have

$$\begin{aligned}
&\|(\widetilde{t} - \widehat{t}_h, \widetilde{u} - \widehat{u}_h)\|^2_{H^{-1/2}(\Gamma)\times H^{1/2}(\Gamma)} \\
&\qquad \leq 2\,\|(\widetilde{t} - \widetilde{t}_h, \widetilde{u} - \widetilde{u}_h)\|^2_{H^{-1/2}(\Gamma)\times H^{1/2}(\Gamma)} + 2\,\|(\widetilde{t}_h - \widehat{t}_h, \widetilde{u}_h - \widehat{u}_h)\|^2_{H^{-1/2}(\Gamma)\times H^{1/2}(\Gamma)} \\
&\qquad \leq 2ch^3 \left[|\widetilde{t}|^2_{H^1_{\mathrm{pw}}(\Gamma)} + |\widetilde{u}|^2_{H^2(\Gamma)}\right] + 2\,\|(\widetilde{t}_h - \widehat{t}_h, \widetilde{u}_h - \widehat{u}_h)\|^2_{H^{-1/2}(\Gamma)\times H^{1/2}(\Gamma)}.
\end{aligned}$$

Next, by using the ellipticity estimate (2.14), and by considering the difference of the variational formulations (2.8)–(2.9) and (3.13)–(3.14), we further conclude

$$\begin{aligned}
c_1^A\,\|(\widetilde{t}_h - \widehat{t}_h, \widetilde{u}_h - \widehat{u}_h)\|^2_{H^{-1/2}(\Gamma)\times H^{1/2}(\Gamma)} &\leq a(\widetilde{t}_h - \widehat{t}_h, \widetilde{u}_h - \widehat{u}_h; \widetilde{t}_h - \widehat{t}_h, \widetilde{u}_h - \widehat{u}_h) \\
&= \langle \widetilde{N}_0 f - N_0 f, \widetilde{t}_h - \widehat{t}_h\rangle_{\Gamma_D} + \langle \widetilde{N}_1 f - N_1 f, \widetilde{u}_h - \widehat{u}_h\rangle_{\Gamma_N} \\
&\leq \|\widetilde{N}_0 f - N_0 f\|_{L_2(\Gamma)}\|\widetilde{t}_h - \widehat{t}_h\|_{L_2(\Gamma)} + \|\widetilde{N}_1 f - N_1 f\|_{L_2(\Gamma)}\|\widetilde{u}_h - \widehat{u}_h\|_{L_2(\Gamma)} \\
&\leq c\,h^2\,\|f\|_{L_2(\Omega)}\|\widetilde{t}_h - \widehat{t}_h\|_{L_2(\Gamma)} + \widetilde{c}\,h^{3/2}\|f\|_{L_2(\Omega)}\|\widetilde{u}_h - \widehat{u}_h\|_{L_2(\Gamma)}
\end{aligned}$$

due to the error estimates (3.18) and (3.19). With the inverse inequality

$$\|\widetilde{t}_h - \widehat{t}_h\|_{L_2(\Gamma)} \leq c_I\, h^{-1/2}\,\|\widetilde{t}_h - \widehat{t}_h\|_{H^{-1/2}(\Gamma)}$$

and by using the embedding $H^{1/2}(\Gamma) \subset L_2(\Gamma)$ we further obtain

$$c_1^A\,\|(\widetilde{t}_h - \widehat{t}_h, \widetilde{u}_h - \widehat{u}_h\|^2_{H^{-1/2}(\Gamma)\times H^{1/2}(\Gamma)} \leq c\,h^{3/2}\,\|f\|_{L_2(\Gamma)}\left[\|\widetilde{t}_h - \widehat{t}_h\|_{H^{-1/2}(\Gamma)} + \|\widetilde{u}_h - \widehat{u}_h\|_{H^{1/2}(\Gamma)}\right]$$

and therefore

$$\|(\widetilde{t}_h - \widehat{t}_h, \widetilde{u}_h - \widehat{u}_h\|_{H^{-1/2}(\Gamma)\times H^{1/2}(\Gamma)} \leq c\,h^{3/2}\,\|f\|_{L_2(\Omega)}$$

follows. □

Instead of the multipole approximation $\widetilde{N}_1 f$ we may also use the indirect approximation $\widehat{N}_1 f$ as defined in (3.12). Hence we need to estimate the related error $N_1 f - \widehat{N}_1 f$.

Lemma 3.5. *Let* $\widehat{N}_1 f = (-\frac{1}{2}I + K')\widetilde{w}_h$ *be an approximation of the Newton potential* $N_1 f$*, where* $\widetilde{w}_h \in S_h^0(\Gamma)$ *is the unique solution of the variational problem* (3.11)*. Assume* $w = V^{-1}N_0 f \in H^1_{pw}(\Gamma)$*. Then there holds the error estimate*

$$\|N_1 f - \widehat{N}_1 f\|_{H^{-1/2}(\Gamma)} \leq c\, h^{3/2} \left[\|w\|_{H^1_{pw}(\Gamma)} + \|f\|_{L_2(\Omega)}\right].$$

Proof. Recall that $\widetilde{w}_h \in S_h^0(\Gamma)$ is the unique solution of the perturbed variational problem

$$\langle V\widetilde{w}_h, \tau_h\rangle_\Gamma = \langle \widetilde{N}_0 f, \tau_h\rangle_\Gamma \quad \text{for all } \tau_h \in S_h^0(\Gamma),$$

while $w \in H^{-1/2}(\Gamma)$ is the unique solution of the variational problem

$$\langle Vw, \tau\rangle_\Gamma = \langle N_0 f, \tau\rangle_\Gamma \quad \text{for all } \tau \in H^{-1/2}(\Gamma).$$

In addition, $w_h \in S_h^0(\Gamma)$ is the unique solution of the Galerkin variational problem

$$\langle Vw_h, \tau_h\rangle_\Gamma = \langle N_0 f, \tau_h\rangle_\Gamma \quad \text{for all } \tau_h \in S_h^0(\Gamma).$$

By the triangle inequality we first have

$$\|w - \widetilde{w}_h\|_{H^{-1/2}(\Gamma)} \leq \|w - w_h\|_{H^{-1/2}(\Gamma)} + \|w_h - \widetilde{w}_h\|_{H^{-1/2}(\Gamma)}.$$

While the first term can be estimated by using Cea's lemma, we use the $H^{-1/2}(\Gamma)$–ellipticity of the single layer potential V to obtain for the second term

$$\begin{aligned} c_1^V \|w_h - \widetilde{w}_h\|^2_{H^{-1/2}(\Gamma)} &\leq \langle V(w_h - \widetilde{w}_h), w_h - \widetilde{w}_h\rangle_\Gamma \\ &= \langle N_0 f - \widetilde{N}_0 f, w_h - \widetilde{w}_h\rangle_\Gamma \\ &\leq \|N_0 f - \widetilde{N}_0 f\|_{L_2(\Gamma)} \|w_h - \widetilde{w}_h\|_{L_2(\Gamma)}. \end{aligned}$$

By using the error estimate (3.18) and the inverse inequality in $S_h^0(\Gamma)$ we further have

$$\|N_0 f - \widetilde{N}_0 f\|_{L_2(\Gamma)} \leq c\, h^2 \|f\|_{L_2(\Omega)}, \quad \|w_h - \widetilde{w}_h\|_{L_2(\Gamma)} \leq c_I\, h^{-1/2} \|w_h - \widetilde{w}_h\|_{H^{-1/2}(\Gamma)}.$$

Hence we conclude

$$\|w_h - \widetilde{w}_h\|_{H^{-1/2}(\Gamma)} \leq c\, h^{3/2} \|f\|_{L_2(\Omega)}$$

Finally, when assuming $w = V^{-1}N_0 f \in H^1_{\rm pw}(\Gamma)$ we obtain

$$\|w - \widetilde{w}_h\|_{H^{-1/2}(\Gamma)} \leq c\, h^{3/2} \left[\|w\|_{H^1_{\rm pw}(\Gamma)} + \|f\|_{L_2(\Omega)}\right].$$

The assertion now follows from

$$\|N_1 f - \widehat{N}_1 f\|_{H^{-1/2}(\Gamma)} = \|(-\frac{1}{2}I + K')(w - \widetilde{w}_h)\|_{H^{-1/2}(\Gamma)} \leq c\, \|w - \widetilde{w}_h\|_{H^{-1/2}(\Gamma)}.$$

□

As in Theorem 3.4 we are now able to derive an error estimate for the approximate solution when using the indirect approximation $\widehat{N}_1 f$ of the Newton potential $N_1 f$. Since the proof is based on the standard use of the Strang lemma we skip the details.

Theorem 3.6. *Let $(\widehat{t}_h, \widehat{u}_h) \in S_h^0(\Gamma_D) \times S_h^1(\Gamma_N)$ be the unique solution of the variational problem (3.13) and (3.14), where the multipole approximation $\widetilde{N}_1 f$ is replaced by the indirect approximation $\widehat{N}_1 f$. Assume $\widetilde{g}_N \in H^1_{pw}(\Gamma)$, $\widetilde{g}_D \in H^2(\Gamma)$, and $w = V^{-1}N_0 f \in H^1_{pw}(\Gamma)$. Then there holds the error estimate*

$$\|\widetilde{t}-\widehat{t}_h\|^2_{H^{-1/2}(\Gamma)} + \|\widetilde{u}-\widehat{u}_h\|^2_{H^{1/2}(\Gamma)} \le c\,h^3 \left[|\widetilde{t}|^2_{H^1_{pw}(\Gamma)} + |\widetilde{u}|^2_{H^2(\Gamma)} + \|f\|^2_{L_2(\Omega)} + \|V^{-1}N_0 f\|_{H^1_{pw}(\Gamma)} \right].$$

Remark 3.2. *The assumptions of Theorems 3.4 and 3.6, i.e. $\widetilde{t} \in H^1_{pw}(\Gamma)$ and $\widetilde{u} \in H^2(\Gamma)$ are satisfied if we can ensure $u \in H^{5/2}(\Omega)$ for the solution u of the mixed boundary value problem (2.1), and $u_f \in H^{5/2}(\Omega)$ where*

$$-\Delta u_f = f \text{ in } \Omega, \quad u_f = 0 \text{ on } \Gamma.$$

Note that u_f is given by the representation formula

$$u_f(x) = (Vw)(x) - (N_0 f)(x) \qquad \text{for } x \in \Omega$$

where

$$w = \frac{\partial}{\partial n} u_f = V^{-1} N_0 f.$$

Hence, if $u_f \in H^{5/2}(\Omega)$ is satisfied, $w = V^{-1}N_0 f \in H^1_{pw}(\Gamma)$ follows.
The regularity assumption $u \in H^{5/2}(\Omega)$ ensures an optimal convergence of Galerkin boundary element methods of lowest order, as used in this paper. However, when the solution u of the mixed boundary value problem (2.1) has only reduced regularity [3, 8, 24], we only obtain error estimates with a reduced order of convergence. But this is not reflected by the use of fast boundary element methods.

Remark 3.3. *In addition to the energy error estimates as presented in Theorems 3.4 and 3.6 we can also derive error estimates in $L_2(\Gamma)$. By using standard arguments, see, e.g., [20], we finally obtain the following error estimates:*

$$\|\widetilde{t} - \widetilde{t}_h\|_{L_2(\Gamma)} \le c\,h \left[|\widetilde{t}|^2_{H^1_{pw}(\Gamma)} + |\widetilde{u}|^2_{H^2(\Gamma)} + \|f\|^2_{L_2(\Omega)} + \|V^{-1}N_0 f\|_{H^1_{pw}(\Gamma)} \right]^{1/2}, \quad (3.20)$$

$$\|\widetilde{u} - \widetilde{u}_h\|_{L_2(\Gamma)} \le c\,h^2 \left[|\widetilde{t}|^2_{H^1_{pw}(\Gamma)} + |\widetilde{u}|^2_{H^2(\Gamma)} + \|f\|^2_{L_2(\Omega)} + \|V^{-1}N_0 f\|_{H^1_{pw}(\Gamma)} \right]^{1/2}. \quad (3.21)$$

4 Numerical results

In the following numerical example, a standard Galerkin boundary element method is compared to the proposed fast multipole boundary element method to solve an inhomogeneous partial differential equation. First we consider the Dirichlet boundary value problem

$$-\Delta u(x) = -2 \quad \text{for } x \in \Omega = (0,1)^3, \quad u(x) = x_1^2 \qquad \text{for } x \in \Gamma = \partial\Omega, \qquad (4.1)$$

where the exact solution is $u(x) = x_1^2$. Starting from a uniform volume mesh, the cube is uniformly refined. The boundary element mesh is the restriction of the volume mesh to the boundary. The boundary element discretization of the boundary value problem (4.1) results in the linear system

$$V_h \underline{t} = (\frac{1}{2} M_h + K_h)\underline{g} - \underline{N}_0$$

which is solved by a conjugate gradient method with an algebraic BPX preconditioner [19]. The numerical results are given in Table 2.

N_Γ	N_Ω	$\underline{N}_0$	Setup	Solve	It	$\|t - t_h\|_{L_2(\Gamma)}$
384	1536	3	8	0	28	1.70e-01
		0	2	0	28	1.70e-01
1536	12288	94	168	1	30	8.55e-02
		3	6	1	30	8.56e-02
6144	98204	2997	4188	6	34	4.28e-02
		13	24	6	34	4.29e-02
24576	786432	(26.6 h)	(32 h)	(107)		
		77	112	32	38	2.15e-02
98304	6291456	(35.5 d)	(39 d)	(1852)		
		466	611	278	41	1.07e-02

Table 2: Comparison of a standard and a fast multipole boundary element method.

For each refinement level, the first line states the results of the standard Galerkin boundary element method, whereas the second line contains the results for the proposed fast multipole boundary element method. The first and the second column contain the number N_Γ of boundary elements and the number N_Ω of tetrahedral volume elements, respectively. Furthermore, the time in seconds is given for the evaluation of the Newton potential $N_0 f$, followed by the total time for the setup of the system of linear equations. In Columns 5 and 6, the time for solving the linear system and the number of CG iterations are given. Finally, the L_2–norm of the error $t - t_h$ is given. The parameters for the fast multipole method were chosen such that the related approximation error is almost the same as of the standard method. According to the error estimate (3.20) a linear convergence is observed for both approaches. The standard approach could be applied only up to 6144 boundary elements due to memory restrictions. As N_Γ and N_Ω increase by a factor of 4 and 8, respectively, the times for computing the Newton potential $\underline{N}_0$ increase by a factor of 32 for the standard boundary element method. In the case of the fast multipole method, the factor is smaller than 8 and thus better than estimated. This was achieved by various optimizations of the cluster hierarchy. However, it is expected that this factor will tend to 8 for calculations on higher levels. The rest of the setup time increases as expected for the standard approach with the factor 16, and for the fast multipole approach by the factor

of about 4. Already in the first refinement level the fast multipole method is faster than the standard method. On the finest level, it outperforms the standard method with about 8 minutes compared to about 35.5 days for the direct evaluation of the Newton potential $\underline{N}_0$.

In a second example, we compare the direct and the indirect evaluation of the Newton potential $\underline{N}_1$. We consider the mixed boundary value problem

$$\begin{aligned} -\Delta u(x) &= -2 && \text{for } x \in \Omega = (0,1)^3, \\ u(x) &= g_D(x) && \text{for } x \in \Gamma_D, \\ \frac{\partial}{\partial n_x} u(x) &= g_N(x) && \text{for } x \in \Gamma_N \end{aligned} \tag{4.2}$$

where the Dirichlet boundary is $\Gamma_D = \{x \in \partial\Omega : x_3 = 0\}$, and the Neumann boundary is $\Gamma_N = \partial\Omega \setminus \overline{\Gamma}_D$. We choose $u(x) = x^2$ as exact solution, and the given Cauchy data g_D and g_N are given accordingly. The linear system (2.10) is solved by a preconditioned GMRES method where the single layer potential V_h is preconditioned by an algebraic BPX [19], while the discrete hypersingular integral operator D_h is preconditioned by the single layer potential discretized by using piecewise linear basis functions [21]. The setup times for both approaches are given in Table 3.

N_Γ	N_Ω	Indirect evaluation			FMM evaluation		
		$\overline{\underline{N}}_0$	$\overline{V}_h \underline{w} = \overline{\underline{N}}_0$	overall time	$\tilde{\underline{N}}_0$	$\tilde{\underline{N}}_1$	overall time
96	192	0	0	1	0	0	1
384	1536	1	0	10	1	2	10
1536	12288	5	1	49	1	13	49
6144	98304	27	2	160	5	66	174
24576	789432	219	15	667	40	510	895
98304	6291456	1022	76	2710	196	2486	3996

Table 3: Comparison of fast multipole and indirect evaluation of $N_1 f$.

The overall setup time for the system of linear equations is smaller for the indirect approach compared to the direct computation by the fast multipole method. To understand this difference the setup time was split up. The computational times for the Newton potential $\overline{\underline{N}}_0$ and for solving the system $\overline{V}_h \underline{w} = \overline{\underline{N}}_0$ are given in the the case of the indirect approach, while the times for the direct evaluation of the Newton potentials $\tilde{\underline{N}}_0$ and $\tilde{\underline{N}}_1$ are stated in the case of the direct fast multipole approach. The setup times for all boundary integral operators and the preconditioners are included in the overall setup times, too. In the case of the direct approach, the Newton potentials $\tilde{\underline{N}}_0$ and $\tilde{\underline{N}}_1$ have to be evaluated on the Dirichlet part and the Neumann part of the boundary, respectively. In the case of the indirect approach, the Newton potential $\overline{\underline{N}}_0$ has to be evaluated on the whole boundary. The Newton potential $\overline{\underline{N}}_0$ can be evaluated more efficiently, since only one constant test function per element has to be considered compared to three linear form functions for

$\underline{\tilde{N}}_1$. In the case of the indirect evaluation, the additional time for computing the enlarged matrices $\overline{V}_h$ and $\overline{K}_h$ and for solving the system of linear equations to compute $\underline{\widehat{N}}_1$ is rather small compared to the expensive direct evaluation of $\underline{\tilde{N}}_1$. The numerical example shows that the indirect evaluation is faster than the direct fast multipole evaluation.

N_Γ	N_Ω	indirect evaluation		direct FMM evaluation	
		$\|\tilde{u}-\tilde{u}_h\|_{L_2(\Gamma)}$	$\|\tilde{t}-\tilde{t}_h\|_{L_2(\Gamma)}$	$\|\tilde{u}-\tilde{u}_h\|_{L_2(\Gamma)}$	$\|\tilde{t}-\tilde{t}_h\|_{L_2(\Gamma)}$
96	192	5.83e-02	1.55e-01	5.65e-02	1.55e-01
384	1536	1.47e-02	8.15e-02	1.43e-02	8.17e-02
1536	12288	3.70e-03	4.17e-02	3.60e-03	4.18e-02
6144	98304	9.28e-04	2.12e-02	8.95e-04	2.12e-02
24576	789432	2.34e-04	1.06e-02	2.28e-04	1.06e-02
98304	6291456	5.96e-05	5.34e-03	5.08e-05	5.35e-03

Table 4: Comparison of approximation errors.

Finally, we list the approximation errors which were obtained in both approaches in Table 4. All errors are as predicted in the error estimates (3.21) and (3.20), in particular we get linear convergence for the Neumann data, and quadratic convergence for the Dirichlet data. While the Neumann error almost coincide in both approaches, the Dirichlet error for the indirect error is slightly larger, due to the additional approximation error when computing $\underline{\widehat{N}}_1$.

5 Linear elasticity problems

In this section the fast evaluation of the multipole method will be applied to the inhomogeneous system of linear elasticity

$$\begin{aligned} -\sum_{j=1}^{3} \frac{\partial}{\partial x_j}\sigma_{ij}(u,x) =& f_i(x) \text{ for } x \in \Omega,\ i=1,\dots,3, \\ u_i(x) =& g_{D,i}(x) \text{ for } x \in \Gamma_D, \quad i=1,\dots,3 \\ \sum_{j=1}^{3} \sigma_{ij}(u,x)n_j(x) =& g_{N,i}(x) \text{ for } x \in \Gamma_N, \quad i=1,\dots,3. \end{aligned} \tag{5.1}$$

The fundamental solution can be represented as the fundamental solution of the Poisson equation and its derivatives in the following way

$$\begin{aligned} U^*_{k\ell}(x,y) = \frac{1+\nu}{8\pi E(1+\nu)}\Bigg[&(3-4\nu)\frac{\delta_{k\ell}}{|x-y|} - \frac{1}{2}x_\ell\frac{\partial}{\partial x_k}\frac{1}{|x-y|} - \frac{1}{2}y_\ell\frac{\partial}{\partial y_k}\frac{1}{|x-y|} \\ &- \frac{1}{2}x_k\frac{\partial}{\partial x_\ell}\frac{1}{|x-y|} - \frac{1}{2}x_k\frac{\partial}{\partial x_\ell}\frac{1}{|x-y|}\Bigg]. \end{aligned}$$

The fast multipole method can therefore be applied in an analogue way. The boundary integral operators for the system of linear elasticity were realized for example in [12, 13]; see also the references given therein. In a straightforward manner, those techniques and the techniques described in Sect. 3 can be combined for a fast evaluation of Newton potentials in linear elasticity. The same error estimates as for the approximation of the Newton potentials in the case of the Poisson equation can be found in a similar way [22].

5.1 Numerical example

For $\Omega = (0,1)^3$ the boundary value problem (5.1) is considered. The Dirichlet boundary is defined as $\Gamma_D = \{(x,y,z)^\top \in \partial\Omega : z = 0\}$ and the Neumann boundary as $\Gamma_N = \partial\Omega \setminus \Gamma_D$. The solution is given as $u(x,y,z) = (x^3, y^3, z^3)^T$ and the Cauchy data and the volume function $f(x)$ are chosen accordingly. The Newton potential $N_1 f$ was calculated with the indirect approach as described in Sect. 3.3. This alternative representation is obviously also valid for the system of linear elasticity. The resulting system of linear equations is solved by a preconditioned GMRES method where the single layer potential V_h is preconditioned by an algebraic BPX [19] componentwise, while the discrete hypersingular integral operator D_h is preconditioned by the single layer potential of the Laplacian [21] componentwise.
In Table 5 the results are summarized. The same notations are used as in Table 2. Additionally, the approximation errors $\|\tilde{u} - \tilde{u}_h\|_{L_2(\Gamma)}$ for the Dirichlet data and $\|\tilde{t} - \tilde{t}_h\|_{L_2(\Gamma)}$ for the Neumann data are given in the L_2-Norm.

N_Γ	N_Ω	$\overline{\underline{N}}_0$	Setup	Solve	it	$\|\tilde{u} - \tilde{u}_h\|_{L_2(\Gamma)}$	$\|\tilde{t} - \tilde{t}_h\|_{L_2(\Gamma)}$
384	1536	8	22	1	34	5.11e-02	6.14e+01
		4	16	2	34	5.11e-02	6.14e+01
1536	12288	249	462	14	39	1.50e-02	3.07e+01
		18	91	21	39	1.51e-02	3.08e+01
6144	98304	8032	11509	352	43	4.29e-03	1.54e+01
		102	440	117	43	4.34e-03	1.54e+01
24576	786432	(3 d)	(3.6 d)	(1.82 h)			
		631	2132	890	50	1.22e-03	7.70e+00
98304	6291456	(95 d)	(105 d)	(1.3 d)			
		3935	9829	4064	53	3.36e-04	3.88e+00

Table 5: Comparison: Direct evaluation - FMM

Due to limits in memory, the computation of the last two levels was not possible by the standard boundary element method. As expected, the time to evaluate the Newton potential $\overline{\underline{N}}_0$ increases the most, with the factor 32 for the standard boundary element method and with factor 8 for the FMM. This means that at the last refinement level the standard boundary element method would require approximately 95 days just to evaluate the Newton potential $\overline{\underline{N}}_0$, whereas the FMM only requires little over an hour.

The error of the Neumann data halves as expected. The Dirichlet error decreases with a factor of about 3.4 and not 4. The reduced convergence order seems due to reduced regularity of the density function w, which is based on the regularity of u_f as stated in Remark 3.2. The reduced oder of convergence is not caused by the approximation of the FMM.

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