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Raport Badawczy Research Report

RB/23/2010

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Recovering gradients from surface integrals and applications

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1 Introduction

1.1 Domain decomposition with Steklov-Poincaré operators for linear problems

We start with a simple model problem on applications of the Steklov-Poincaré operators to the topological sensitivity analysis of linear variational problems. The shape functional is given by the associated energy functional to the boundary value problem. Given domains Ω , $\Omega(\varepsilon) = \Omega \setminus \overline{\mathbb{B}}_{\varepsilon} \subset \mathbb{R}^d$, $d \geq 2$, with a small hole $\mathbb{B}_{\varepsilon} = \{x \in \mathbb{R}^d \mid ||x|| < \varepsilon \text{ of radius } \varepsilon \to 0$, the associated energy functional to the elliptic boundary value problem under considerations is introduced for the singularly perturbed equation:

Find $u_{\varepsilon} = u(\Omega(\varepsilon))$ such that

$$-\Delta u_{\varepsilon} = f \quad \text{in} \quad \Omega(\varepsilon) , \qquad (1)$$

$$u_{\varepsilon} = 0 \quad \text{on} \quad \Gamma = \partial \Omega ,$$
 (2)

$$\frac{\partial u_{\varepsilon}}{\partial n} = 0 \quad \text{on} \quad \Gamma_{\varepsilon} = \partial \mathbb{B}_{\varepsilon} ,$$
 (3)

where $f \in L^2(\mathbb{R}^d)$ is a given element which vanishes in the vicinity of the origin $\mathcal{O} \in \omega$.

The boundary value problem corresponds to the minimization of the

quadratic functional

$$I_{\varepsilon}(\varphi) = \frac{1}{2} \int_{\Omega(\varepsilon)} |\nabla \varphi|^2 - \int_{\Omega(\varepsilon)} f \varphi$$
 (4)

over the linear subspace $V\subset H^1(\Omega(\varepsilon))$ of the form

$$V = \{ \varphi \in H^1(\Omega(\varepsilon)) \mid \varphi = 0 \text{ on } \Gamma \}$$
 (5)

The shape functional

$$J(\Omega(\varepsilon)) := \frac{1}{2} \int_{\Omega(\varepsilon)} |\nabla u_{\varepsilon}|^2 - \int_{\Omega(\varepsilon)} f u_{\varepsilon} = -\frac{1}{2} \int_{\Omega(\varepsilon)} f u_{\varepsilon} . \tag{6}$$

defined by the equality

$$J(\Omega(\varepsilon)) = I_{\varepsilon}(u_{\varepsilon}) \tag{7}$$

is the energy for the singularly perturbed domain $\Omega(\varepsilon)$. We know already that the energy admits the expansion with respect to the small parameter $\varepsilon \to 0$ of the following form

$$J(\Omega(\varepsilon)) = J(\Omega) - C(d)\varepsilon^{d} e_{u}(\mathcal{O}) + o(\varepsilon^{d}) , \qquad (8)$$

where $e_u(\mathcal{O})$ is the bulk energy density at the origin \mathcal{O} , in general the bulk energy density at a point a point $x_0, x_0 = (x_{1,0}, \dots, x_{d,0}) \in \mathbb{R}^d$ is given by the formula

$$e_u(x_0) = \|\nabla u(x_0)\|^2$$
.

1.2 Two spatial dimensions

The results for the Laplacian in two spatial dimensions are obtained explicitly. We have

$$J(\Omega(\varepsilon)) = J(\Omega) - \frac{1}{2}\pi\varepsilon^2 e_u(\mathcal{O}) + o(\varepsilon^2) , \qquad (9)$$

where $e_u(\mathcal{O})$ is the bulk energy density at the origin \mathcal{O} , in general the bulk energy density at a point $x_0, x_0 = (x_{1,0}, x_{2,0}) \in \mathbb{R}^2$ is given by the formula

$$e_u(x_0) = ||\nabla u(x_0)||^2$$
.

If the function u is harmonic in a ball $\mathbb{B}_R \subset \mathbb{R}^2$, of radius R > 0 and the centre x_0 then the expressions for the first order derivatives of u in the following form

$$u_{/1}(x_0) = \frac{1}{\pi R^3} \int_{\Gamma_R(x_0)} u \cdot (x_1 - x_{1,0}) \, ds, \qquad u_{/2}(x_0) = \frac{1}{\pi R^3} \int_{\Gamma_R(x_0)} u \cdot (x_2 - x_{2,0}) \, ds.$$
(10)

are exact.

Here we use the notation

$$u_{/i}(x_0) = \frac{\partial u}{\partial x_i}, \quad i = 1, \cdots, d.$$

In view of this, expansion (9) can be rewritten in the equivalent form

$$J(\Omega(\varepsilon)) = J(\Omega) - \frac{\varepsilon^2}{2\pi R^6} \left[\left(\int_{\Gamma_R} u_{\Omega} x_1 \, ds \right)^2 + \left(\int_{\Gamma_R} u_{\Omega} x_2 \, ds \right)^2 \right] + o(\varepsilon^2) ,$$
(11)

which is interesting on its own, as it is observed in [2], [3], since (11) can be rewritten as follows

$$J(\Omega(\varepsilon)) = J(\Omega) + \varepsilon^2 \langle Bu, u \rangle_{\Gamma_R} + o(\varepsilon^2) . \tag{12}$$

with a certain integral boundary operator B. The operator B is selfadjoint since it is defined by the symmetric an positive bilinear form

$$\langle Bu, u \rangle = b(\Gamma_R; u, u) = -\frac{1}{2\pi R^6} \left[\left(\int_{\Gamma_R} u x_1 \, ds \right)^2 + \left(\int_{\Gamma_R} u x_2 \, ds \right)^2 \right] \tag{13}$$

From the above representation, since the line integrals on Γ_R are well defined for functions in $L_2(\Gamma_R)$, or even in $L_1(\Gamma_R)$, it follows that the operator B can be extended to the bounded operator on $L_2(\Gamma_R)$,

$$B \in \mathcal{L}(L_2(\Gamma_R) \to L_2(\Gamma_R))$$
 (14)

since the symmetric bilinear form of the operator, given by the equality

$$\langle Bu, v \rangle = b(\Gamma_R; u, v) =$$

$$-\frac{1}{2\pi R^6} \left[\left(\int_{\Gamma_R} ux_1 \, ds \right) \left(\int_{\Gamma_R} vx_1 \, ds \right) + \left(\int_{\Gamma_R} ux_2 \, ds \right) \left(\int_{\Gamma_R} vx_2 \, ds \right) \right]$$
(15)

is continuous for all $u, v \in L_2(\Gamma_R)$. In fact, the bilinear form

$$L_2(\Gamma_R) \times L_2(\Gamma_R) \ni (u, v) \mapsto b(\Gamma_R; u, v) \in \mathbb{R}$$

is continuous with respect to the weak convergence since it has the simple structure

$$b(\Gamma_R; u, v) = L_1(u)L_1(v) + L_2(u)L_2(v)$$
 $u, v \in L_1(\Gamma_R)$

with two linear forms $v \to L_i(v), i=1,2$, given by the line integrals on Γ_R . This gives us an additional regularity for approximation of the singular perturbation of geometrical domain by the regular non-local perturbation B of the pseudo-differential Steklov-Poincaré boundary operator A_{ε} . The Steklov-Poincaré boundary operator A_{ε} is defined in the following way. For given element $v \in H^{1/2}(\Gamma_R)$ solve the boundary value problem

$$-\Delta w = 0$$
 in $C(R, \varepsilon)$, $\frac{\partial w}{\partial \nu} = 0$ on Γ_{ε} , $w = v$ on Γ_{R} , (16)

and set

$$A_{\varepsilon}v = \frac{\partial w}{\partial \nu}$$
 on Γ_R , (17)

where ν is the unit exterior normal vector on $\partial C(R,\varepsilon)$, note that the unit exterior normal vector n on $\Gamma_R \subset \partial \Omega_R$ is $n=-\nu$. We denote by $C(R,\varepsilon)$ the annulus $\mathbb{B}_R \setminus \overline{\mathbb{B}}_{\varepsilon}$, in our application we also introduce the truncated domain

 $\Omega_R=\Omega\setminus\overline{\mathbb{B}}_R$ and use the domain decomposition technique with the Steklov-Poincaré operator.

Since the energy functional in $\Omega(\varepsilon)$ takes the form

$$J(\Omega(\epsilon)) = \frac{1}{2} \int_{\Omega_R} |\nabla u_{\epsilon}|^2 - \int_{\Omega_R} f u_{\epsilon} + \frac{1}{2} \langle A_{\epsilon} u_{\epsilon}, u_{\epsilon} \rangle_{\Gamma_R} , \qquad (18)$$

provided the source term f vanishes in the small ball \mathbb{B}_R around the origin, and the Steklov-Poincaré operator admits the expansion

$$A_{\varepsilon} = A + \varepsilon^2 B + R_{\varepsilon} \,, \tag{19}$$

where the remainder R_{ϵ} is of order $o(\epsilon^2)$ in the operator norm $\mathcal{L}(\mathcal{H}^{1/2}(\Gamma_R) \mapsto \mathcal{H}^{-1/2}(\Gamma_R))$. We obtain another approach to the evaluation of the topological derivative for the energy type functional. The approach is based on the representation of the energy functional in the form of a minimization procedure for regularly perturbed quadratic functional in view of (18),

$$J(\Omega(\varepsilon)) = \inf_{\varphi \in H_{\Gamma}^1(\Omega_R)} \left\{ \frac{1}{2} \int_{\Omega_R} |\nabla \varphi|^2 - \int_{\Omega_R} f \varphi + \frac{1}{2} \langle A_{\varepsilon} \varphi, \varphi \rangle_{\Gamma_R} \right\}, \tag{20}$$

where $H^1_{\Gamma}(\Omega_R)$ is a subset of $H^1(\Omega_R)$ with the functions which vanish on Γ . This approach is of some importance for the variational inequalities since allow us to derive the formulae for the topological derivatives which coincide with the formulae obtained for the corresponding liner boundary value problems.

2 Energy functionals and Steklov-Poincaré operators for variational inequalities

Let us assume that $\Omega\subset\mathbb{R}^d$ is a given domain. If \mathbb{B}_ϱ denotes the sphere with the centre at the origin

$$\mathbb{B}_{\varrho} = \{ x \in \mathbb{R}^d \mid |x| \le \varrho \}$$

then we consider the domain $\Omega(\varepsilon) = \Omega \setminus \mathbb{B}_{\varepsilon}$ and the truncated domain $\Omega_R = \Omega \setminus \mathbb{B}_R$.

The same mathematical model (20) can serve us in order to derive the topological derivatives of the energy shape functional for variational inequalities. It means that we replace in (20) the linear space $H^1_{\Gamma}(\Omega_R)$ by the convex and closed subset $K \subset H^1_{\Gamma}(\Omega_R)$, and consider

$$I_{\varepsilon}^{R}(u_{\varepsilon}^{R}) = \inf_{\varphi \in K \subset H_{\Gamma}^{1}(\Omega_{R})} \left\{ \frac{1}{2} \int_{\Omega_{R}} |\nabla \varphi|^{2} - \int_{\Omega_{R}} f\varphi + \frac{1}{2} (A_{\varepsilon}\varphi, \varphi)_{\Gamma_{R}} \right\} . \tag{21}$$

The assumption we need now is simple, that the minimizer u_{ε}^{R} in (21) coincides with the restriction to Ω_{R} of the minimizer $u_{\varepsilon} := u(\Omega(\varepsilon))$ of the corresponding quadratic functional defined in the whole singularly perturbed domain $\Omega(\varepsilon)$,

$$J(\Omega(\varepsilon)) = \inf_{\varphi \in K \subset H^1_{\Gamma}(\Omega(\varepsilon))} \frac{1}{2} \int_{\Omega(\varepsilon)} |\nabla \varphi|^2 - \int_{\Omega(\varepsilon)} f\varphi . \tag{22}$$

In this way the equality

$$J(\Omega(\varepsilon)) = \frac{1}{2} \int_{\Omega(\varepsilon)} |\nabla u_{\varepsilon}|^{2} - \int_{\Omega(\varepsilon)} f u_{\varepsilon} = I_{\varepsilon}^{R}(u_{\varepsilon}^{R}) =$$

$$= \frac{1}{2} \int_{\Omega_{R}} |\nabla u_{\varepsilon}|^{2} - \int_{\Omega_{R}} f u_{\varepsilon} + \frac{1}{2} \langle A_{\varepsilon} u_{\varepsilon}, u_{\varepsilon} \rangle_{\Gamma_{R}}$$
(23)

holds for $\varepsilon \to 0$ and we can determine the topological derivative of $J(\Omega)$ by using the expansion of $I_{\varepsilon}^R(u_{\varepsilon}^R)$. The assumption we need to perform the derivation of $I_{\varepsilon}^R(u_{\varepsilon}^R)$ with respect to the parameter ε at $\varepsilon = 0^+$ is the strong convergence for R > 0,

$$u_{\varepsilon}^R \to u^R$$
 strongly in $H^1(\Omega_R)$, (24)

i.e., there is no need to require any differentiability properties of the minimizer $u_{\varepsilon}^R \in H^1(\Omega_R)$ with respect to ε . In fact, we establish the existence of the conical differential for the mapping

$$[0, \varepsilon_0) \ni \varepsilon \mapsto u_\varepsilon^R \in H^1(\Omega_R) ,$$
 (25)

and of the expansion

$$u_{\varepsilon}^{R} = u^{R} + \varepsilon^{d} q^{R} + o^{R}(\varepsilon)$$
 in $H^{1}(\Omega_{R})$. (26)

The element $q^R \in H^1(\Omega_R)$ is uniquely determined by a solution of an associated variational problem with the constraints defined in function of the solution u^R and its coincidence set for the unilateral constraints imposed by the cone K.

We describe the framework in details. The abstract model of an energy functional for the non-linear boundary value problem in the form of variational inequality considered in this paper can be described in the following way in three spatial dimensions.

Given a domain $\Omega(\varepsilon) = \Omega \setminus \overline{\mathbb{B}}_{\varepsilon} \subset \mathbb{R}^3$, with a small cavity $\mathbb{B}_{\varepsilon} \subset \mathbb{B}_R$ of radius $\varepsilon \to 0$, denote by $\Omega_R = \Omega \setminus \overline{\mathbb{B}}_R$ the domain without the cavity, and by $C(R,\varepsilon) = \mathbb{B}_R \setminus \overline{\mathbb{B}}_{\varepsilon}$ the annulus with the small cavity. It means that the domain $\Omega(\varepsilon)$ is decomposed into two subdomains, the truncated domain Ω_R and the annulus $C(R,\varepsilon)$. The main idea which is employed here is to restrict the asymptotic analysis to the annulus $C(R,\varepsilon)$, and apply the obtained result to the variational inequality considered only in the truncated domain Ω_R . In this way the singular domain perturbation in the annulus influences the variational inequality by a pseudodifferential operator of Steklov-Poincaré type, which is localised on the exterior boundary Γ_R of the annulus, since at the same time Γ_R is the interior boundary of the truncated domain Ω_R . In other words, the variational inequality in the truncated domain takes the following form:

Find $u_{\epsilon} \in K \subset V^R$ which is the unique minimizer of the quadratic energy functional defined in the Sobolev space $V^R = \mathcal{H}^1(\Omega_R)$,

$$I_{\epsilon}^{R}(\varphi) = \frac{1}{2}a^{R}(\varphi, \varphi) - L^{R}(\varphi) + \frac{1}{2}(A_{\epsilon}(\gamma^{R}\varphi), \gamma^{R}\varphi)_{R},$$
 (27)

where A_{ε} stands for the Steklov-Poincaré operator for the ring $C(R,\varepsilon)$. The linear mapping $\gamma^R: \mathcal{H}^1(\Omega_R) \mapsto \mathcal{H}^{1/2}(\Gamma_R)$ denotes the trace operator on the interface Γ_R created by the domain decomposition, and $\langle \cdot, \cdot \rangle_R$ is the duality pairing defined for the fractional Sobolev spaces $\mathcal{H}^{-1/2}(\Gamma_R) \times \mathcal{H}^{1/2}(\Gamma_R)$ on the interface Γ_R , associated with the corresponding Steklov-Poincaré operator $A_{\varepsilon}: \mathcal{H}^{1/2}(\Gamma_R) \mapsto \mathcal{H}^{-1/2}(\Gamma_R)$. The Steklov-Poincaré operator is evaluated in the ring $C(R,\varepsilon)$ for $\varepsilon \geq 0$, ε small enough, and it admits the expansion

$$A_{\varepsilon} = A + \varepsilon^3 B + R_{\varepsilon}, \tag{28}$$

where the remainder R_{ϵ} is of order $o(\epsilon^3)$ in the operator norm $\mathcal{L}(\mathcal{H}^{1/2}(\Gamma_R) \mapsto \mathcal{H}^{-1/2}(\Gamma_R))$.

We want to replace the original variational inequality defined in the domain $\Omega(\varepsilon)$ by the variational inequality defined in the truncated domain Ω_R , i.e. we want to replace for the purposes of asymptotic analysis the original quadratic functional defined in the domain of integration $\Omega(\varepsilon)$

$$I_{\varepsilon}(\psi) = \frac{1}{2} a_{\varepsilon}(\psi, \psi) - L_{\varepsilon}(\psi) , \quad \psi \in \mathcal{H}^{1}(\Omega(\varepsilon)) ,$$
 (29)

by the functional $I_{\varepsilon}^{R}(\varphi)$ defined in the truncated domain without any hole. To this end, we require the following property for the minimizers u_{ε} and u_{ε}^{R} of $I_{\varepsilon}(\psi)$ and $I_{\varepsilon}^{R}(\varphi)$, respectively. For $\varepsilon > 0$ small enough the minimizer u_{ε}^{R} in the truncated domain is given the restriction to the truncated domain Ω_{R} of the minimizer u_{ε} in the singularly perturbed domain $\Omega(\varepsilon)$. If it is the case, we can determine the topological derivative of the energy functional

$$J(\Omega(\varepsilon)) = \frac{1}{2} a_{\varepsilon}(u_{\varepsilon}, u_{\varepsilon}) - L_{\varepsilon}(u_{\varepsilon})$$
(30)

from the expansion of the energy functional in the truncated domain

$$I_{\varepsilon}^{R}(u_{\varepsilon}^{R}) = \frac{1}{2}a^{R}(u_{\varepsilon}^{R}, u_{\varepsilon}^{R}) - L^{R}(u_{\varepsilon}^{R}) + \frac{1}{2}\langle A_{\varepsilon}(\gamma^{R}u_{\varepsilon}^{R}), \gamma^{R}u_{\varepsilon}^{R}\rangle_{R}$$
 (31)

which takes the form

$$I_{\varepsilon}^{R}(u_{\varepsilon}^{R}) = J(\Omega) + \varepsilon^{d} \langle B(\gamma^{R}u), \gamma^{R}u \rangle_{R} + o(\varepsilon^{d}) , \qquad (32)$$

where $u^R = u(\Omega_R)$ stands for the restriction to the truncated domain of the solution $u = u(\Omega)$ of the original variational inequality in the unperturbed domain Ω .

This result is based on the equality

$$J(\Omega(\varepsilon)) = I_{\varepsilon}^{R}(u_{\varepsilon}^{R}), \tag{33}$$

and the following characterisation of the energy functional for the specific case

$$I_{\varepsilon}^{R}(u_{\varepsilon}^{R}) = \inf_{\varphi \in K} \left\{ \frac{1}{2} a^{R}(\varphi, \varphi) - L^{R}(\varphi) + \frac{1}{2} \langle A_{\varepsilon}(\gamma^{R}\varphi), \gamma^{R}\varphi \rangle_{R} \right\} . \tag{34}$$

The domain decomposition method can be applied under the assumption that the quadratic term $\varepsilon \mapsto \langle A_{\varepsilon}(\gamma^R u_{\varepsilon}), \gamma^R u_{\varepsilon} \rangle_R$ is a regular perturbation of the bilinear form.

Proposition 2.1 Assume that (28) holds in the operator norm and that the strong convergence takes place

$$u_{\epsilon}^{R} \to u^{R}$$
 (35)

in the energy norm for the functional (34). Then we have

$$I_{\varepsilon}^{R}(u_{\varepsilon}^{R}) = I^{R}(u^{R}) + \varepsilon^{3} \langle B(u^{R}), u^{R} \rangle_{R} + o(\varepsilon^{3}),$$
 (36)

where $o(\varepsilon^3)/\varepsilon^3 \to 0$ with $\varepsilon^3 \to 0$ in the same energy norm.

The proof of Proposition 2.1 is based on the evident inequalities

$$\frac{I_{\varepsilon}^{R}(u_{\varepsilon}^{R}) - I^{R}(u_{\varepsilon}^{R})}{\varepsilon^{3}} \leq \frac{I_{\varepsilon}^{R}(u_{\varepsilon}^{R}) - I^{R}(u^{R})}{\varepsilon^{3}} \leq \frac{I_{\varepsilon}^{R}(u^{R}) - I^{R}(u^{R})}{\varepsilon^{3}} , \quad (37)$$

which imply the existence of the limit

$$\limsup_{\varepsilon^{3} \to 0} \frac{I_{\varepsilon}^{R}(u_{\varepsilon}^{R}) - I^{R}(u_{\varepsilon}^{R})}{\varepsilon^{3}} = \lim_{\varepsilon^{3} \to 0} \frac{I_{\varepsilon}^{R}(u_{\varepsilon}^{R}) - I^{R}(u^{R})}{\varepsilon^{3}} =$$

$$\liminf_{\varepsilon^{3} \to 0} \frac{I_{\varepsilon}^{R}(u^{R}) - I^{R}(u^{R})}{\varepsilon^{3}} = \langle B(u^{R}), u^{R} \rangle_{R}.$$
(38)

In the subsequent sections the explicit form of the bilinear form which gives rise to the operator B is presented for the laplacian and for the linear elasticity in three spatial dimensions.

3 Case of Laplace equation in \mathbb{R}^3

Let us consider the equation

$$\Delta u = 0$$
 in $\Omega \subset \mathbb{R}^3$ (39)

with some, unspecified for the moment, boundary conditions. We assume also that $0 \in \operatorname{int} \Omega$, so that we may surround it with the sphere of some radius R, $S(R) \subset \operatorname{int} \Omega$. Our goal is to express $\operatorname{grad} u = (u_{/1}, u_{/2}, u_{/3})^{\mathsf{T}}$ in terms of integrals of u on S(R). As it is known, the solution to (39) is analytic in the interior of domain, so we may use for this derivation the formal series method, as mentioned already in [2] for the 2D case.

To this end we shall assume that in the neighbourhood of 0 the solution has the form

$$u(\mathbf{x}) = a_{000} + \sum_{\alpha=1}^{\infty} \sum_{k_1 + k_2 + k_3 = \alpha} \frac{1}{k_1! k_2! k_3!} a_{k_1 k_2 k_3} x_1^{k_1} x_2^{k_2} x_3^{k_3}$$
(40)

where k_1, k_2, k_3 are positive integers. In spherical coordinate system around

0 we have also

$$x_1(\varphi, \theta) = R\cos\theta\cos\varphi, \quad x_2(\varphi, \theta) = R\cos\theta\sin\varphi, \quad x_3(\varphi, \theta) = R\sin\theta$$

and we may define $A(\varphi, \theta) = R^2 \cos \theta$, where $\varphi \in (-\pi, \pi]$, $\theta \in [-\pi/2, \pi/2]$.

We shall define also functions

$$I(k_1, k_2, k_3) = \int_{S(R)} x_1^{k_1} x_2^{k_2} x_3^{k_3} ds =$$

$$\int_{-\pi/2}^{\pi/2} \int_{-\pi}^{\pi} x_1^{k_1} (\varphi, \theta) x_2^{k_2} (\varphi, \theta) x_3^{k_3} (\varphi, \theta) A(\varphi, \theta) d\varphi d\theta.$$
(41)

For example,

$$I(2,0,0) = \frac{4}{3}\pi R^4$$
, $I(4,0,0) = \frac{4}{5}\pi R^6$, $I(2,2,0) = I(2,0,2) = \frac{4}{15}\pi R^6$. (42)

From representation of the solution (40) results the following expression for the surface integral

$$\begin{split} \int_{S(R)} ux_1 \, ds = & I(2,0,0)a_{100} + \\ & \frac{1}{6}I(4,0,0)a_{300} + \frac{1}{2}I(2,2,0)a_{120} + \frac{1}{2}I(2,0,2)a_{102} + \\ & \frac{30}{120}I(2,2,2)a_{122} + \frac{10}{120}I(4,2,0)a_{320} + \frac{10}{120}I(4,0,2)a_{302} + \\ & \frac{5}{120}I(2,4,0)a_{140} + \frac{5}{120}I(2,0,4)a_{104} + \frac{1}{120}I(6,0,0)a_{500} + \\ \end{split}$$

terms corresponding to $\alpha=7,9,\ldots$

(43)

The terms corresponding to even values of α disappear for antisymmetry reasons.

Exploiting once more the representation (40), we may explicitly compute that

$$\Delta u_{/1}|_{\mathbf{x}=0} = a_{300} + a_{120} + a_{102} = 0 \tag{44}$$

what means, in view of (42), that

$$\frac{1}{6}I(4,0,0)a_{300} + \frac{1}{2}I(2,2,0)a_{120} + \frac{1}{2}I(2,0,2)a_{102} = 0.$$

This takes care of the part corresponding to $\alpha = 3$. For $\alpha = 5$ we shall differentiate (39) more times, obtaining

$$\Delta \Delta u_{/1} \mid_{\mathbf{x}=0} = a_{500} + a_{140} + a_{104} + 2(a_{320} + a_{302} + a_{122}) = 0 \tag{45}$$

Taking into account that

$$I(2,2,2) = \frac{4}{105}\pi R^8$$
, $I(4,2,0) = I(4,0.2) = I(2,4,0) = I(2,0,4) = \frac{12}{105}\pi R^8$,
$$I(6,0,0) = \frac{60}{105}\pi R^8$$
,

the appropriate part of (42) also vanishes

$$\begin{split} &\frac{30}{120}I(2,2,2)a_{122} + \frac{10}{120}I(4,2,0)a_{320} + \frac{10}{120}I(4,0,2)a_{302} + \\ &\frac{5}{120}I(2,4,0)a_{140} + \frac{5}{120}I(2,0,4)a_{104} + \frac{1}{120}I(6,0,0)a_{500} = 0. \end{split}$$

In the same way we may cancel further terms.

As a result we get

$$a_{100} = u_{/1}(0) = \frac{3}{4\pi R^4} \int_{S(R)} ux_1 \, ds$$

or, in general

$$u_{/1}(0) = \frac{3}{4\pi R^4} \int_{S(R)} ux_1 \, ds,$$

$$u_{/2}(0) = \frac{3}{4\pi R^4} \int_{S(R)} ux_2 \, ds,$$

$$u_{/3}(0) = \frac{3}{4\pi R^4} \int_{S(R)} ux_3 \, ds.$$
(46)

To test the formula, let us take the function $u(\mathbf{x}) = 1/|\mathbf{x} - \mathbf{p}|$, where $\mathbf{p} = (2, 2, 2)^{\mathsf{T}}$, and R = 1. Then the exact value of $u_{/1}(0)$ is $\sqrt{3}/36 = 0.04811252243$ and numerical integration using Maple gives

$$u_{/1}(0) = \frac{3}{4\pi R^4} \int_{S(R)} ux_1 ds = 0.04811252242.$$

Using (46) one can easily write down the bilinear form

$$\begin{split} b_R(u,v) = & \Big(\frac{3}{4\pi R^4}\Big)^2 \Big(\int_{S(R)} ux_1 \, ds \cdot \int_{S(R)} vx_1 \, ds \\ & + \int_{S(R)} ux_2 \, ds \cdot \int_{S(R)} vx_2 \, ds + \int_{S(R)} ux_3 \, ds \cdot \int_{S(R)} vx_3 \, ds \Big) \end{split}$$

such, that energy density at 0 is $\frac{1}{2}b_R(u,u)$. From the computational point of view, the effort in comparison to 2D case [2] grows similarly as the difficulty of computing integrals over circle versus integrals over sphere.

4 Case of elasticity system in \mathbb{R}^3

Let us now consider the same domain as in the last section, but a different problem, namely the elasticity system

$$(1 - 2\nu)\Delta \mathbf{u} + \operatorname{grad}\operatorname{div}\mathbf{u} = 0, \tag{47}$$

where $\mathbf{u} = (u_1, u_2, u_3)^{\mathsf{T}}$, $\nu = \lambda/(2(\lambda + \mu) - \text{Poisson ratio}$ and λ, μ are Lame coefficients. Our goal is to express elements of strain tensor ε_{ij} at $\mathbf{x} = 0$ in terms of integrals of u_i over S(R). In principle it could be done in the same way as in case of Laplace equation in the last section or 2-D elasticity in [2]. However, the calculations would be extremely complicated, as we shall see later. Therefore we will use the knowledge of the form of the solution for Dirichlet problem in the ball, as proposed by Trefftz,

$$\mathbf{u} = \mathbf{U} + (r^2 - R^2) \mathbf{grad} \, \Psi, \tag{48}$$

where U is a harmonic vector, Ψ – harmonic scalar and $r = \sqrt{\mathbf{x}^{\mathsf{T}}\mathbf{x}}$. In the sequel we shall follow partially the derivation from [1], chapter 5. We introduce standard polar coordinates

$$x_1 = r \sin \theta \cos \varphi, \quad x_2 = r \sin \theta \sin \varphi, \quad x_3 = r \cos \theta.$$

with $\theta \in [0, \pi]$, $\varphi \in (-\pi, \pi]$. It is well known that a harmonic vector **U** has the form

$$U = \sum_{n=0}^{\infty} \left(\frac{r}{R}\right)^n Y_n(\theta, \varphi), \quad r < R, \quad (49)$$

where $Y_n(\theta, \varphi)$ consists of Laplace spherical vectors

$$Y_n = a_{n0}P_n(\tau) + \sum_{m=1}^n [a_{nm}\cos(m\varphi) + b_{nm}\sin(m\varphi)]P_n^m(\tau).$$
 (50)

Here $\tau = \cos \theta$, $\mathbf{a}_{nm} = (a_{nm}^1, a_{nm}^2, a_{nm}^3)^{\top}$, $\mathbf{b}_{nm} = (b_{nm}^1, b_{nm}^2, b_{nm}^3)^{\top}$ and

$$P_n(\tau) = \frac{1}{2^n n!} \frac{d^n}{d\tau^n} (\tau^2 - 1)^n, \qquad P_n^m(\tau) = (1 - \tau^2)^{m/2} \frac{d^m}{d\tau^m} P_n(\tau).$$

The explicit forms of these polynomials for values of n, m which are needed in our calculations are given in Appendix.

We introduce the scalar product and the corresponding norm on S(R),

$$\langle f, g \rangle_R = \int_{S(R)} fg \, ds, \quad ||f||_R = \sqrt{\langle f, f \rangle_R}.$$
 (51)

Furthermore we denote

$$U_n = \frac{r^n}{R^n} Y_n(\theta, \varphi) = \frac{1}{R^n} \hat{Y}_n(\mathbf{x}) \qquad (52)$$

where

$$\hat{Y}_n(\mathbf{x}) = \mathbf{a}_{n0}\hat{P}_n(\mathbf{x}) + \sum_{n=1}^{n} [\mathbf{a}_{nm}\hat{P}_n^{m,c}(\mathbf{x}) + \mathbf{b}_{nm}.\hat{P}_n^{m,s}(\mathbf{x})].$$
 (53)

The polynomials \hat{P} are given by identities

$$\hat{P}_{n}(\mathbf{x}) = r^{n} P_{n}(\cos \theta),$$

$$\hat{P}_{n}^{m,c}(\mathbf{x}) = r^{n} P_{n}^{m}(\cos \theta) \cos(m\varphi),$$

$$\hat{P}_{n}^{m,\theta}(\mathbf{x}) = r^{n} P_{n}^{m}(\cos \theta) \sin(m\varphi).$$
(54)

These are homogeneous polynomials of n-th order in terms of variables x_1, x_2, x_3 . Their normalized versions are defined as

$$d_{n}(\mathbf{x}) = \frac{1}{\|\hat{P}_{n}\|_{R}} \hat{P}_{n}(\mathbf{x}),$$

$$c_{n}^{m}(\mathbf{x}) = \frac{1}{\|\hat{P}_{n}^{m,c}\|_{R}} \hat{P}_{n}^{m,c}(\mathbf{x}),$$

$$s_{n}^{m}(\mathbf{x}) = \frac{1}{\|\hat{P}_{n}^{m,e}\|_{R}} \hat{P}_{n}^{m,e}(\mathbf{x}).$$
(55)

The set of functions

$$\{d_0;\ d_1,c_1^1,s_1^1;\ d_2,c_2^1,s_2^1,c_2^2,s_2^2;\ d_3,c_3^1,s_3^1,c_3^2,s_3^2,c_3^3,s_3^3;\ \ldots\}$$

constitutes a system of harmonic polynomials orthonormal on S(R). In these terms

$$U_n = \frac{1}{R^n} [a_{n0} d_n(\mathbf{x}) + \sum_{m=1}^n (a_{nm} c_n^m(\mathbf{x}) + b_{nm} s_n^m(\mathbf{x}))].$$
 (56)

Now from (48) it follows that

$$\mathbf{u}_{|r=R} = \mathbf{U}_{|r=R} = \sum_{n=0}^{\infty} \mathbf{U}_{n|r=R}.$$
 (57)

Using (56) and orthonormality we easily compute constant coefficients for $n \ge 0, m = 1..n, i = 1, 2, 3$:

$$a_{n0}^{i} = R^{n} \langle u_{i}, d_{n}(\mathbf{x}) \rangle_{R},$$

$$a_{nm}^{i} = R^{n} \langle u_{i}, c_{n}^{m}(\mathbf{x}) \rangle_{R},$$

$$b_{nm}^{i} = R^{n} \langle u_{i}, s_{n}^{m}(\mathbf{x}) \rangle_{R}.$$
(58)

The harmonic scalar Ψ in (48) also has a representation

$$\Psi = \sum_{n=0}^{\infty} \Psi_n = \sum_{n=0}^{\infty} \frac{r^n}{R^n} Z_n(\theta, \varphi).$$
 (59)

Using (47) one can obtain [1] the relation

$$\Psi_{n-1} = -\frac{1}{2[(3-2\nu)n - 2(1-\nu)]} \operatorname{div} \mathbf{U}_n. \tag{60}$$

After denoting $k_n(\nu)=1/2[(3-2\nu)n-2(1-\nu)]$ the solution of the elasticity system in the ball takes on the form

$$\mathbf{u} = \sum_{n=0}^{\infty} [\mathbf{U}_n + (R^2 - r^2)k_n(\nu) \operatorname{grad} \operatorname{div} \mathbf{U}_n]. \tag{61}$$

Since we are looking for $\varepsilon_{ij}(0)$, only the part of \mathbf{u} which is linear in \mathbf{x} is relevant. It contains only two terms:

$$\hat{\mathbf{u}} = \mathbf{U}_1 + R^2 k_3(\nu) \operatorname{grad} \operatorname{div} \mathbf{U}_3. \tag{62}$$

Since, for any f(x), grad div $(af) = H(f) \cdot a$, where H(f) is the Hessian matrix of f, we obtain

$$\hat{\mathbf{u}} = \frac{1}{R} [\mathbf{a}_{10} d_1(\mathbf{x}) + \mathbf{a}_{11} c_1^1(\mathbf{x}) + \mathbf{b}_{11} s_1^1(\mathbf{x})] + R^2 k_3(\nu) \frac{1}{R^3} \left[H(d_3)(\mathbf{x}) \mathbf{a}_{30} + \sum_{m=1}^3 \left(H(c_3^m)(\mathbf{x}) \mathbf{a}_{3m} + H(s_3^m)(\mathbf{x}) \mathbf{b}_{3m} \right) \right]$$
(63)

From the above we may single out the coefficients standing at x_1, x_2, x_3 in u_1, u_2, u_3 . In particular, see Appendix,

$$\begin{split} \varepsilon_{11}(0) &= u_{1/1}(0) = \frac{1}{R^3} \sqrt{\frac{3}{4\pi}} a_{11}^1 + \frac{1}{R^5} k_3(\nu) \Big[-3\sqrt{\frac{7}{4\pi}} a_{30}^3 - 9\sqrt{\frac{7}{24\pi}} a_{31}^1 \\ &- 3\sqrt{\frac{7}{24\pi}} b_{31}^2 + 30\sqrt{\frac{7}{240\pi}} a_{32}^3 + 90\sqrt{\frac{7}{1440\pi}} a_{33}^3 + 90\sqrt{\frac{7}{1440\pi}} b_{33}^2 \Big], \\ \varepsilon_{22}(0) &= u_{2/2}(0) = \frac{1}{R^3} \sqrt{\frac{3}{4\pi}} b_{11}^2 + \frac{1}{R^5} k_3(\nu) \Big[-3\sqrt{\frac{7}{4\pi}} a_{30}^3 - 3\sqrt{\frac{7}{24\pi}} a_{31}^1 \\ &- 9\sqrt{\frac{7}{24\pi}} b_{31}^2 - 30\sqrt{\frac{7}{240\pi}} a_{32}^3 - 90\sqrt{\frac{7}{1440\pi}} a_{33}^1 - 90\sqrt{\frac{7}{1440\pi}} b_{33}^2 \Big], \\ \varepsilon_{33}(0) &= u_{3/3}(0) = \frac{1}{R^3} \sqrt{\frac{3}{4\pi}} a_{10}^3 + \frac{1}{R^5} k_3(\nu) \Big[6\sqrt{\frac{7}{4\pi}} a_{30}^3 + 12\sqrt{\frac{7}{24\pi}} a_{31}^1 \\ &+ 12\sqrt{\frac{7}{24\pi}} b_{31}^2 \Big], \end{split}$$

Observe that

$$\varepsilon_{11}(0) + \varepsilon_{22}(0) + \varepsilon_{33}(0) = \frac{1}{R^3} \sqrt{\frac{3}{4\pi}} \left(R\langle u_1, c_1^1 \rangle_R + R\langle u_2, s_1^1 \rangle_R + R\langle u_3, d_1 \rangle_R \right)$$
 and $c_1^1 = \frac{1}{R^2} \sqrt{\frac{3}{4\pi}} x_1$, $s_1^1 = \frac{1}{R^2} \sqrt{\frac{3}{4\pi}} x_2$, $d_1 = \frac{1}{R^2} \sqrt{\frac{3}{4\pi}} x_3$, exactly the same as for the case of Laplace equation. This should be expected, since $\operatorname{tr} \varepsilon$ is a

harmonic function.

$$\begin{split} \varepsilon_{12}(0) &= \frac{1}{2}(u_{1/2}(0) + u_{2/1}(0)) = \frac{1}{R^3}\sqrt{\frac{3}{4\pi}}(b_{11}^1 + a_{11}^2) \\ &+ \frac{1}{R^5}k_3(\nu)\Big[-3\sqrt{\frac{7}{24\pi}}a_{31}^2 - \sqrt{\frac{7}{24\pi}}b_{31}^1 + 15\sqrt{\frac{7}{60\pi}}b_{32}^3 \\ &- 90\sqrt{\frac{7}{1440\pi}}a_{33}^2 + 90\sqrt{\frac{7}{1440\pi}}b_{33}^1\Big], \end{split}$$

and similarly for $\varepsilon_{13}(0)$, $\varepsilon_{23}(0)$ In order to test these formulas, they were applied to one of the fundamental solutions of the elasticity system. Let $\mathbf{p} = (2, 2, 2)^{\mathsf{T}}$, $r = |\mathbf{x} - \mathbf{p}|$; then the displacement corresponding to the unit concentrated force in the direction x_1 has the form

$$V_1 = ((3-4\nu)/r + (x_1-p_1)^2/r^3, (x_1-p_1)(x_2-p_2)/r^3, (x_1-p_1)(x_3-p_3)/r^3)^{\top}$$
. Hence for $R=1$ and $\nu=0.25$ we have $\varepsilon_{11}(0)=1/12\sqrt{3}=0.04811252245$. The value obtained from the above expression, after numerical integration for computing a_{nm}^i, b_{nm}^i (Maple), was $\varepsilon_{11}(0)=0.04811252241$.

Again, as in the case of Laplace equation in the last section, one can construct the bilinear form representing the energy density at 0. In 2D case [2] it was necessary to compute to this goal 8 integrals over circle using 1-st (x_1, x_2) and 3-rd order (x_1^3, x_2^3) polynomials. Here we must compute 24 such integrals over sphere, and polynomials, even if more complicated, are still explicitly given. The computational effort grows only slightly more as in the case of Laplace equation

5 Appendix

The Laplace spherical polynomials have the following explicit form.

For n=1:

$$\hat{P}_1(\mathbf{x}) = x_3, \quad \hat{P}_1^{1,c}(\mathbf{x}) = x_1, \quad \hat{P}_1^{1,s}(\mathbf{x}) = x_2,$$

$$\|\hat{P}_1\|_R = \|\hat{P}_1^{1,c}\|_R = \|\hat{P}_1^{1,s}\|_R = R^2 \sqrt{\frac{4\pi}{3}},$$

and for n=3:

$$\begin{split} \hat{P}_3(\mathbf{x}) &= x_3^3 - \frac{3}{2} x_2^2 x_3 - \frac{3}{2} x_1^2 x_3, & \|\hat{P}_3\|_R = R^4 \sqrt{\frac{4\pi}{7}}, \\ \hat{P}_3^{1,c}(\mathbf{x}) &= 6 x_1 x_3^2 - \frac{3}{2} x_1^3 - \frac{3}{2} x_1 x_2^2, & \|\hat{P}_3^{1,c}\|_R = R^4 \sqrt{\frac{24\pi}{7}}, \\ \hat{P}_3^{1,s}(\mathbf{x}) &= 6 x_2 x_3^2 - \frac{3}{2} x_2^3 - \frac{3}{2} x_1^2 x_2, & \|\hat{P}_3^{1,s}\|_R = R^4 \sqrt{\frac{24\pi}{7}}, \\ \hat{P}_3^{2,c}(\mathbf{x}) &= 15 x_1^2 x_3 - 15 x_2^2 x_3, & \|\hat{P}_3^{2,c}\|_R = R^4 \sqrt{\frac{240\pi}{7}}, \\ \hat{P}_3^{2,s}(\mathbf{x}) &= 15 x_1 x_2 x_3, & \|\hat{P}_3^{2,s}\|_R = R^4 \sqrt{\frac{60\pi}{7}}, \\ \hat{P}_3^{3,c}(\mathbf{x}) &= 15 x_1^3 - 45 x_1 x_2^2, & \|\hat{P}_3^{3,c}\|_R = R^4 \sqrt{\frac{1440\pi}{7}}, \\ \hat{P}_3^{3,s}(\mathbf{x}) &= 45 x_1^2 x_2 - 15 x_2^3, & \|\hat{P}_3^{3,s}\|_R = R^4 \sqrt{\frac{1440\pi}{7}}, \end{split}$$

The Hessian matrices of d_3 , c_3^i , s_3^i are

$$H(d_3) = \frac{1}{R^4} \sqrt{\frac{7}{4\pi}} \begin{bmatrix} -3x_3 & , & 0 & , & -3x_1 \\ 0 & , & -3x_3 & , & -3x_2 \\ -3x_1 & , & -3x_2 & , & 6x_3 \end{bmatrix}$$

$$H(c_3^1) = \frac{1}{R^4} \sqrt{\frac{7}{24\pi}} \begin{bmatrix} -9x_1 & , & -3x_2 & , & 12x_3 \\ -3x_2 & , & -3x_1 & , & 0 \\ 12x_3 & , & 0 & , & 12x_1 \end{bmatrix}$$

$$H(s_3^1) = \frac{1}{R^4} \sqrt{\frac{7}{24\pi}} \begin{bmatrix} -3x_2 & , & -3x_1 & , & 0 \\ -3x_1 & , & -9x_2 & , & 12x_3 \\ 0 & , & 12x_3 & , & 12x_2 \end{bmatrix}$$

$$H(c_3^2) = \frac{1}{R^4} \sqrt{\frac{7}{240\pi}} \begin{bmatrix} 30x_3 & , & 0 & , & 30x_1 \\ 0 & , & -30x_3 & , & -30x_2 \\ 30x_1 & , & -30x_2 & , & 0 \end{bmatrix}$$

$$H(s_3^2) = \frac{1}{R^4} \sqrt{\frac{7}{60\pi}} \begin{bmatrix} 0 & , & 15x_3 & , & 15x_2 \\ 15x_3 & , & 0 & , & 15x_1 \\ 15x_2 & , & 15x_1 & , & 0 \end{bmatrix}$$

$$H(c_3^3) = \frac{1}{R^4} \sqrt{\frac{7}{1440\pi}} \begin{bmatrix} 90x_1 & , & -90x_2 & , & 0 \\ -90x_2 & , & -90x_1 & , & 0 \\ 0 & , & 0 & , & 0 \end{bmatrix}$$

$$H(s_3^3) = \frac{1}{R^4} \sqrt{\frac{7}{1440\pi}} \begin{bmatrix} 90x_2 & , & 90x_1 & , & 0 \\ 90x_1 & , & -90x_2 & , & 0 \\ 0 & , & 0 & , & 0 \end{bmatrix}$$

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