Supporting Information for "A shape optimization approach towards improving the understanding of magmatic plumbing system"

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Introduction

Text S1. Calculation of the shape derivative of $J_{\mathrm{LS}}(\Omega)$ using Cea's method

For completeness, we provide a formal outline of the calculation of the shape derivative of the function $J_{\mathrm{LS}}(\Omega)$ in (2). We essentially reproduce the argument from (Allaire et al., 2004), based on Céa's method (Cea, 1986).

Let us first recall a classical result, which is often referred to as the Reynolds transport theorem, see e.g. (Henrot & Pierre, 2018).

Proposition 0.1 *Let $f : \mathbb{R}^3 \to \mathbb{R}$ be a smooth function, and let $F(\Omega)$ be defined by:*

$$F(\Omega) := \int_{\Omega^c} f \, \mathrm{d}\boldsymbol{x}.$$

The shape derivative of the functional $F(\Omega)$ then reads:

$$F'(\Omega)(\boldsymbol{\theta}) = -\int_{\Gamma} f(\boldsymbol{\theta} \cdot \boldsymbol{n}) \, \mathrm{d}s,$$

where $\boldsymbol{n}$ is the unit normal vector to Γ, pointing outward Ω.

We now turn the proof of the formula (2), properly speaking. Let V be the space of vector-valued functions $\mathbf{u} : \mathbb{R}^3 \to \mathbb{R}$ vanishing on the region Γ_{b}, and let $\mathcal{L}(\Omega, \cdot, \cdot) : V \times V \to \mathbb{R}$ be defined by:

$$\mathcal{L}(\Omega, \mathbf{u}, \mathbf{p}) = \int_{\Gamma_{\mathrm{u}}} |\mathbf{u} - \mathbf{u}_{\mathrm{obs}}|^2 \, \mathrm{d}s + \int_{\Omega^c} Ae(\mathbf{u}) : e(\mathbf{p}) \, \mathrm{d}\mathbf{x} - \Delta P \int_{\Gamma} \mathbf{p} \cdot \mathbf{n} \, \mathrm{d}s.$$

Intuitively, $\mathcal{L}(\Omega, \mathbf{u}, \mathbf{p})$ is the Lagrangian associated to the minimization problem (2), in the equivalent formulation where the elasticity problem (1) for the displacement $\mathbf{u}_\Omega$ of the underground is seen as a constraint and $\mathbf{p}$ is the associated Lagrange multiplier, that is:

$$\min_{\Omega, \mathbf{u}} \int_{\Gamma_u} |\mathbf{u} - \mathbf{u}_{\mathrm{obs}}|^2 \, \mathrm{d}s \text{ s.t. } \begin{cases} -\mathrm{div}(Ae(\mathbf{u})) = \mathbf{0} & \text{in } \Omega^c, \\ \mathbf{u} = \mathbf{0} & \text{on } \Gamma_{\mathrm{b}}, \\ Ae(\mathbf{u})(-\mathbf{n}) = \Delta P \mathbf{n} & \text{on } \Gamma, \\ Ae(\mathbf{u})\mathbf{n} = \mathbf{0} & \text{on } \partial D \setminus \overline{\Gamma_{\mathrm{b}}}, \end{cases} \tag{S.1}$$

By construction, it holds:

$$\forall \mathbf{p} \in V, \quad J_{\mathrm{LS}}(\Omega) = \mathcal{L}(\Omega, \mathbf{u}_\Omega, \mathbf{p}). \tag{S.2}$$

Introducing a smooth function $\chi : \mathbb{R}^3 \to \mathbb{R}$, which equals 1 on Ω and 0 on ∂D, and applying the Green's formula, we may rewrite the last integral as an integral over the domain Ω^c:

$$\mathcal{L}(\Omega, \mathbf{u}, \mathbf{p}) = \int_{\Gamma_{\mathrm{u}}} |\mathbf{u} - \mathbf{u}_{\mathrm{obs}}|^2 \,\mathrm{d}s + \int_{\Omega^c} Ae(\mathbf{u}) : e(\mathbf{p}) \,\mathrm{d}\mathbf{x} + \Delta P \int_{\Omega^c} \mathrm{div}(\chi \mathbf{p}) \,\mathrm{d}\mathbf{x}.$$

For a given shape Ω, $\mathbf{u}$ attains the minimum in (S.1) if there exists $\mathbf{p} \in V$ such that $(\mathbf{u}, \mathbf{p}) \in V \times V$ is a saddle point of the function $\mathcal{L}(\Omega, \cdot, \cdot)$. We then search for these saddle points. To achieve this, we equate the partial derivatives of $\mathcal{L}(\Omega, \cdot, \cdot)$ to 0. This yields:

$$\forall \widehat{\mathbf{p}} \in V, \quad \int_{\Omega^c} Ae(\mathbf{u}) : e(\widehat{\mathbf{p}}) \,\mathrm{d}\mathbf{x} - \Delta P \int_{\Gamma} \widehat{\mathbf{p}} \cdot \mathbf{n} \,\mathrm{d}s = 0, \tag{S.3}$$

and

$$\forall \widehat{\mathbf{u}} \in V, \quad 2 \int_{\Gamma_{\mathrm{u}}} (\mathbf{u} - \mathbf{u}_{\mathrm{obs}}) \cdot \widehat{\mathbf{u}} \,\mathrm{d}s + \int_{\Omega^c} Ae(\widehat{\mathbf{u}}) : e(\mathbf{p}) \,\mathrm{d}\mathbf{x} = 0. \tag{S.4}$$

From the first relation (S.3), it immediately follows that $\mathbf{u}$ is the unique solution $\mathbf{u}_\Omega$ to the state equation (1). From the second relation (S.4), we see that $\mathbf{p}$ is the solution $\mathbf{p}_\Omega$ to the adjoint system (5).

Let us now return to the equation (S.2). Taking derivatives with respect to the shape Ω in both sides, the chain rule yields:

$$\forall \mathbf{p} \in V, \quad J'_{\mathrm{LS}}(\Omega)(\boldsymbol{\theta}) = \frac{\partial \mathcal{L}}{\partial \Omega}(\Omega, \mathbf{u}_\Omega, \mathbf{p})(\theta) + \frac{\partial \mathcal{L}}{\partial \mathbf{u}}(\Omega, \mathbf{u}_\Omega, \mathbf{p})(\mathbf{u}'_\Omega(\boldsymbol{\theta})). \tag{S.5}$$

The first partial derivative in the above right-hand side is the derivative of the mapping $\Omega \mapsto \mathcal{L}(\Omega, \mathbf{u}, \mathbf{p})$ (for fixed $\mathbf{u}$, $\mathbf{p} \in V$), which is eventually evaluated at $\mathbf{u} = \mathbf{u}_\Omega$ and $\mathbf{p}$. This quantity is easily computed thanks to Proposition 0.1. The function $\mathbf{u}'_\Omega(\boldsymbol{\theta})$ appearing in the second term is the so-called "Eulerian derivative" of the mapping $\Omega \mapsto \mathbf{u}_\Omega$. Although the latter can be characterized by a boundary value problem, we wish to eliminate this difficult contribution. To achieve this, we now select $\mathbf{p} = \mathbf{p}_\Omega$ in (S.5), so that the second integral in the above right-hand side vanishes, see (S.4). We are thus left with:

$$J'_{\mathrm{LS}}(\Omega)(\boldsymbol{\theta}) = \frac{\partial \mathcal{L}}{\partial \Omega}(\Omega, \mathbf{u}_\Omega, \mathbf{p}_\Omega)(\boldsymbol{\theta}).$$

A simple calculation based on Proposition 0.1 now yields:

$$J'_{\mathrm{LS}}(\Omega)(\boldsymbol{\theta}) = -\int_\Gamma Ae(\mathbf{u}_\Omega) : e(\mathbf{p}_\Omega)(\boldsymbol{\theta} \cdot \mathbf{n}) \,\mathrm{d}s - \Delta P \int_\Gamma \mathrm{div}(\mathbf{p}_\Omega)(\boldsymbol{\theta} \cdot \mathbf{n}) \,\mathrm{d}s,$$

as desired.

Data Set S1.

Movie S1.

Audio S1.

References

Allaire, G., Jouve, F., & Toader, A.-M. (2004). Structural optimization using sensitivity analysis and a level-set method. *Journal of computational physics*, *194*(1), 363–393.

Cea, J. (1986). Conception Optimale Ou Identification de Formes, Calcul Rapide de La Dérivée Directionnelle de La Fonction Coût. *ESAIM: Modélisation mathématique et analyse numérique*, *20*(3), 371–402.

Henrot, A., & Pierre, M. (2018). *Shape Variation and Optimization.* EMS Tracts in Mathematics Vol. 28.