SUPPLEMENTARY MATERIAL: A RENORMALIZED NEWTON METHOD FOR LIQUID CRYSTAL DIRECTOR MODELING

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This note of Supplementary Material extends the modeling, analysis, and numerical experiments of the main paper. The general forms of the macroscopic liquid crystal director models in the presence of electric and/or magnetic fields are discussed; they are carefully compared and contrasted with the Landau-Lifshitz free energy models for ferromagnetic materials; and a typical non-dimensionalization for our prototype problem is presented. In addition, a simple example is given showing that liquid crystal free-energy functionals in general do not possess the kind of "energy decay property" (with respect to rescaling the director field $\boldsymbol{n}$) that was used in earlier work to analyze the "Harmonic Mapping Problem." Finally, we include results from additional numerical experiments, which validate certain properties of the Truncated Newton Method discussed in the main paper.

S1. Liquid crystal director models. Many experiments and devices involving liquid crystal materials can be effectively modeled using a macroscopic continuum framework in which the orientational state of the system is described by a *director field* (a unit-length vector field representing the average orientation of the molecules in a fluid element at a point), traditionally denoted by $\boldsymbol{n}$: with respect to an orthonormal frame,

$$\boldsymbol{n} = n_1\boldsymbol{e}_1 + n_2\boldsymbol{e}_2 + n_3\boldsymbol{e}_3, \quad |\boldsymbol{n}|^2 = n_1^2 + n_2^2 + n_3^2 = 1.$$

One of the main difficulties in dealing with models such as these numerically is the *unit-vector constraint* on $\boldsymbol{n}$, which must be satisfied at each point in the region occupied by the liquid crystal material. If the director field is simple enough (e.g., a modest tilting or twisting), this can be managed by representing $\boldsymbol{n}$ in terms of orientation angles (e.g., $\boldsymbol{n} = \cos\theta\,\boldsymbol{e}_1 + \sin\theta\,\boldsymbol{e}_2$, in a 2-D setting), which recasts the problem as an *unconstrained* problem for the scalar fields associated with these angles. For more complicated director fields, there can be degeneracies associated with the orientation angles, and an angle representation can't be employed. In such cases, it is common to enforce the constraint $|\boldsymbol{n}| = 1$ either by Lagrange multipliers or by penalty methods. Several other liquid crystal models involve unit-length vector fields and constraints—see [8] for more discussion. Standard references on liquid crystals include [2, 3, 9, 10]. Unit-vector constraints arise in other areas as well, including the modeling of ferromagnetic materials—see [4, 6, 7].

S1.1. Coupled electric fields. Most devices and many experiments involve the interaction between a liquid crystal material and an applied electric field (which is used to control the liquid crystal orientational properties). The electric fields are usually created by sandwiching a liquid crystal film between electrodes to which a voltage is applied. This is a coupled interaction, with the electric field influencing the orientations of the liquid crystal molecules and the molecular orientational properties

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in turn influencing the local electric fields through their effect on the dielectric tensor. The *free energy* (expressed as an integral functional of the field variables) is the thermodynamic potential that determines equilibrium states of systems such as these. For a uniaxial nematic liquid crystal material in equilibrium with a coupled electric field (at constant potential), the free energy has the generic form

$$\mathcal{F} = \int_\Omega \Big[W(\boldsymbol{n}, \nabla \boldsymbol{n}) - \frac{1}{2} \boldsymbol{D} \cdot \boldsymbol{E} \Big], \quad \boldsymbol{D} = \boldsymbol{\varepsilon}(\boldsymbol{n}) \boldsymbol{E}, \quad \boldsymbol{E} = -\nabla U.$$

Here Ω is the region occupied by the liquid crystal, W is the distortional elastic energy density, $\boldsymbol{D}$ is the electric displacement (or flux), $\boldsymbol{E}$ is the local electric field, $\boldsymbol{\varepsilon}$ is the dielectric tensor, and U is the electrostatic potential.

The form of W commonly used to model experiments and devices with real (uniaxial nematic) materials is the Oseen-Frank model [9, §2.2], [10, §3.2]:

$$\begin{aligned} 2W = {} & K_1 (\operatorname{div} \boldsymbol{n})^2 + K_2 (\boldsymbol{n} \cdot \operatorname{curl} \boldsymbol{n})^2 + K_3 |\boldsymbol{n} \times \operatorname{curl} \boldsymbol{n}|^2 \\ & + (K_2 + K_4) \big[\operatorname{tr}(\nabla \boldsymbol{n})^2 - (\operatorname{div} \boldsymbol{n})^2 \big], \end{aligned} \tag{S1.1}$$

where $K_1, \ldots, K_4$ are material-dependent and temperature-dependent "elastic constants." A simplified form, which embodies the essential features of importance to us here, is the so-called "equal elastic constant" model ($K_1 = K_2 = K_3 = K$, $K_4 = 0$):

$$W = \frac{K}{2} |\nabla \boldsymbol{n}|^2, \quad |\nabla \boldsymbol{n}|^2 = \sum_{i,j=1}^{3} \left(\frac{\partial n_i}{\partial x_j} \right)^2, \quad K > 0.$$

The expression for $|\nabla \boldsymbol{n}|^2$ above is for a fixed Cartesian frame. This is the form that we use in the main paper. We emphasize that this is done for simplicity and does not limit the applicability of the ideas or analysis.

The anisotropy of the medium is reflected in the tensorial nature of the "dielectric constant," which here corresponds to the real, symmetric, positive-definite tensor field $\boldsymbol{\varepsilon}$ (which is a function of $\boldsymbol{n}$). At a point in a uniaxial nematic liquid crystal, the $\boldsymbol{\varepsilon}$ tensor is transversely isotropic with respect to the local director $\boldsymbol{n}$, that is, it has a distinguished eigenvector parallel to $\boldsymbol{n}$ and a degenerate eigenspace perpendicular to $\boldsymbol{n}$:

$$\boldsymbol{\varepsilon}(\boldsymbol{n}) = \varepsilon_0 \big(\varepsilon_\perp \mathbf{I} + \varepsilon_{\mathrm{a}} \boldsymbol{n} \otimes \boldsymbol{n} \big) \quad \leftrightarrow \quad \varepsilon_{ij} = \varepsilon_0 (\varepsilon_\perp \delta_{ij} + \varepsilon_{\mathrm{a}} n_i n_j), \quad \varepsilon_{\mathrm{a}} := \varepsilon_\parallel - \varepsilon_\perp. \tag{S1.2a}$$

In an eigenframe with third eigenvector $\boldsymbol{n}$ at a point, for example, the $\boldsymbol{\varepsilon}$ tensor would have Cartesian components

$$\boldsymbol{\varepsilon} = \varepsilon_0 \begin{bmatrix} \varepsilon_\perp & & \\ & \varepsilon_\perp & \\ & & \varepsilon_\parallel \end{bmatrix}_{\boldsymbol{l}, \boldsymbol{m}, \boldsymbol{n}}, \qquad \boldsymbol{l}, \boldsymbol{m}, \boldsymbol{n} = \text{orthonormal triple.} \tag{S1.2b}$$

Here ε_0 is a positive constant, and $\varepsilon_\parallel$ and $\varepsilon_\perp$ are positive, material-dependent, relative dielectric permittivities (for $\boldsymbol{E}$ oriented "parallel" to $\boldsymbol{n}$, as opposed to "perpendicular" to $\boldsymbol{n}$). For situations involving AC electric fields (with the liquid crystal director responding to the time-averaged electric field, at sufficiently high frequencies), $\varepsilon_\parallel$ and $\varepsilon_\perp$ would also depend on the frequency of the AC field. The dielectric anisotropy ε_{a} can be positive or negative.

The total free energy of our simplified model then takes the form

$$\mathcal{F}[\boldsymbol{n}, U] = \frac{1}{2}\int_\Omega \big[K|\nabla \boldsymbol{n}|^2 - \boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U \cdot \nabla U\big]. \tag{S1.3}$$

This is the simplest prototype model that contains the essential features of importance to us. One can see the intrinsic saddle-point nature of the electric-field coupling: equilibria are *minimizing* with respect to $\boldsymbol{n}$ but *maximizing* with respect to U. In a generic sense, the variational problem has the form

$$\min_{|\boldsymbol{n}|=1}\max_{U} \mathcal{F}[\boldsymbol{n}, U],$$

where the extremal elements are sought over sufficiently regular fields that conform to any essential boundary conditions. The strong form of the constrained equilibrium equations for (S1.3) (with $\boldsymbol{\varepsilon}$ of the form (S1.2)) is

$$-K\Delta \boldsymbol{n} = \lambda \boldsymbol{n} + \varepsilon_0 \varepsilon_{\mathrm{a}}\big(\nabla U \cdot \boldsymbol{n}\big)\nabla U, \quad \operatorname{div}\big(\boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U\big) = 0, \quad |\boldsymbol{n}| = 1, \tag{S1.4}$$

which is to be solved in Ω subject to appropriate boundary conditions on $\boldsymbol{n}$ and U. The Lagrange multiplier field λ is associated with the pointwise unit-vector constraint. In terms of Cartesian components (with respect to a fixed frame), the electrostatics equation takes the form

$$\operatorname{div}\big(\boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U\big) = \sum_{i,j}\frac{\partial}{\partial x_i}\left(\varepsilon_{ij}\frac{\partial U}{\partial x_j}\right) = 0.$$

By virtue of (S1.2), we see that the eigenvalues of $\boldsymbol{\varepsilon}(\boldsymbol{n})$ are independent of $\boldsymbol{n}$, are strictly positive, and are given by

$$\text{eigenvalues of } \boldsymbol{\varepsilon}(\boldsymbol{n}) = \varepsilon_0 * \{\varepsilon_\parallel, \varepsilon_\parallel, \varepsilon_\perp\},$$

from which follows

$$\varepsilon_0 \min\{\varepsilon_\parallel, \varepsilon_\perp\}\int_\Omega |\nabla U|^2 \le \int_\Omega \boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U \cdot \nabla U \le \varepsilon_0 \max\{\varepsilon_\parallel, \varepsilon_\perp\}\int_\Omega |\nabla U|^2.$$

Thus any combination of boundary conditions for U (as well as interface conditions and far-field asymptotic conditions, if $\boldsymbol{E}$ extends beyond Ω) that yield a well-posed problem for $\Delta U = 0$ will also give a well-posed problem for $\operatorname{div}\big(\boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U\big) = 0$. Assuming the auxiliary conditions on U to be such, then, for any given (sufficiently regular) director field $\boldsymbol{n}$, the associated electric potential field U is uniquely determined.

In (S1.4) one again sees the coupled nature of the problem, the electric field influencing the director equilibrium solution via the ∇U terms in the first equation and the director field influencing the electric potential through $\boldsymbol{\varepsilon}(\boldsymbol{n})$ in the second equation. Modeling a realistic system of interest can bring in multiple other complications (in addition to the extra distortional elastic terms in (S1.1)), including chirality (favored spontaneous twisting distortions of the director field), polarization (existence of a net, macroscopic, electric dipole moment per unit volume), weak boundary conditions and surface anchoring potentials, periodic solutions with a-priori unknown periodicity, extended electric fields (if the region Ω is not completely enclosed by electrodes), etc. See [5] for a recent example.

S1.2. Comparison with ferromagnetics. The Landau-Lifshitz free energy provides a phenomenological model for equilibrium states of magnetization in ferromagnetic materials and bears some similarity to the Oseen-Frank model for liquid crystals [4, 6, 7]. The free-energy density is expressed in terms of a unit-length vector field $\boldsymbol{m}$, which corresponds to a normalized (saturated) magnetization vector $\boldsymbol{M}$, analogous to the liquid crystal director $\boldsymbol{n}$ but differing from it in the sense that $\boldsymbol{m}$ is a *proper* vector ($\boldsymbol{m}$ and $-\boldsymbol{m}$ are *not* equivalent). The density contains terms proportional to $|\nabla \boldsymbol{m}|^2$, penalizing spatial variations in $\boldsymbol{m}$ (as do the terms in $W(\boldsymbol{n}, \nabla \boldsymbol{n})$ to $\boldsymbol{n}$). The magnetic stray field is given in terms of a magnetostatic potential via $\boldsymbol{H}_{\mathrm{s}} = -\nabla U$ (as with the local electric field and electrostatic potential in liquid crystals, $\boldsymbol{E} = -\nabla U$). The magnetic medium can be regarded as isotropic and homogeneous, however, so that the magnetic potential solves $\Delta U = \operatorname{div} \boldsymbol{M}$ (in the material domain); whereas the electric potential for liquid crystals satisfies $\operatorname{div}\big(\boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U\big) = 0$. This last equation would become $\operatorname{div}\big(\boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U\big) = \operatorname{div} \boldsymbol{P}$ in a ferroelectric liquid crystal with polarization $\boldsymbol{P}$.

The contribution of the (spontaneous) stray field to the magnetic free-energy density is *positive* ($\frac{1}{2}\boldsymbol{B}\cdot\boldsymbol{H}_{\mathrm{s}},\ \boldsymbol{B} = \mu_0(\boldsymbol{H}_{\mathrm{s}} + \boldsymbol{M})$); whereas in a liquid crystal system at constant voltage, the coupling to an applied electric field is *negative* ($-\frac{1}{2}\boldsymbol{D}\cdot\boldsymbol{E},\ \boldsymbol{D} = \boldsymbol{\varepsilon}(\boldsymbol{n})\boldsymbol{E}$). Any externally applied magnetic field $\boldsymbol{H}_{\mathrm{e}}$ is treated as uniform throughout the sample and acts as a fixed force (or torque) on the magnetization in much the same way that external magnetic fields influence liquid crystals. Juxtaposing the two free energies (for our model problem with an external magnetic field contribution included), we would have

$$\mathcal{F}[\boldsymbol{n}] = \frac{1}{2}\int_\Omega \big[K|\nabla \boldsymbol{n}|^2 - \boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U\cdot\nabla U - \mu_0\Delta\chi(\boldsymbol{H}_{\mathrm{e}}\cdot\boldsymbol{n})^2\big]$$
$$\operatorname{div}(\boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U) = 0 \ \text{ in } \Omega, \quad \text{plus BCs}$$

versus

$$\mathcal{F}[\boldsymbol{m}] = \int_\Omega \Big[C_{\mathrm{ex}}|\nabla \boldsymbol{m}|^2 + \frac{\mu_0}{2}|\nabla U|^2 - \mu_0 \boldsymbol{H}_{\mathrm{e}}\cdot\boldsymbol{M} + \Phi(\boldsymbol{m})\Big] + \frac{\mu_0}{2}\int_{\mathbb{R}^d\setminus\Omega} |\nabla U|^2$$
$$\Delta U = \begin{cases} \operatorname{div} \boldsymbol{M}, & \text{in } \Omega \\ 0, & \text{in } \mathbb{R}^d\setminus\Omega \end{cases}, \quad \text{plus BCs and interface conditions.}$$

Here μ_0 is the vacuum magnetic permeability (the magnetic analogue of ε_0), $\Delta\chi$ is the diamagnetic anisotropy of the liquid crystal material (the magnetic analogue of ε_{a}), C_{ex} is the exchange constant, and $\Phi(\boldsymbol{m})$ is the anisotropy energy density of the ferromagnetic material (a potential favoring certain preferred directions of magnetization). See, for example, [9, §2.2 and §2.3] or [10, §3.2 and §4.1] concerning the Oseen-Frank expression, and [4, §1], [6, §1], or [7, Part I, Summary and Results] for the Landau-Lifshitz expression.

Thus, while ferromagnetic systems have to deal with the extended nature of the magnetic stray field and potential U, they do not have to cope with the indefiniteness (lack of coercivity) that the U variables cause in liquid crystal systems. Furthermore, in the liquid-crystal setting, it is not possible to introduce a Newtonian potential representation for U, as is done in computational micromagnetics, since the liquid crystal electrostatic problem $\operatorname{div}(\boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U) = 0$ (or $\operatorname{div}(\boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U) = \operatorname{div} \boldsymbol{P}$) does not reduce to a Laplace (or Poisson) equation. The combination of inhomogeneity, anisotropy, and negative-definiteness of the coupling between $\boldsymbol{n}$ and U add to the challenge of numerical modeling of liquid crystal systems.

S1.3. Non-dimensionalization. It is convenient for analysis and appropriate for numerical explorations in general to express all aspects of the problem (free-energy functional, Euler-Lagrange equations, etc.) in dimensionless form. This renders all variables independent of changes of the system of units employed, reduces the total number of parameters, and identifies the combinations of parameters upon which the equilibrium solutions actually depend. If the problem were to be left in fully dimensional form, then the vectors of unknowns in the discretized model in the paper would contain mixtures of quantities of different physical dimensions, and the norms of those vectors that are employed in our analysis would need to contain additional weight factors to balance these physical dimensions appropriately.

As an example of a reasonable non-dimensionalization, consider the model free-energy functional $\mathcal{F}$ in (S1.3) in d space dimensions ($\Omega \subset \mathbb{R}^d$). The director $\boldsymbol{n}$ is dimensionless by definition, as are $\varepsilon_{\parallel}$ and $\varepsilon_{\perp}$, their difference $\varepsilon_{\rm a}$, and the relative dielectric tensor

$$\boldsymbol{\varepsilon}_{\rm r} := \frac{1}{\varepsilon_0}\,\boldsymbol{\varepsilon} = \varepsilon_{\perp}\mathbf{I} + \varepsilon_{\rm a}\boldsymbol{n}\otimes\boldsymbol{n}.$$

One can scale lengths by the diameter of Ω and scale the electrostatic potential by the applied voltage V,

$$\overline{x}_i := \frac{x_i}{L}, \quad L := \mathrm{diam}(\Omega), \quad \overline{U} := \frac{U}{V},$$

to obtain the following dimensionless form:

$$\overline{\mathcal{F}}[\boldsymbol{n},\overline{U}] = \frac{1}{2}\int_{\overline{\Omega}} \left[\, |\overline{\nabla}\boldsymbol{n}|^2 - \alpha^2\boldsymbol{\varepsilon}_{\rm r}(\boldsymbol{n})\overline{\nabla}\,\overline{U}\cdot\overline{\nabla}\,\overline{U}\,\right], \quad \overline{\mathcal{F}} := \frac{\mathcal{F}}{KL^{d-2}}, \quad \alpha^2 := \frac{\varepsilon_0 V^2}{K}.$$

Here $\overline{\Omega}$ is the domain Ω in the rescaled coordinate system, and $\overline{\nabla}$ is the spatial gradient operator with respect to the rescaled coordinates ($\overline{\nabla} = L^{-1}\nabla$). The functional has the same form as before in (S1.3) but now with $K = 1$ and $\varepsilon_0 = \alpha^2$ (and all quantities dimensionless). The Euler-Lagrange equations (S1.4) would transform in a similar way. In the paper, we assume that the problem has been non-dimensionalized in a reasonable way such as this, but we drop the overbars for convenience of notation.

S2. Lack of an energy decay property in general. Those familiar with the analysis of the "harmonic mapping case" in [1] will wonder if any of those results are relevant to the analysis in the main paper here. We address this now. The "Harmonic Mapping Problem" is a special case of the types of models we consider here. It consists of a normalized equal-elastic-constant model with no magnetic or electric fields (the "Dirichlet Energy"):

$$\mathcal{F}[\boldsymbol{n}] = \frac{1}{2}\int_{\Omega} |\nabla\boldsymbol{n}|^2, \quad \min \mathcal{F}[\boldsymbol{n}], \;\; \text{subject to } |\boldsymbol{n}| = 1 \text{ in } \Omega,\; \boldsymbol{n} = \boldsymbol{n}_0 \text{ on } \partial\Omega.$$

In [1], a convergence analysis was presented for an iterative scheme that involved a renormalization step ($\boldsymbol{n} \leftarrow \boldsymbol{n}/|\boldsymbol{n}|$) similar to that employed in Algorithm 4.1 in the main paper. The analysis relied upon the fact that renormalizing a director field that is greater than unit length necessarily reduces the Dirichlet energy:

$$|\boldsymbol{n}| \geq 1 \text{ on } \Omega \quad \Rightarrow \quad |\nabla(\boldsymbol{n}/|\boldsymbol{n}|)| \leq |\nabla\boldsymbol{n}| \quad \Rightarrow \quad \mathcal{F}[\boldsymbol{n}/|\boldsymbol{n}|] \leq \mathcal{F}[\boldsymbol{n}].$$

Unfortunately, this decay property seems to be tied to the simple form of the Dirichlet energy and does not hold for liquid crystal free-energy functionals in general. To see this, consider, for example, an equal-elastic-constant model with an external magnetic field:

$$\mathcal{F}[\boldsymbol{n}] = \frac{1}{2}\int_\Omega \left[K|\nabla \boldsymbol{n}|^2 - \mu_0 \Delta\chi(\boldsymbol{H}\cdot\boldsymbol{n})^2\right], \quad \boldsymbol{H} = \text{const}, \quad K, \mu_0, \Delta\chi > 0. \tag{S2.1}$$

If $\boldsymbol{n}$ is un-normalized with $|\boldsymbol{n}| \geq 1$ on Ω, then rescaling $\boldsymbol{n} \leftarrow \boldsymbol{n}/|\boldsymbol{n}|$ will lower the contribution of the distortional elasticity ($|\nabla \boldsymbol{n}|^2$ term) but will increase (make less negative) the contribution of the magnetic energy density ($(\boldsymbol{H}\cdot\boldsymbol{n})^2$ term). Thus one may have in principle either $\mathcal{F}[\boldsymbol{n}/|\boldsymbol{n}|] \leq \mathcal{F}[\boldsymbol{n}]$ or $\mathcal{F}[\boldsymbol{n}/|\boldsymbol{n}|] > \mathcal{F}[\boldsymbol{n}]$. For the special case of rescaling $\boldsymbol{n}$ in (S2.1) by a *constant* multiplicative factor, we would have

$$\mathcal{F}[c\,\boldsymbol{n}] = c^2\mathcal{F}[\boldsymbol{n}], \quad c = \text{const},$$

for which

$$|c| < 1 \text{ and } \mathcal{F}[\boldsymbol{n}] < 0 \quad \Rightarrow \quad \mathcal{F}[c\,\boldsymbol{n}] > \mathcal{F}[\boldsymbol{n}].$$

It is common to have negative free energies for stable liquid crystal equilibrium director fields with external magnetic fields or coupled electric fields, and this is the case, for example, with all Fréedericksz-transition problems (classical magnetic-field or electric-field induced distortions) beyond the "switching threshold"—see for example [9, §3.4 and §3.5] or [10, §4.2].

We do not know under what circumstances one can have an energy decay property for the general Oseen-Frank distortional elastic energy density (S1.1) (with unequal elastic constants), even in the absence of magnetic or electric fields. The problems mainly of interest to us (with coupled electric fields) are not even free-energy minimization problems. They are minimax problems, and our analysis in §4.1 of the main paper applies to any regular saddle-point equilibrium solution of such problems (locally stable or unstable).

S3. Numerical experiments on the Truncated Newton Method. Numerical experiments were conducted to explore some aspects of the Truncated Newton Method (as discussed in §4.3 and §4.4): spectral properties of the projected Hessian $H(\mathbf{n})$ of (4.18) and solutions of the Truncated Newton step $H(\mathbf{n})\mathbf{p} = -\mathbf{G}(\mathbf{n})$. For this we used the same model problem (5.1), discretized as in (5.3). With $N = (n-1)^2$ total free nodes, the projected Hessian $H(\mathbf{n})$ is $3N \times 3N$, and the projected gradient $\mathbf{G}(\mathbf{n})$ is a $3N$-vector. Proposition 4.6 of §4.4 indicates that for a regular constrained discrete equilibrium solution $\mathbf{n}^*$ of this model problem, the nullity of $H(\mathbf{n}^*)$ should be equal to N. This was borne out for small-scale examples for which the full set of eigenvalues of $H(\mathbf{n}^*)$ could be computed using Matlab's eigensolver for full (dense) arrays, utilizing solution vectors $\mathbf{n}^*$ that were computed to machine attainable accuracy by the Renormalized Newton Method solver. Results are reported in Table S3.1 for $n = 4$ using a fully converged upward "escape" solution for $\mathbf{n}^*$. In this case, $N = 9$, $H(\mathbf{n}^*)$ is 27×27, and the first nine eigenvalues are of the order of the machine epsilon, while the last 18 eigenvalues are order one.

Proposition 4.7 of §4.4 indicates that $\mathbf{p} = \mathbf{n}$ is always a solution for the Truncated Newton step $H(\mathbf{n})\mathbf{p} = -\mathbf{G}(\mathbf{n})$, the only solution if $H(\mathbf{n})$ is nonsingular. To test this, we took for $\mathbf{n}$ the crude initial guess $\mathbf{n}^{\text{init}}$ of (5.6) for an upward escape solution with $\alpha = 0.6$ and solved $H(\mathbf{n})\mathbf{p} = -\mathbf{G}(\mathbf{n})$ using Matlab's backslash operator

TABLE S3.1

Eigenvalues of the projected Hessian $H(\mathbf{n}^*)$ (4.18) of the Truncated Newton step (4.19) evaluated at a fully converged "escape" solution $\mathbf{n}^*$ (see §5.1 and Fig. 5.1 right) for $n = 4$ and $N = 9$. $H(\mathbf{n}^*)$ is 27×27, and the eigenvalues are scaled and given in increasing sequence, left to right, top to bottom. The eigenvalues were calculated using Matlab's `eig()` function.

scale	scaled eigenvalues of $H(\mathbf{n}^*)$								
10^{-15}	−1.06	−0.88	−0.57	−0.49	−0.43	−0.16	0.34	0.87	1.20
1	0.55	0.59	0.98	1.59	1.97	2.27	2.52	2.53	2.92
1	3.18	3.52	3.54	4.00	4.06	4.66	4.71	5.56	5.69

TABLE S3.2

Numerical aspects of the Truncated Newton step $H(\mathbf{n})\mathbf{p} = -\mathbf{G}(\mathbf{n})$ (4.19) for the model Harmonic Mapping Problem (5.1), discretized as in (5.3). Here $\mathbf{n}$ is the crude initial guess for the upward "escape" solution (5.6) with $\alpha = 0.6$, and $H(\mathbf{n})$ is the projected Hessian of the Truncated Newton Method (4.18). 1-norm condition numbers were estimated using Matlab's `condest()` function, and minimum and maximum eigenvalues of $H(\mathbf{n})$ were computed using Matlab's `eigs()` function. $\mathbf{p}$ is the solution of $H(\mathbf{n})\mathbf{p} = -\mathbf{G}(\mathbf{n})$ computed using Matlab's backslash operator (with $H(\mathbf{n})$ stored as a symmetric sparse Matlab array).

		eigenvalues		
n	cond($H(\mathbf{n})$)	min	max	$\|\mathbf{n}-\mathbf{p}\|_\infty$
4	7.67(+02)	−.824	6.06	3.44(−15)
8	1.64(+05)	−.846	7.52	6.34(−13)
16	8.61(+06)	−.855	7.88	7.34(−11)
32	2.34(+08)	−.857	7.97	1.92(−09)
64	5.04(+09)	−.857	7.99	7.24(−08)
128	9.16(+10)	−.857	8.00	1.23(−06)

for $n = 4, 8, \ldots, 128$. Also computed were the 1-norm condition number of $H(\mathbf{n})$ (estimated by Matlab's `condest()` function), the minimum and maximum eigenvalues of $H(\mathbf{n})$ (computed by Matlab's `eigs()` function), and the max norm of the difference between the computed solution vector $\mathbf{p}$ and the true solution $\mathbf{n}$ (for $H(\mathbf{n})$ nonsingular). The results are reported in Table S3.2. The projected Hessian $H(\mathbf{n})$ was found to be indefinite but nonsingular, although ill-conditioned with condition numbers much larger than those of M and Z^TAZ in Table 5.5. The condition numbers grow with n but don't appear to follow a regular scaling law. The relationship between cond($H(\mathbf{n})$) and $\|\mathbf{n}-\mathbf{p}\|_\infty$ for the different values of n is as one would expect (in double precision).

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