Norm-preserving discretization of integral equations for elliptic PDEs with internal layers I: the one-dimensional case

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Abstract

We investigate the behavior of integral formulations of variable coefficient elliptic partial differential equations (PDEs) in the presence of steep internal layers. In one dimension, the equations that arise can be solved analytically and the condition numbers estimated in various L^p norms. We show that high-order accurate Nyström discretization leads to well-conditioned finite-dimensional linear systems if and only if the discretization is both norm-preserving in a correctly chosen L^p space and adaptively refined in the internal layer.

Keywords: integral equations, integral operator norms, divergence-form elliptic equations, internal layers, adaptive discretization

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1. Introduction

A number of problems in computational physics require the solution of divergence-form elliptic equations

$$\nabla \cdot (\epsilon(\mathbf{x}) \nabla u(\mathbf{x})) = f(\mathbf{x}) \tag{1}$$

where $\epsilon(\mathbf{x})$ is a scalar function with steep internal layers in a domain Ω . We assume for the sake of concreteness that $u(\mathbf{x})$ satisfies a Dirichlet boundary condition

$$u(\mathbf{x}) = g(\mathbf{x}) \tag{2}$$

for $\mathbf{x} \in \partial \Omega$, but the basic approach outlined below applies equally well to other types of boundary conditions. Equations of the form (1) arise, for example, in fluid dynamics [2, 22], where $\epsilon(\mathbf{x})$ is the inverse of the fluid density and in semiconductor device simulation [23], where $\epsilon(\mathbf{x})$ can be either the semiconductor permittivity, or a complicated function determined by electron and hole mobilities and diffusion coefficients. They also arise in phase field models for microstructure evolution in materials science [7]. When ϵ is piecewise constant, boundary integral equation methods are well-known to be extremely effective (see, for example, [13, 14, 17, 24, 25]). When ϵ is smooth but has a steep internal layer, however, the domain itself must be discretized. In that setting, it is most common to use finite difference or finite element approximations based on the partial differential equation itself [4, 21, 27].

Volume integral equations can also been used for problems such as (1). There is a substantial literature in this area, which we do not attempt to review, except to observe that there are a variety *Preprint submitted to*September 5, 2021

of analytic methods which can be used to derive integral formulations, a variety of numerical methods which can be used for their discretization, and a variety of fast algorithms which can be used for iterative or direct solution [5, 6, 8, 9, 10, 11, 16, 18, 20, 26].

In this paper, we focus on the behavior of volume integral methods in one dimension, where the divergence form equation reduces to

$$\frac{\partial}{\partial x} \left(\epsilon(x) \frac{\partial u}{\partial x} \right) = f. \tag{3}$$

For the sake of simplicity, we assume the solution is subject to homogeneous Dirichlet conditions on the interval [a,b], that is u(a)=u(b)=0. We assume that $\epsilon(x)$ is positive, smooth and bounded, but may have steep gradients, so that its derivative $\epsilon_x(x)$ can be arbitrarily large, corresponding to an internal layer. Without care, this can lead to arbitrarily badly conditioned linear systems. While there is some literature on analyzing the conditioning of second kind integral equations (see, for example, [1, 19]), the influence of the choice of L^p space has received relatively little attention. Here, we show that a combination of adaptivity and a suitable norm-preserving discretization, to be defined below, leads to condition numbers that depend only weakly on ϵ_x . In particular, we show that for a Lippmann-Schwinger type integral equation with the second derivative u_{xx} as the unknown, a discretization that is norm-perserving in L^1 leads to nearly optimal schemes.

Our work was motivated, in part, by Bremer's analysis of boundary integral equations for scattering problems in the presence of corners [3]. He showed that naive Nyström discretization leads to ill-conditioned linear systems, but that suitable L^2 -weighting corrects the difficulty both in theory and in practice.

2. The integral equation

There are several standard methods for converting the ordinary differential equation (3) to an integral equation, typically making use of the Green's function G(x, t) that satisfies

$$\frac{d^2}{dx^2}G(x,t) = \delta(x-t), \qquad G(a,t) = G(b,t) = 0.$$

It is well-known [15] and easy to verify that

$$G(x,t) = \begin{cases} (x-a)(t-b)/(b-a) & \text{if } x < t \\ (x-b)(t-a)/(b-a) & \text{if } x \ge t \end{cases}$$
 (4)

Rewriting the equation (3) in the form

$$u_{xx} + \frac{\epsilon_x}{\epsilon} u_x = \frac{f}{\epsilon} \tag{5}$$

and representing the solution as

$$u(x) = \int_{a}^{b} G(x, t)\sigma(t) dt, \qquad (6)$$

we obtain an integral equation for the unknown density σ :

$$\sigma(x) + \frac{\epsilon_x(x)}{\epsilon(x)} \int_a^b G_x(x, t) \sigma(t) dt = g(x),$$
 (7)

or

$$(I + K_1)\sigma(x) = g(x) \tag{8}$$

where $g = f/\epsilon$ and

$$K_1\sigma(x) = \frac{\epsilon_x(x)}{\epsilon(x)} \int_a^b G_x(x,t)\sigma(t) dt.$$

Alternatively, one can rewrite (3) in the form

$$(\epsilon u)_{xx} - (\epsilon_x u)_x = f. \tag{9}$$

Integrating (9) against G(x, t) yields

$$u(x) + \frac{1}{\epsilon(x)} \int_0^1 G_x(x, t) (\epsilon_x(t)u(t)) dt = \frac{1}{\epsilon(x)} \int_0^1 G(x, t) f(t) dt$$
 (10)

or

$$(I + K_2)u(x) = \frac{1}{\epsilon(x)} \int_a^b G(x, t) f(t) dt, \qquad (11)$$

where

$$K_2 u(x) = \frac{1}{\epsilon(x)} \int_0^1 G_x(x,t) (\epsilon_x(t) u(t)) \, dt \, .$$

The principal difference between (7) and (10) is that, in the former, $\sigma(x) = u_{xx}(x)$ is the unknown while, in the latter, u(x) is the unknown. Both are Fredholm equations of the second kind.

2.1. Analytic solution of the integral equation

For the sake of simplicty, let us assume in this section that [a, b] = [0, 1]. ¿From the original ODE, we have

$$(\epsilon(x)u_x(x))_x = g(x)\epsilon(x)$$

$$\epsilon(x)u_x(x) = \int_0^x g(t)\epsilon(t) dt + \epsilon(0)u_x(0)$$

$$u_x(x) = \frac{1}{\epsilon(x)} \int_0^x g(t)\epsilon(t) dt + \frac{\epsilon(0)u_x(0)}{\epsilon(x)}$$
(12)

Using the fact that $\sigma = u_{xx}$, we may write

$$\sigma(x) = g(x) - \frac{\epsilon_x(x)}{\epsilon(x)^2} \left(\int_0^x g(t)\epsilon(t) dt + \epsilon(0)u_x(0) \right). \tag{13}$$

To remove the $\epsilon(0)u_x(0)$ term from the expression, we integrate the equation (12).

$$u(1) - u(0) = \int_0^1 \frac{1}{\epsilon(x)} \int_0^x g(t)\epsilon(t) \, dt \, dx + \epsilon(0)u_x(0) \int_0^1 \frac{1}{\epsilon(x)} \, dx$$

so that

$$\epsilon(0)u_x(0) = -\frac{\int_0^1 \frac{1}{\epsilon(x)} \int_0^x g(t)\epsilon(t) dt dx}{\int_0^1 \frac{1}{\epsilon(x)} dx}.$$
 (14)

Letting $A_1 = I + K_1$ denote the operator applied to σ on the left-hand side of (7), we now have an expression for its inverse in the form $A_1^{-1} = I - R_1$. From (13) and (14),

$$\sigma(x) = g(x) - \frac{\epsilon_x(x)}{\epsilon(x)^2} \left(\int_0^x g(t)\epsilon(t) dt - \frac{\int_0^1 \frac{1}{\epsilon(s)} \int_0^s g(t)\epsilon(t) dt ds}{\int_0^1 \frac{1}{\epsilon(s)} ds} \right).$$

¿From this, it is straightforward to obtain the following formula for the resolvent kernel R_1 :

$$R_1(x,t) = \frac{\epsilon_x(x)}{\epsilon(x)^2} \left(H(x-t)\epsilon(t) - \frac{\epsilon(t)}{\int_0^1 \frac{1}{\epsilon(s)} ds} \int_t^1 \frac{1}{\epsilon(s)} ds \right), \tag{15}$$

where H(x) is the standard Heavyside function.

Letting $A_2 = I + K_2$ denote the operator applied to u on the left-hand side of (10), a similar calculation yields an expression for its inverse in the form $A_2^{-1} = I - R_2$. In this case, R_2 is

$$R_2(x,t) = -\frac{\epsilon_x(t)}{\epsilon(t)^2} \left(H(x-t)\epsilon(t) - \frac{\epsilon(t)}{\int_0^1 \frac{1}{\epsilon(s)} ds} \int_0^x \frac{1}{\epsilon(s)} ds \right). \tag{16}$$

Having analytic expressions for the resolvent kernels permits us to obtain simple estimates for the condition number of the operators A_1 and A_2 acting on L_p spaces for $1 \le p \le \infty$. It is worth noting an important difference between the two resolvent kernels: the term ϵ_x/ϵ^2 in (16) is evaluated at t rather than x. It is integrated when applying the inverse operator:

$$u(x) = h(x) + \int_0^x h(t) \frac{\epsilon_x(t)}{\epsilon(t)} dt - \frac{\int_0^1 h(s) \frac{\epsilon_x(s)}{\epsilon(s)} ds}{\int_0^1 \frac{1}{\epsilon(s)} ds} \int_0^x \frac{1}{\epsilon(t)} dt$$
 (17)

3. Integral Equation Operator Bounds

We wish to characterize functions $\epsilon(x)$ that (a) are fairly flat on some subinterval of [a, b] and (b) are uniformly bounded from above and below. These conditions are formalized as follows:

Definition 1. Let \mathcal{E} denote a family of functions on the interval [a, b].

• \mathcal{E} satisfies Property 1 if there exists $0 \le \delta \ll 1$ and a constant c > 0 such that, for each $\epsilon \in \mathcal{E}$, there is a neighborhood $V = B(\zeta(\epsilon), c) \subset [a, b]$ such that

$$\left\| \frac{\epsilon_x}{\epsilon} \cdot 1_V \right\|_p \le \delta \left\| \frac{\epsilon_x}{\epsilon} \right\|_p$$

for all $1 \le p \le \infty$.

• \mathcal{E} satisfies Property 2 if m > 0 and $M < \infty$ where

$$m = \inf_{\epsilon \in \mathcal{E}} \left[\min_{x \in [a,b]} \epsilon(x) \right] \ and \ M = \sup_{\epsilon \in \mathcal{E}} \left[\max_{x \in [a,b]} \epsilon(x) \right]$$

We then have the following result on the condition number of the operator A_1 , the Fredholm operator on the left-hand side of (7).

Theorem 1. Let \mathcal{E} be a family of functions satisfying Properties 1 and 2. Then

$$C_1\left(\left\|\frac{\epsilon_x}{\epsilon}\right\|_p^2\right) - 1 \le cond_p(A_1(\epsilon)) \le C_2\left(\left\|\frac{\epsilon_x}{\epsilon}\right\|_p^2\right) + 1,$$

where $cond_p(A_1(\epsilon))$ is the condition number of $A_1(\epsilon)$ as an operator from $L^p[a,b] \to L^p[a,b]$ for $1 \le p < \infty$ and as an operator from $L^{\infty}[a,b] \cap C[a,b] \to L^{\infty}[a,b] \cap C[a,b]$ for $p = \infty$.

A proof can be found in the Appendix. Theorem 1 gives us a sense of the qualitative behavior of $A_1(\epsilon)$ acting on L^p spaces. In particular, its condition number is well-controlled in L^1 , even when there are steep internal layers (where ϵ_x/ϵ can be large). In L^1 , it is the total variation of ϵ that matters. In the L_{∞} norm, on the other hand, the operator norm can be seen to be large by inspection. A dual result can be obtained for the integral operator $A_2(\epsilon) = I + K_2$ in (11).

Theorem 2. Let \mathcal{E} be a family of functions satisfying Properties 1 and 2. Then

$$C_1\left(\left\|\frac{\epsilon_x}{\epsilon}\right\|_q^2\right) - 1 \le cond_p(A_2(\epsilon)) \le C_2\left(\left\|\frac{\epsilon_x}{\epsilon}\right\|_q^2\right) + 1$$

where 1/p + 1/q = 1 and $cond_p(A_2(\epsilon))$ is the condition number of $A_2(\epsilon)$ as an operator from $L^p[a,b] \to L^p[a,b]$ for $1 \le p < \infty$ and as an operator from $L^\infty[a,b] \cap C[a,b] \to L^\infty[a,b] \cap C[a,b]$ for $p = \infty$.

Since the condition number in L^p depends on the L^q norm of ϵ_x/ϵ in this case, it is clear that the condition number of $A_2(\epsilon)$ will be modest in L^∞ and very large in L^1 in the presence of internal layers.

4. Norm-Preserving Discretization

In order to analyze the condition number of discretized integral equations, it is convenient to introduce the following definition.

Definition 2. A mapping $\Phi: V \subset L^p[a,b] \to \mathbb{C}^n$ is said to be norm-preserving if

$$\|\Phi(g)\|_{l^p} = \|g\|_{L^p[a,b]}$$

for all $g \in V$.

Let A be an invertible, bounded integral operator mapping V to U. We say that a matrix $A_h(V)$ is a norm-preserving discretization of A on the subspace V if there exist norm-preserving mappings Φ and Ψ such that the diagram

$$V \subset L^{p}[a,b] \xrightarrow{A} U \subset L^{p}[a,b]$$

$$\downarrow^{\Psi} \qquad \qquad \downarrow^{\Phi}$$

$$\mathbb{C}^{n} \xrightarrow{A_{h}} \mathbb{C}^{n}$$

commutes.

In the Hibert space case (p = 2), it was shown in [3] that inner product preserving discretizations have singular values which approximate those of the original operator. In the Banach space setting, it is easy to show something equally useful, namely that the condition number of a norm-preserving discretization approximates that of the original operator.

For this, let $B|_W$ denote the restriction of an operator B to a subspace W. Let A be an invertible, bounded operator mapping V to U, let Ψ , Φ be norm-preserving mappings and let A_h be a norm-preserving discretization of A, as above. Then,

$$||A_h|_{\Psi(V)}||_{l^p} = \sup_{v \in \Psi(V)} \frac{||A_h v||_{l^p}}{||v||_{l^p}} = \sup_{g \in V} \frac{||Ag||_{L^p}}{||g||_{L^p}} = ||A|_V||_{L^p},$$
(18)

$$||A_h^{-1}|_{\Phi(U)}||_{l^p} = \sup_{w \in \Psi(V)} \frac{||w||_{l^p}}{||A_h w||_{l^p}} = \sup_{f \in V} \frac{||f||_{L^p}}{||Af||_{L^p}} = ||A^{-1}|_U||_{L^p}.$$
(19)

Thus, the condition number of A_h restricted to $\Psi(V)$ and of A restricted to V are the same.

4.1. Norm-preserving Nyström discretizations

We build (approximate) norm-preserving Nyström discretizations for A by applying a quadrature rule to the integral operator A = I + K:

$$Af(x) = f(x) + \int_a^b K(x, y) f(y) \, dy.$$

For this, we assume that we are given an *n*-point quadrature rule

$$\int_a^b f(x) dx \approx \sum_{k=1}^n f(x_k) w_k,$$

with positive weights. This induces a mapping Φ : $L^p[a,b] \to \mathbb{C}^n$:

$$\Phi(f) = \begin{pmatrix} f(x_1)w_1^{1/p} \\ \vdots \\ f(x_n)w_n^{1/p} \end{pmatrix}$$
 (20)

If the quadrature rule is exact for functions of the form $|g|^p$ for $g \in V$ and $|f|^p$ for $f \in U$, then Φ is a norm-preserving mapping from V into \mathbb{C}^n and U into \mathbb{C}^n . Further, suppose that the quadrature rule is exact for functions of the form $K(x,\cdot)g(\cdot)$ where $g \in V$, and that A_h is given by th Nyström discretization:

$$(A_h)_{ij} = \delta_{ij} + K(x_i, x_j) w_i^{1/p} w_j^{1-1/p}.$$
(21)

Then A_h is norm-preserving, since

$$[A_h \Phi(g)]_i = g(x_i) w_i^{1/p} + w_i^{1/p} \sum_{j=1}^n K(x_i, x_j) w_j^{1-1/p} g(x_j) w_j^{1/p}$$
(22)

$$= w_i^{1/p} \left(g(x_i) + \int_a^b K(x_i, y) g(y) \, dy \right). \tag{23}$$

We note that discretization by sampling, i.e. where

$$\Phi(f) = \begin{pmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{pmatrix}$$

corresponds to a norm-preserving Nyström discretization on the space $L^{\infty}[a,b] \cap C[a,b]$. In particular, suppose we let $V \subset L^{\infty}[a,b] \cap C[a,b]$ be equicontinuous and let $0 < \delta \ll 1$. Then, by taking a fine enough mesh we can clearly satisfy

$$||f||_{L^\infty} = ||\Phi(f)||_{l^\infty}(1+\delta)$$

for any $f \in V$. In short, the simplest Nyström discretization, corresponding to sampling the unknown on a grid, results in a discrete operator whose condition number approximates that of the continuous operator acting on $L^{\infty}[a,b] \cap C[a,b]$.

4.2. Discrete condition number estimates in alternate norms

Two aspects of norm-preserving discretations should be noted here. First, the fact that a discretized operator equation is well-conditioned in l^p for some p may not be very informative if we solve the finite-dimensional linear algebra problem using a different norm. Suppose, for example, that we wish to solve the equation (7), which is well-conditioned in L^1 . After discretization using (21), it is well-conditioned in l^1 as well. However, if we use an iterative scheme such as GMRES [28], we would like to ensure rapid convergence, which depends on the condition number in l^2 . (One could, of course, solve linear systems iteratively in l^p spaces, but the procedures are nonlinear and much more expensive.)

Fortunately, in finite dimensional spaces, norms and condition numbers are all equivalent and satisfy simple relations [12]. For instance,

$$\operatorname{cond}_2(A_h) \le n \operatorname{cond}_1(A_h). \tag{24}$$

Thus, if the system size is modest and we employ a norm-preserving discretization for L^1 , we will have an acceptable bound on the l^2 condition number of the system matrix (21).

A second, closely related, feature of norm-preserving discretizations is that spatial adaptivity is *essential* for the choice of L^p to have an impact. One can see from (21) that for a uniform mesh (with $w_i = h = \frac{1}{n}$ for all i), the resulting matrix A_h is the same for every p. Thus, if the continuous operator equation has a large condition number in L^2 , the discretized equation will be ill-conditioned in l^2 as well.

We will return to these issues in section 6, following an exploration of the behavior of the l^1 , l^2 and l^{∞} discretizations on some model problems.

5. Numerical Examples

To investigate the utility of the analysis outlined above, let us first consider functions $\epsilon(x)$ in (3) of the form

$$\epsilon_{\delta}(x) = 2 + \tanh(\delta(x - x_0))$$
 (25)

on the interval [0, 2], where $x_0 \in (0, 2)$. For large values of δ , these functions have a steep internal layer centered at $x = x_0$. They are relatively flat away from the internal layer. and they are bounded in the range [1, 3]. As a result, the family

$$\mathcal{E} = \{ \epsilon_{\delta} \in L^p : \delta \ge 10 \} \tag{26}$$

satisfies Properties 1 and 2 as given in Definition 1. Note that the derivative $(\epsilon_{\delta})_x = \delta \operatorname{sech}^2(\delta(x - x_0))$, so that

$$\|(\epsilon_{\delta})_{x}\|_{p} = \left(\int_{0}^{2} \delta^{p} \operatorname{sech}^{2p}(\delta(x - x_{0})) dx\right)^{1/p}$$

$$\leq \delta \left(\int_{0}^{2} \operatorname{sech}^{2}(\delta(x - x_{0})) dx\right)^{1/p}$$

$$= \delta^{(1-1/p)} \left(\tanh(\delta(2 - x_{0})) + \tanh(\delta x_{0}) \right)^{1/p}$$

$$\|(\epsilon_{\delta})_{x}\|_{p} = \left(\int_{0}^{2} \delta^{p} \operatorname{sech}^{2p}(\delta(x - x_{0})) dx\right)^{1/p}$$

$$\geq \frac{\delta}{2} \left(2 \operatorname{cosh}^{-1}(\sqrt{2})/\delta\right)^{1/p}$$

$$= C(p)\delta^{(1-1/p)} \tag{28}$$

Combining (27) with (28) and the fact that the ϵ_{δ} are uniformly bounded above and below, we have

$$\left\| \frac{(\epsilon_{\delta})_x}{\epsilon_{\delta}} \right\|_p = \Theta\left(\delta^{(1-1/p)}\right) \tag{29}$$

for $1 \le p < \infty$, using the standard "Big Theta" notation. It is straightforward to check that

$$\left\| \frac{(\epsilon_{\delta})_x}{\epsilon_{\delta}} \right\|_{\infty} = \Theta(\delta). \tag{30}$$

Letting $A_1(\epsilon)$ and $A_2(\epsilon)$ be the operators given by the left hand sides of (8) and (11), respectively, and applying Theorem 1 to the family \mathcal{E} , we see that

$$\operatorname{cond}_1(A_1(\epsilon_\delta)) = \Theta(1),$$

 $\operatorname{cond}_2(A_1(\epsilon_\delta)) = \Theta(\delta),$
 $\operatorname{cond}_\infty(A_1(\epsilon_\delta)) = \Theta(\delta^2).$

Likewise, we have

$$\operatorname{cond}_1(A_2(\epsilon_\delta)) = \Theta(\delta^2),$$

 $\operatorname{cond}_2(A_2(\epsilon_\delta)) = \Theta(\delta),$
 $\operatorname{cond}_\infty(A_2(\epsilon_\delta)) = \Theta(1).$

We discretize the integral equations (7) and (10), using a norm-preserving Nyström discretization scheme, as described in section 4.1. For this, we adaptively refine the interval [a, b] so

that the function $\epsilon(x)$ is well resolved with a piecewise Legendre polynomial approximation to a user-specified precision. More precisely, we use piecewise 16th order approximations, and refine each interval until the quadrature error in integrating ϵ is less than 10^{-15} . On each subinterval, we sample all functions involved (u, ϵ, f) at the scaled Gauss-Legendre nodes of order 16. We use the standard Gauss-Legendre quadrature weights scaled to each subinterval. Given these nodes and weights, the norm-preserving discretization (21) in L^p applied to equation (7) yields

$$\sigma(x_i)w_i^{1/p} + \frac{\epsilon_x(x_i)}{\epsilon(x_i)} \sum_j G_x(x_i, x_j)w_j^{1-1/p}w_i^{1/p}\sigma(x_j)w_j^{1/p} = g(x_i)w_i^{1/p}.$$
 (31)

Likewise, equation (10) yields

$$u(x_i)w_i^{1/p} + \frac{1}{\epsilon(x_i)} \sum_j G_x(x_i, x_j) \epsilon_x(x_j) w_j^{1-1/p} w_i^{1/p} u(x_i) w_i^{1/p} = h(x_i) w_i^{1/p}$$
(32)

where h is simply the right hand side of (10). We will use $A_{1,p}(\epsilon)$ and $A_{2,p}(\epsilon)$ to denote the p-norm-preserving discretizations of these integral operators. Because the unknowns σ and u are weighted by $w_i^{1/p}$, we see that the entries of the discrete operators are given by

$$\begin{aligned} \left[A_{1,p}(\epsilon) \right]_{ij} &= \delta_{ij} + \frac{\epsilon_x(x_i)}{\epsilon(x_i)} G_x(x_i, x_j) w_j^{1-1/p} w_i^{1/p} \\ \left[A_{2,p}(\epsilon) \right]_{ij} &= \delta_{ij} + \frac{\epsilon_x(x_j)}{\epsilon(x_i)} G_x(x_i, x_j) w_j^{1-1/p} w_i^{1/p} \end{aligned}$$

5.1. Condition Numbers

Using the family of functions \mathcal{E} defined above, we may study the l^p condition numbers of our discrete operators $A_{1,p}(\epsilon_{\delta})$ and $A_{2,p}(\epsilon_{\delta})$ for p=1,2, and ∞ . Because of the norm-preserving discretization, we expect $\operatorname{cond}_1(A_{1,1}(\epsilon_{\delta})) = \Theta(1)$, $\operatorname{cond}_2(A_{1,2}(\epsilon_{\delta})) = \Theta(\delta)$, and $\operatorname{cond}_\infty(A_{1,\infty}(\epsilon_{\delta})) = \Theta(\delta^2)$ since that is the behavior of the continous operators (Theorem 1). Similarly, we expect $\operatorname{cond}_1(A_{2,1}(\epsilon_{\delta})) = \Theta(\delta^2)$, $\operatorname{cond}_2(A_{2,2}(\epsilon_{\delta})) = \Theta(\delta)$, and $\operatorname{cond}_\infty(A_{2,\infty}(\epsilon_{\delta})) = \Theta(1)$ (from Theorem 2).

In Figs. 1 and 2, we plot numerical results for the family of functions ϵ_{δ} , where $\delta = 100j$, with j = 1, ..., 100. For each ϵ_{δ} , we formed the system matrices for an adaptive norm-preserving discretization of the domain [0, 2] as described above. The l^p condition numbers were computed by brute force (using the singular value decomposition in MATLAB).

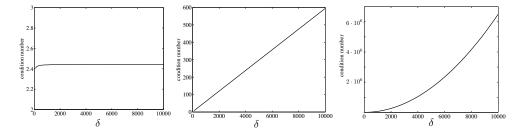


Figure 1: l^p condition numbers of $A_{1,p}(\epsilon_\delta)$ for p=1 (left), p=2 (center), and $p=\infty$ (right). The slope of the internal layer is approximately δ and the thickness of the internal layer is approximately $1/\delta$.

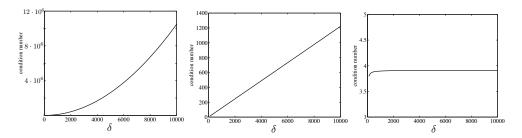


Figure 2: l^p condition numbers of $A_{2,p}(\epsilon_\delta)$ for p=1 (left), p=2 (center), and $p=\infty$ (right).

We see from the data that the condition numbers of the discrete operators do, indeed, exhibit the scaling properties expected from our analysis of the continuous operators. Note that the 1-norm-preserving scheme to discretize (7) and the ∞-norm-preserving scheme to discretize (10) result in very well-conditioned matrices, independent of the steepness of the internal layer.

5.2. Convergence behavior using GMRES

As discussed in section 4.2, it is reasonable to ask how standard iterative schemes work when applied to l^p -norm-preserving discretizations. We use GMRES here, whose convergence behavior depends formally on the l^2 condition number of the system matrix. It is reasonable to expect that the better conditioned systems (the 1-norm-preserving system for $A_1(\epsilon)$ and the ∞ -norm-preserving system for $A_2(\epsilon)$) will fare better.

For these experiments, we solve the ODE (3), i.e.

$$\frac{\partial}{\partial x} \left(\epsilon(x) \frac{\partial u}{\partial x} \right) = f$$

subject to inhomogeneous Dirichlet conditions, $u(a) = \gamma_a$ and $u(b) = \gamma_b$. If we let l(x) = mx + c be a linear function satisfying the boundary conditions, then v = u - l satisfies homogeneous Dirichlet conditions and the ODE with a modificed right-hand side:

$$\frac{\partial}{\partial x} \left(\epsilon(x) \frac{\partial v}{\partial x} \right) = f - m \epsilon_x.$$

This problem can be addressed using one of the integral equations (7) or (10), from which the solution to the original problem is u = v + l. Here, we consider $f \equiv 1$, $\gamma_a = 1$ and $\gamma_b = 2$. We consider two types of functions $\epsilon(x)$ that contain multiple internal layers by adding together several hyperbolic tangent functions, as in (25), with multiple centers and $\delta = 500$, as shown in Fig. 3. We refer to the left-hand profile as a "double hill" and the right-hand profile as a "double well".

Using adaptive refinement, we obtain linear systems (31) and (32) as described above, for p = 1, 2, and ∞ . We solve the systems using GMRES and record the relative residuals for each step in Figs. 4 and 5. The l^2 condition numbers of the discrete operators are shown in Table 1.

Note that the l^2 condition numbers for $A_{1,1}(\epsilon)$ and $A_{2,\infty}(\epsilon)$ operators are the smallest, as expected. Note also that these linear systems are solved much more easily using GMRES. The other discretizations fail to reach the desired tolerance (10⁻¹⁵) in a reasonable number of iterations.

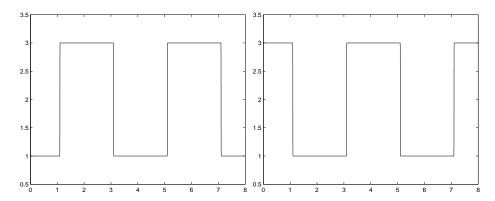


Figure 3: The "double hill" (left) and "double well" (right) functions $\epsilon(x)$.

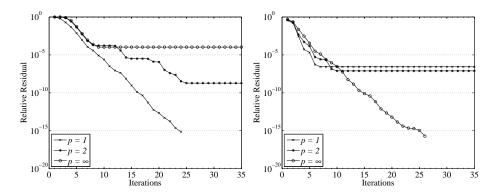


Figure 4: Convergence of GMRES for the "double hill" $\epsilon(x)$. The relative residual of the error at each iteration is shown using the $A_{1,p}(\epsilon)$ operator (left) and the $A_{2,p}(\epsilon)$ operator (right).

6. Discussion

Our work in this paper was motivated by the observation that boundary integral equations are extremely robust when solving problems of the type (1) when ϵ is piecewise constant. In particular, a *charge* distribution on the dielectric interface leads to well-conditioned integral equations involving the single layer potential [13, 14, 17, 24, 25]). That charge density, however, is not a smooth function in the ambient space - it is a singular function supported on the interface alone.

In the variable coefficient case, setting the unknown to be $\sigma = \Delta u$, as in (7), corresponds to seeking the solution in terms of a *volume* charge distribution. As the internal layer becomes steeper and steeper, the function $\sigma(x)$ blows up, since it is converging to a distribution and not a bounded function. One interpretation of the L^1 norm-preserving discretization is that, in the discontinuous limit, the l^1 -scaled unknown approximates the *strength* of the δ -function along the steep interface, rather than trying to sample the δ -function itself.

One concern with using the integral equation (7) is that we are only guaranteed tight bounds on accuracy in L^1 , using the standard estimate

$$\frac{\|e\|_1}{\|x\|_1} \le \operatorname{cond}_1(A_1) \frac{\|r\|_1}{\|b\|_1}$$

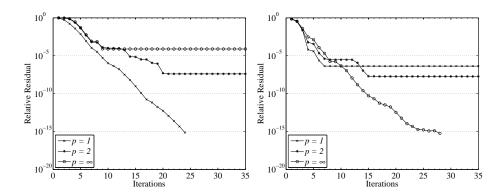


Figure 5: Convergence of GMRES for the "double well" $\epsilon(x)$. The relative residual of the error at each iteration is shown using the $A_{1,p}(\epsilon)$ operator (left) and the $A_{2,p}(\epsilon)$ operator (right).

$\epsilon(x)$	$A_{1,1}(\epsilon)$	$A_{1,2}(\epsilon)$	$A_{1,\infty}(\epsilon)$	$A_{2,1}(\epsilon)$	$A_{2,2}(\epsilon)$	$A_{2,\infty}(\epsilon)$
"Double Hill"	35.1453	979.052	86459.5	116010	978.240	31.1643
"Double Well"	33.1648	977.744	98620.1	147328	977.411	27.9858

Table 1: ℓ^2 condition numbers for the discretized $A_{1,p}(\epsilon)$ and $A_{2,p}(\epsilon)$ operators.

where \tilde{x} is an approximate solution, $e = x - \tilde{x}$, and $r = A_1 \tilde{x} - b$ is the residual. (This estimate applies to invertible Fredholm equations of the second kind as well as to finite-dimensional linear systems). Fortunately, the quantities of interest u, u_x are computed as integral functionals of σ using the representation (6) and are obtained with high accuracy. The integral equation (10) can be discretized naively, corresponding, as noted earlier, to norm-preservation in l^{∞} . While in some respects simpler, derivative data (u_x) must then be computed numerically.

We are currently working on the extension of our analysis to higher-dimensional problems, and will report on the performance of such solvers at a later date.

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Appendix A. Proof of Theorem 1

Let $\mathcal E$ be a family of functions satisfying Properties 1 and 2 from Definition 1. Let ϵ be an arbitrary function in $\mathcal E$ and let A_1 be given by

$$A_1\sigma(x) = (I + K_1)\sigma(x) = \sigma(x) + \frac{\epsilon_x(x)}{\epsilon(x)} \int G_x(x, y)\sigma(y) \, dy.$$

We now establish bounds for A_1 as on operator on $L^{\infty}[0,1] \cap C[0,1]$. To begin, we note that $|G_x(x,y)|$ is bounded by 1. Thus,

$$||A_1||_{\infty} = \sup_{\|\sigma\|_{\infty} = 1} \sup_{x \in [0,1]} \left| \sigma(x) + \frac{\epsilon_x(x)}{\epsilon(x)} \int G_x(x,y) \sigma(y) \, dy \right| \tag{A.1}$$

$$\leq 1 + \left\| \frac{\epsilon_x}{\epsilon} \right\|_{\infty}$$
 (A.2)

Let x_* be the maximizer of $|\epsilon_x/\epsilon|$ and define the functions σ_n by

$$\sigma_n(y) = \begin{cases} 1 & \text{if} \quad y \le x_* \\ 1 - 2n(y - x_*) & \text{if} \quad x_* < y < x_* + 1/n \\ -1 & \text{if} \quad y \ge x_* + 1/n \end{cases}.$$

These functions are continuous and approximate the sign of $G_x(x_*, y)$. A straightforward computation shows that

$$||A_1||_{\infty} = \sup_{\|\sigma\|_{\infty} = 1} \sup_{x \in [0,1]} \left| \sigma(x) + \frac{\epsilon_x(x)}{\epsilon(x)} \int G_x(x,y) \sigma(y) \, dy \right| \tag{A.3}$$

$$\geq \sup_{x \in [0,1]} \left| \sigma_n(x) + \frac{\epsilon_x(x)}{\epsilon(x)} \int G_x(x,y) \sigma_n(y) \, dy \right| \tag{A.4}$$

$$\geq \left| \frac{\epsilon_{x}(x_{*})}{\epsilon(x_{*})} \right| \left(\int |G_{x}(x_{*}, y)| \, dy - \frac{2}{n} \right) - \sigma_{n}(x_{*}) \tag{A.5}$$

$$\geq \left\| \frac{\epsilon_x}{\epsilon} \right\|_{\infty} \left(\frac{1}{4} - \frac{2}{n} \right) - 1 \tag{A.6}$$

so that

$$||A_1||_{\infty} \geq \frac{1}{4} \left\| \frac{\epsilon_x}{\epsilon} \right\|_{\infty} - 1.$$

We note that A_1^{-1} is given by

$$A_1^{-1}g(x) = (I - R_1)g(x) = g(x) - \frac{\epsilon_x(x)}{\epsilon(x)^2} \left(\int_0^x g(t)\epsilon(t) \, dt - \frac{\int_0^1 \frac{1}{\epsilon(s)} \int_0^s g(t)\epsilon(t) \, dt \, ds}{\int_0^1 \frac{1}{\epsilon(s)} \, ds} \right).$$

It is straightforward to see that

$$||A_1^{-1}||_{\infty} = \sup_{\|g\|_{\infty} = 1} ||(I - R_1)g||_{\infty}$$
(A.7)

$$\leq 1 + \sup_{\|g\|_{\infty} = 1} \sup_{x \in [0,1]} \left| \frac{\epsilon_x(x)}{\epsilon(x)^2} \left(\int_0^x g(t)\epsilon(t) dt - \frac{\int_0^1 \frac{1}{\epsilon(s)} \int_0^s g(t)\epsilon(t) dt ds}{\int_0^1 \frac{1}{\epsilon(s)} ds} \right) \right|$$
(A.8)

$$\leq 1 + \left\| \frac{\epsilon_x}{\epsilon} \right\|_{\infty} \frac{1}{m} \left(1 + \frac{M}{m} \right) \|\epsilon\|_1. \tag{A.9}$$

Again, let x_* be the maximizer of $|\epsilon_x/\epsilon|$ and let m_ϵ be the minimum of ϵ on [0, 1]. We define the function g_ϵ as follows

$$g_{\epsilon}(x) = \begin{cases} m_{\epsilon}/\epsilon(x) & \text{if} & x \le x_*/2 \\ -m_{\epsilon}/\epsilon(x) & \text{if} & x_*/2 < x \le x_* \\ m_{\epsilon}/\epsilon(x) & \text{if} & x_* < x \le (1+x_*)/2 \\ -m_{\epsilon}/\epsilon(x) & \text{if} & (1+x_*)/2 < x \le 1 \end{cases}.$$

The function g_{ϵ} is such that the integral $\int_0^x g_{\epsilon}(t) \epsilon(t) dt$ is zero at $x = x^*, 0$, and 1 and positive otherwise. Let g_n be continuous functions which satisfy $||g_n||_{\infty} = 1$ and converge pointwise to g_{ϵ} . A few straightforward computations and an application of the dominated convergence theorem yield

$$||A_1^{-1}||_{\infty} = \sup_{\|g\|_{\infty} = 1} ||(I - R_1)g||_{\infty}$$
(A.10)

$$\geq \lim_{n \to \infty} \left\| (I - R_1) g_n \right\|_{\infty} \tag{A.11}$$

$$\geq \lim_{n \to \infty} |R_1 g_n(x_*)| - 1 \tag{A.12}$$

$$\geq \left| \frac{\epsilon_{x}(x_{*})}{\epsilon(x_{*})^{2}} \right| \lim_{n \to \infty} \frac{\int_{0}^{1} \frac{1}{\epsilon(s)} \int_{0}^{s} g_{n}(t) \epsilon(t) dt ds}{\int_{0}^{1} \frac{1}{\epsilon(s)} ds} - \left| \frac{\epsilon_{x}(x_{*})}{\epsilon(x_{*})^{2}} \right| \lim_{n \to \infty} \int_{0}^{x_{*}} g_{n}(t) \epsilon(t) dt - 1$$
 (A.13)

$$= \left| \frac{\epsilon_x(x_*)}{\epsilon(x_*)^2} \right| \frac{\int_0^1 \frac{1}{\epsilon(s)} \int_0^s g_{\epsilon}(t) \epsilon(t) dt ds}{\int_0^1 \frac{1}{\epsilon(s)} ds} - 1$$
(A.14)

$$\geq \frac{1}{M} \left\| \frac{\epsilon_x}{\epsilon} \right\|_{\infty} \frac{m_{\epsilon} m}{8M} - 1 \tag{A.15}$$

$$\geq \left\| \frac{\epsilon_x}{\epsilon} \right\|_{\infty} \frac{m^2}{8M^2} - 1. \tag{A.16}$$

We next establish bounds on A_1 as an operator on $L^p[0,1]$, for 1 .

$$||A_1||_p = \sup_{||\sigma|| = 1} ||(I + K_1)\sigma||_p$$
(A.17)

$$\leq 1 + \sup_{\|\sigma\|_p = 1} \left(\int \left| \frac{\epsilon_x(x)}{\epsilon(x)} \int G_x(x, y) \sigma(y) \, dy \right|^p \, dx \right)^{1/p} \tag{A.18}$$

$$\leq 1 + \sup_{\|\sigma\|_p = 1} \left\| \left(\frac{\epsilon_x(x)}{\epsilon(x)} \right)^p \right\|_1^{1/p} \left\| \int |G_x(\cdot, y)\sigma(y)|^p \ dy \right\|_{\infty}^{1/p} \tag{A.19}$$

$$\leq 1 + \left\| \frac{\epsilon_{x}(\cdot)}{\epsilon(\cdot)} \right\|_{p} . \tag{A.20}$$

Because \mathcal{E} satisfies Property 1, we may choose $0 \le \delta \ll 1$ and a neighborhood $V = B(\xi, c) \subset [0, 1]$ centered at ξ and of radius c such that

$$\left\| \frac{\epsilon_x}{\epsilon} \cdot 1_V \right\|_p \le \delta \left\| \frac{\epsilon_x}{\epsilon} \right\|_p.$$

For concreteness, assume $c \le 1/2$. Note now that a density σ is the second derivative of a function u with homogeneous Dirichlet boundary values. In particular, $u'(x) = \int G_x(x, y)\sigma(y)\,dy$. As a result, the function u' integrates to zero (since u(1) = u(0) = 0). This observation permits us to build densities σ with the desired properties. In particular, we'd like a density σ such that $u'(x) = \int G_x(x, y)\sigma(y)\,dy$ is small only in the neighborhood where ϵ_x/ϵ satisfies the above property. We choose u' to be of the form

$$u'(x) = \begin{cases} a(x - \xi)^2 & \text{for } x \le \xi \\ b(x - \xi)^2 & \text{for } x > \xi \end{cases}$$

where a and b are chosen such that u' integrates to zero. Setting b = 1 and $a = (\xi - 1)^3/\xi^3$ is sufficient. This yields

$$\sigma(x) = \begin{cases} \frac{2(\xi - 1)^3}{\xi^3} (x - \xi) & \text{for } x \le \xi \\ 2(x - \xi) & \text{for } x > \xi \end{cases}$$

The L_p norm of the above function satisfies

$$\|\sigma\|_p \le \|\sigma\|_{\infty} \le \frac{2(1-c)}{c^3} .$$

Let $\sigma_{\epsilon} = \sigma/||\sigma||_p$. Then the corresponding $u'(x) = \int G_x(x, y)\sigma_{\epsilon}(y) dy$ is given by

$$\int G_x(x,y)\sigma_\epsilon(y)\,dy = \left\{ \begin{array}{ll} \frac{1}{\|\sigma\|_p}\frac{(\xi-1)^3}{\xi^3}(x-\xi)^2 & \text{for} \quad x \leq \xi \\ \frac{1}{\|\sigma\|_p}(x-\xi)^2 & \text{for} \quad x > \xi \end{array} \right..$$

This provides a minimum value of $|\int G_x(x,y)\sigma_{\epsilon}(y)\,dy|$ on $[0,1]\setminus V$ which satisfies

$$\min_{x \in [0,1] \setminus V} \left| \int G_x(x,y) \sigma_{\epsilon}(y) \, dy \right| \ge \frac{c^8}{(1-c)^4} \, .$$

We then have

$$||A_1||_p = \sup_{\|\sigma\|_p = 1} ||(I + K_1)\sigma||_p$$
(A.21)

$$\geq \sup_{\|\sigma\|_{p}=1} \left(\int \left(\frac{\epsilon_{x}(x)}{\epsilon(x)} \int G_{x}(x,y)\sigma(y) \, dy \right)^{p} \, dx \right)^{1/p} - 1 \tag{A.22}$$

$$\geq \left(\int \left(\frac{\epsilon_x(x)}{\epsilon(x)} \int G_x(x, y) \sigma_{\epsilon}(y) \, dy\right)^p \, dx\right)^{1/p} - 1 \tag{A.23}$$

$$\geq (1 - \delta) \frac{c^8}{1 - c^4} \left\| \frac{\epsilon_x(\cdot)}{\epsilon(\cdot)} \right\|_p - 1 \tag{A.24}$$

$$= C(c, \delta) \left\| \frac{\epsilon_{x}(\cdot)}{\epsilon(\cdot)} \right\|_{p} - 1. \tag{A.25}$$

Let 1 and <math>1/p + 1/q = 1. Then

$$||A_1^{-1}||_p = \sup_{\|g\|=1} ||(I - R_1)g||_p$$
(A.26)

$$\leq 1 + \sup_{\|g\|_p = 1} \|R_1 g\|_p \tag{A.27}$$

$$\leq 1 + \sup_{\|g\|_p = 1} \left(\int_0^1 \left| \frac{\epsilon_x(x)}{\epsilon(x)^2} \left(\int_0^x g(t)\epsilon(t) dt - \frac{\int_0^1 \frac{1}{\epsilon(s)} \int_0^s g(t)\epsilon(t) dt ds}{\int_0^1 \frac{1}{\epsilon(s)} ds} \right) \right|^p dx \right)^{1/p}$$
(A.28)

$$\leq 1 + \left\| \left(\frac{\epsilon_x}{\epsilon^2} \right)^p \right\|_{1}^{1/p} \sup_{\|g\|_p = 1} \left(\sup_{x \in [0,1]} \left| \int_0^x g(t)\epsilon(t) \, dt - \frac{\int_0^1 \frac{1}{\epsilon(s)} \int_0^s g(t)\epsilon(t) \, dt \, ds}{\int_0^1 \frac{1}{\epsilon(s)} \, ds} \right|^p \right)^{1/p} \tag{A.29}$$

$$\leq 1 + \left\| \frac{\epsilon_x}{\epsilon^2} \right\|_{p \, \|g\|_p = 1} \left(\int_0^1 |g(t)\epsilon(t)| \, dt + \frac{\int_0^1 \frac{1}{\epsilon(s)} \int_0^1 |g(t)\epsilon(t)| \, dt \, ds}{\int_0^1 \frac{1}{\epsilon(s)} \, ds} \right) \tag{A.30}$$

$$\leq 1 + \left\| \frac{\epsilon_x}{\epsilon^2} \right\|_p \left(1 + \frac{M}{m} \right) \sup_{\|g\|_p = 1} \|g\epsilon\|_1 \tag{A.31}$$

$$\leq 1 + \left\| \frac{\epsilon_x}{\epsilon^2} \right\|_p \left(1 + \frac{M}{m} \right) \|\epsilon\|_q \tag{A.32}$$

$$\leq 1 + \left\| \frac{\epsilon_x}{\epsilon} \right\|_p \left(1 + \frac{M}{m} \right) \frac{M}{m} \,. \tag{A.33}$$

Let $V = B(\xi, c) \subset [0, 1]$ as above. We define a function g_{ϵ} as follows:

$$g_{\epsilon}(x) = \begin{cases} 0 & \text{if} \quad x \le \xi - c \\ \frac{1}{\epsilon(x)} & \text{if} \quad \xi - c < x \le \xi \\ -\frac{1}{\epsilon(x)} & \text{if} \quad \xi < x \le \xi + c \\ 0 & \text{if} \quad x > \xi + c \end{cases}.$$

It is easy to see that

$$\int_0^x g_\epsilon(t)\epsilon(t)\,dt = \left\{ \begin{array}{rcl} 0 & \text{if} & x \leq \xi - c \\ x - \xi + c & \text{if} & \xi - c < x \leq \xi \\ \xi - x + c & \text{if} & \xi < x \leq \xi + c \\ 0 & \text{if} & x > \xi + c \end{array} \right.,$$

that

$$\int_0^1 \frac{1}{\epsilon(s)} \int_0^s g(t)\epsilon(t) dt ds \ge \frac{2}{M} \int_0^c t dt = \frac{c^2}{M},$$

and that

$$||g_{\epsilon}||_p \le \frac{(2c)^{1/p}}{m} \le \frac{1}{m}.$$

¿From these,

$$||A_1^{-1}||_p = \sup_{||g||_p = 1} ||(I - R_1)g||_p$$
(A.34)

$$\geq \sup_{\|g\|_p = 1} \|R_1 g\|_p - 1 \tag{A.35}$$

$$\geq \frac{1}{\|g_{\epsilon}\|_{p}} \left(\int_{0}^{1} \left| \frac{\epsilon_{x}(x)}{\epsilon(x)^{2}} \left(\int_{0}^{x} g_{\epsilon}(t)\epsilon(t) dt - \frac{\int_{0}^{1} \frac{1}{\epsilon(s)} \int_{0}^{s} g_{\epsilon}(t)\epsilon(t) dt ds}{\int_{0}^{1} \frac{1}{\epsilon(s)} ds} \right) \right|^{p} dx \right)^{1/p} - 1 \quad (A.36)$$

$$\geq \frac{1}{\|g_{\epsilon}\|_{p}} \left(\int_{[0,1]\setminus V} \left| \frac{\epsilon_{x}(x)}{\epsilon(x)^{2}} \left(\int_{0}^{x} g_{\epsilon}(t)\epsilon(t) dt - \frac{\int_{0}^{1} \frac{1}{\epsilon(s)} \int_{0}^{s} g_{\epsilon}(t)\epsilon(t) dt ds}{\int_{0}^{1} \frac{1}{\epsilon(s)} ds} \right) \right|^{p} dx \right)^{1/p} - 1$$
(A.37)

$$= \frac{1}{\|g_{\epsilon}\|_{p}} \left(\int_{[0,1]\setminus V} \left| \frac{\epsilon_{x}(x)}{\epsilon(x)^{2}} \left(\frac{\int_{0}^{1} \frac{1}{\epsilon(s)} \int_{0}^{s} g_{\epsilon}(t)\epsilon(t) dt ds}{\int_{0}^{1} \frac{1}{\epsilon(s)} ds} \right) \right|^{p} dx \right)^{1/p} - 1$$
(A.38)

$$\geq \left\| \frac{\epsilon_x}{\epsilon^2} \right\|_{p} m(1 - \delta) \frac{c^2}{M} - 1 \tag{A.39}$$

$$\geq \left\| \frac{\epsilon_x}{\epsilon} \right\|_p (1 - \delta) \frac{mc^2}{M^2} - 1. \tag{A.40}$$

¿From the above, we see that there exist constants C_1' and C_2' – depending only on m, M, c, and δ – such that

$$C_1' \left\| \frac{\epsilon_x}{\epsilon} \right\|_p - 1 \le ||A_1||_p \le C_2' \left\| \frac{\epsilon_x}{\epsilon} \right\|_p + 1$$

$$C_1' \left\| \frac{\epsilon_x}{\epsilon} \right\|_p - 1 \le ||A_1^{-1}||_p \le C_2' \left\| \frac{\epsilon_x}{\epsilon} \right\|_p + 1,$$

so that there are constants C_1 and C_2 – depending only on m, M, c, and δ – such that

$$C_1 \left\| \frac{\epsilon_x}{\epsilon} \right\|_p - 1 \le \operatorname{cond}_p(A_1) \le C_2 \left\| \frac{\epsilon_x}{\epsilon} \right\|_p + 1$$

which completes the proof.

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