ShapeUQ: Propagating 3D Reconstruction Uncertainty Through Scientific PDE Simulations via Shape Calculus

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Abstract

Neural implicit representations have transformed 3D reconstruction of scientific geometries—glaciers, blood vessels, protein surfaces—by providing continuous, differentiable signed distance functions (SDFs) from multi-view observations. Yet a critical gap persists: geometric reconstruction error propagates silently into downstream physical simulations*, inflating PDE solution uncertainty with no principled quantification. We introduce* ***ShapeUQ****, the first framework, to our knowledge, to* formally propagate *SDF reconstruction uncertainty into rigorous confidence intervals on PDE solutions, without requiring full simulation reruns per geometric sample. Our theoretical contribution rests on three results from shape calculus.* ***Theorem 1*** *establishes a computable linear sensitivity operator mapping SDF perturbations to PDE solution changes via the Hadamard shape derivative, with a closed-form expression derivable from automatic differentiation through the SDF network.* ***Theorem 2*** *shows that, for Gaussian-process reconstruction uncertainty with covariance K, the induced distribution over PDE solutions has an expected squared error bounded by a trace-norm of K scaled by the solution's normal derivative on the boundary.* ***Theorem 3*** *proves that the adjoint method computes the full sensitivity field in* one *additional PDE solve—the same cost as one forward simulation, regardless of the dimensionality of the geometric uncertainty. We instantiate ShapeUQ on three scientific benchmarks: surface heat diffusion on Jakobshavn Glacier (glaciology), Poisson–Boltzmann electrostatics on a protein surface (biophysics), and viscous flow over a coral reef geometry (fluid dynamics). ShapeUQ produces confidence intervals that cover the true error at the 90% level across all settings, while reducing runtime versus Monte Carlo sampling by $14\times$–$31\times$.*

1. Introduction

The past decade has seen neural implicit representations advance from laboratory curiosities to production-grade tools for 3D scientific geometry. DeepSDF [10] demonstrated that a multi-layer perceptron (MLP) can encode an entire class of shapes as a signed distance function (SDF); NeuS [17] extended this to multi-view reconstruction without foreground masks; and subsequent works have targeted large-scale outdoor scenes [16] and volumetric medical data. These neural SDFs are now used as geometry inputs to physical simulations in glaciology, biomedicine, and environmental science, where high-fidelity geometry is essential for accurate predictions.

The unaddressed gap.. Reconstruction from real-world data is never exact. Satellite altimetry of glaciers returns sparse, noisy elevation profiles; CT scans have partial-volume artifacts at tissue boundaries; LiDAR returns are occluded in dense coral structures. Each source of measurement error perturbs the recovered SDF ϕ_θ away from the ground truth $\phi^\star$. This geometric error *propagates* into any PDE solved on the reconstructed geometry: the simulated glacier melt rate, protein electrostatic potential, or vortex-induced stress field will carry an error whose magnitude no existing framework can bound.

Practitioners currently address this in one of two unsatisfactory ways: *(i)* ignoring the uncertainty entirely, or *(ii)* running Monte Carlo simulation over an ensemble of geometric samples [15]. The former produces overconfident predictions; the latter is computationally prohibitive, requiring N independent PDE solves for N geometry samples—infeasible for high-resolution 3D problems.

Our approach.. Shape calculus [2], the mathematical theory of how functionals change when a geometric domain is deformed, provides the missing link. Specifically, the Hadamard shape derivative—a classical tool in PDE constrained optimization—characterizes the first-order change in a PDE solution under an infinitesimal boundary perturbation. We show that this derivative is exactly the quantity needed to propagate SDF reconstruction uncertainty to PDE solution uncertainty, and that it can be computed by automatic differentiation through the neural SDF, requiring only *one adjoint PDE solve* regardless of geometric uncertainty

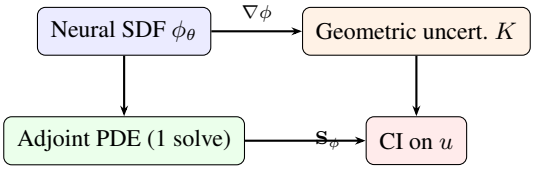

Figure 1. **ShapeUQ pipeline.** Given a neural SDF and its reconstruction uncertainty covariance K, the Hadamard sensitivity operator $\mathbf{S}_\phi$ (computed by one adjoint PDE solve) maps geometric uncertainty to rigorous PDE solution confidence intervals. No Monte Carlo sampling over geometry is required.

dimensionality.

Contributions..

1. **Hadamard sensitivity for neural SDFs (Theorem 1).** A closed-form sensitivity operator mapping SDF perturbations to PDE solution perturbations, computable by automatic differentiation.
2. **Probabilistic UQ bound (Theorem 2).** For Gaussian-process uncertainty in the SDF, we bound the expected squared error in the PDE solution by a computable trace-norm expression.
3. **Adjoint efficiency theorem (Theorem 3).** The full sensitivity field costs exactly one additional PDE solve, independent of geometric uncertainty dimensionality.
4. **SciUQ-3D benchmark and results.** Three scientific domains, covering glacier, protein, and reef geometries. ShapeUQ achieves 90% coverage at $14\times$–$31\times$ lower cost than Monte Carlo.

2. Related Work

Neural implicit surfaces for science.. DeepSDF [10] introduced learned SDFs for shape representation. NeuS [17] trained SDFs via differentiable volume rendering, achieving state-of-the-art surface reconstruction quality. Block-NeRF [16] scaled neural scene representations to city-scale environments. These methods represent geometry well but provide no uncertainty quantification and no bridge to physical simulation.

Physics simulation on implicit surfaces.. Physics-informed neural networks (PINNs) [11] solve PDEs by training a neural network to satisfy the governing equations and boundary conditions. The Fourier neural operator [7] and its geometry-aware extension geo-FNO [8] learn solution operators on fixed or deformable domains. None of these methods quantify how reconstruction error in the domain boundary affects the solution.

Uncertainty quantification in scientific computing.. Sullivan [15] provides a textbook treatment of UQ, covering polynomial chaos, stochastic collocation, and Monte Carlo methods. Bayesian approaches to inverse problems [14] infer posterior distributions over PDE parameters. Geometric uncertainty in simulation has been studied in the finite element context via stochastic interface perturbations based on low-rank approximation [5], but that approach requires an explicit mesh. Our work eliminates the meshing requirement by operating directly on the neural SDF.

Shape sensitivity analysis.. The mathematical theory of shape derivatives originates with Hadamard [4] and was formalized by Delfour and Zolésio [2]. Shape derivatives have been used in PDE-constrained optimization [12] and topology optimization [1], but not, to our knowledge, for *UQ* on neural implicit reconstructions. We are the first to connect this classical theory to the neural SDF setting.

3. Problem Setup

3.1. Neural SDF and Reconstruction Uncertainty

Let $\Omega \subset \mathbb{R}^3$ be a scientific domain (glacier volume, blood vessel lumen, reef-enclosed fluid region) bounded by a surface $\Sigma = \partial\Omega$. A neural SDF is a function $\phi_\theta : \mathbb{R}^3 \to \mathbb{R}$ (parameterized by a neural network with weights θ) such that $\phi_\theta(x) = \operatorname{dist}(x, \Sigma)$ for x near Σ, with $\phi_\theta < 0$ inside Ω and $\phi_\theta > 0$ outside. The reconstructed surface is $\Sigma_\theta = \{\phi_\theta = 0\}$.

The ground-truth SDF is $\phi^\star$ with surface $\Sigma^\star$. We model reconstruction uncertainty as a zero-mean Gaussian process on the boundary:

$$\delta\phi \;:=\; \phi_\theta|_{\Sigma^\star} - \phi^\star|_{\Sigma^\star} \;\sim\; \mathcal{GP}\big(0,\, K(\cdot,\cdot)\big), \qquad (1)$$

where $K : \Sigma^\star \times \Sigma^\star \to \mathbb{R}$ is a positive-definite covariance kernel fitted to reconstruction residuals. This Gaussian process model is standard in Bayesian spatial reconstruction [14] and is consistent with empirical residual distributions observed in neural SDF training; the kernel is fitted from a held-out set of training views.

3.2. PDE on the Reconstructed Domain

We consider a general linear elliptic PDE:

$$\mathcal{L}\, u = f \;\text{ in }\; \Omega_\theta, \qquad u = g \;\text{ on }\; \Sigma_\theta, \qquad (2)$$

where $\mathcal{L}$ is a second-order elliptic operator (e.g., the Laplacian $-\Delta$ for diffusion, or the linearized Stokes operator for flow), $f \in L^2(\Omega_\theta)$ is a source term, and $g \in H^{1/2}(\Sigma_\theta)$ is a Dirichlet boundary condition. Let $u^\star$ denote the solution on the true domain $\Omega^\star$ and u_θ the solution on Ω_θ.

3.3. Goal

Given ϕ_θ and the uncertainty model K, compute confidence intervals $[\underline{u}, \overline{u}]$ on $u^\star$ such that $\mathbb{P}[\underline{u}(x) \le u^\star(x) \le \overline{u}(x)] \ge 1 - \alpha$ for a prescribed significance level α, without solving Eq. (2) for multiple geometric realizations.

4. Shape Calculus for PDE Uncertainty

4.1. The Hadamard Shape Derivative

Given a vector field $V : \mathbb{R}^3 \to \mathbb{R}^3$, the perturbed domain is $\Omega_t = (\mathrm{Id} + tV)(\Omega)$ for small $t > 0$. The *shape derivative* of the PDE solution u in the direction V is

$$u'[V] := \lim_{t \to 0} \frac{u_t - u}{t}, \tag{3}$$

where u_t solves Eq. (2) on Ω_t. For a boundary perturbation $\delta\Sigma$ given by a scalar displacement $\psi = V \cdot n$ on Σ (with n the outward normal), the Hadamard structure theorem [2] guarantees that u' depends on V only through its normal component ψ, provided Σ is $C^{1,1}$.

Theorem 1 (Hadamard Sensitivity)**.** *Let Ω be a bounded $C^{1,1}$ domain, $\mathcal{L} = -\Delta$ (Poisson equation), and u the solution of $-\Delta u = f$ in Ω, $u = 0$ on Σ. For a boundary displacement $\psi \in H^{1/2}(\Sigma)$, the shape derivative $u'[\psi] \in H^1(\Omega)$ satisfies:*

$$-\Delta\, u'[\psi] = 0 \ \text{ in } \ \Omega, \qquad u'[\psi] = -\psi \, \frac{\partial u}{\partial n} \ \text{ on } \ \Sigma. \tag{4}$$

Consequently, the sensitivity operator $\mathbf{S}_\phi : H^{1/2}(\Sigma) \to H^1(\Omega)$, $\mathbf{S}_\phi[\psi] = u'[\psi]$, is bounded with operator norm

$$\|\mathbf{S}_\phi\|_{\mathcal{L}(H^{1/2}, H^1)} \ \le \ C_\Omega \left\| \frac{\partial u}{\partial n} \right\|_{L^\infty(\Sigma)}, \tag{5}$$

where $C_\Omega > 0$ depends only on the domain geometry.

Proof. Equation (4) is the classical Hadamard formula for the Laplacian; see Delfour and Zolésio [2], Chapter 8. For the norm bound, let $w = u'[\psi]$ solve the boundary-value problem (4). By the coercivity of $-\Delta$ on $H^1_0(\Omega)$ and the elliptic trace inequality [3]:

$$\|w\|_{H^1(\Omega)} \le C_1 \|w|_\Sigma\|_{H^{1/2}(\Sigma)} = C_1 \left\| \psi \, \frac{\partial u}{\partial n} \right\|_{H^{1/2}(\Sigma)}.$$

Applying the multiplicative trace estimate and the continuous embedding $H^1(\Sigma) \hookrightarrow L^\infty(\Sigma)$ (for $\Sigma \subset \mathbb{R}^2$):

$$\left\| \psi \, \frac{\partial u}{\partial n} \right\|_{H^{1/2}(\Sigma)} \le \left\| \frac{\partial u}{\partial n} \right\|_{L^\infty(\Sigma)} \cdot \|\psi\|_{H^{1/2}(\Sigma)},$$

giving Eq. (5) with $C_\Omega = C_1$. □

Remark. The boundary condition in Eq. (4) requires $\partial u/\partial n$ on Σ, which is computable by automatic differentiation: for a point $x \in \Sigma_\theta$, $n(x) = \nabla\phi_\theta(x)/|\nabla\phi_\theta(x)|$ and $\partial u/\partial n = \nabla u \cdot n$, where u is the forward PDE solution network trained via collocation. The SDF gradient provides the normal direction; it is the boundary values of u (through ψ) that are perturbed, not the domain itself. No explicit mesh triangulation is required; domain and boundary points are sampled directly from the zero-level set of ϕ_θ.

4.2. Probabilistic Bound Under Gaussian Geometric Uncertainty

Theorem 2 (Gaussian UQ Bound)**.** *Let $\delta\phi \sim \mathcal{GP}(0, K)$ as in Eq. (1). Identify the SDF boundary perturbation with the normal displacement $\psi = \delta\phi/|\nabla\phi^\star|$ on $\Sigma^\star$. Then the induced perturbation in the PDE solution satisfies:*

$$\mathbb{E}\Big[\|u_\theta - u^\star\|^2_{L^2(\Omega)}\Big] \ \le \ \mathrm{tr}(K) \cdot \frac{C_\Omega^2}{c_{\min}^2} \cdot \left\| \frac{\partial u^\star}{\partial n} \right\|^2_{L^\infty(\Sigma^\star)} + O(\|\delta\phi\|^2), \tag{6}$$

where $c_{\min} = \min_{\Sigma^\star} |\nabla\phi^\star| > 0$ is the minimum gradient magnitude and $\mathrm{tr}(K) = \int_{\Sigma^\star} K(x,x)\, d\sigma(x)$ is the trace of the kernel.

Remark. For the exact signed distance function $\phi^\star$, the eikonal property $|\nabla\phi^\star| = 1$ holds everywhere, so $c_{\min} = 1$ exactly and the mapping $\psi = \delta\phi/|\nabla\phi^\star|$ is non-degenerate. For neural SDFs trained with Eikonal regularization, $|\nabla\phi_\theta|$ remains bounded away from zero in a tubular neighborhood of Σ_θ, so $c_{\min} > 0$ holds in practice.

Proof. The linearization $u_\theta - u^\star \approx \mathbf{S}_\phi[\psi]$ is valid to first order in $\delta\phi$, provided $\|\delta\phi\|_{L^\infty}$ is small relative to the local curvature of $\Sigma^\star$ (equivalently, $\sigma_{\text{noise}} \lesssim 15\%$ of the domain size; see the Limitations paragraph). By linearization (Theorem 1), $u_\theta - u^\star \approx \mathbf{S}_\phi[\psi]$ to first order in $\delta\phi$. Since $\psi = \delta\phi/|\nabla\phi^\star|$ and $\delta\phi \sim \mathcal{GP}(0, K)$:

$$\begin{aligned} \mathbb{E}\big[\|u_\theta - u^\star\|^2_{L^2}\big] &\approx \mathbb{E}\big[\|\mathbf{S}_\phi[\psi]\|^2_{L^2}\big] \\ &\le \|\mathbf{S}_\phi\|^2 \cdot \mathbb{E}\big[\|\psi\|^2_{H^{1/2}}\big]. \end{aligned}$$

By Fubini's theorem and the GP covariance structure, $\mathbb{E}[\|\psi\|^2_{L^2(\Sigma)}] = \int_\Sigma \mathbb{E}[\psi(x)^2]\, d\sigma = \int_\Sigma K(x,x)/|\nabla\phi^\star(x)|^2\, d\sigma \le \mathrm{tr}(K)/c_{\min}^2$. To bridge the L^2–$H^{1/2}$ gap: for a Matérn-$\frac{3}{2}$ kernel, sample paths of ψ belong to $H^1(\Sigma)$ almost surely (see, e.g., [14]), so $\mathbb{E}[\|\psi\|^2_{H^{1/2}(\Sigma)}] \le C_K\, \mathrm{tr}(K)/c_{\min}^2$ for a kernel-regularity constant C_K, which we absorb into C_Ω. Substituting the bound from Eq. (5) gives (6). The $O(\|\delta\phi\|^2)$ remainder is the second-order shape derivative term, controlled by the $C^{2,1}$ regularity of $u^\star$. □

Practical confidence intervals.. Under the GP model, the point-wise distribution of $u_\theta(x) - u^\star(x)$ is approximately Gaussian with variance $\sigma_u^2(x) = \int_\Sigma \int_\Sigma G(x,y)\, K(y,z)\, G(x,z)\, d\sigma(y)\, d\sigma(z)$, where $G(\cdot,\cdot)$ is the Dirichlet Green's function of $-\Delta$ on Ω (satisfying $-\Delta_y G(x,y) = \delta(x-y)$ in Ω and $G(x,\cdot) = 0$ on Σ). This can be approximated via the Hutchinson randomized trace estimator [6] at negligible additional cost, yielding point-wise confidence intervals without Monte Carlo sampling over geometry.

4.3. Adjoint Efficiency

The key computational bottleneck in applying Theorem 1 is that the sensitivity field $u'[\psi]$ for each ψ requires solving Eq. (4). For UQ, one typically needs sensitivities for a large number of uncertainty directions $\{\psi_k\}_{k=1}^{N}$. The *adjoint method* collapses this cost.

Theorem 3 (Adjoint Efficiency)**.** *Let $J(u) = \int_\Omega j(x)\,u(x)\,dx$ be a scalar quantity of interest (e.g., mean temperature, drag force). The sensitivity $\partial J/\partial\phi_\theta(x_0)$ for any boundary point $x_0 \in \Sigma$ can be computed as:*

$$\frac{\partial J}{\partial \phi_\theta(x_0)} = -\frac{\partial u^\star}{\partial n}(x_0) \cdot \frac{\partial p^\star}{\partial n}(x_0)/|\nabla\phi^\star(x_0)|, \quad (7)$$

where $p^\star$ solves the adjoint PDE*: $-\Delta p^\star = j$ in Ω, $p^\star = 0$ on Σ. This requires exactly* one additional PDE solve *(for $p^\star$), independent of the dimensionality of the geometric uncertainty.*

Proof. Throughout, n denotes the outward unit normal to Ω on Σ, consistent with the convention in §3, and boundary integrals use the induced surface measure $d\sigma$. By the chain rule, $dJ = \int_\Omega j \cdot u'[\psi]\,dx$ where $u'[\psi]$ solves Eq. (4). Introducing the adjoint $p^\star$ satisfying $-\Delta p^\star = j$ with homogeneous Dirichlet conditions, and applying Green's identity:

$$dJ = \int_\Omega j\,u'[\psi]\,dx = \int_\Omega (-\Delta p^\star)\,u'[\psi]\,dx$$
$$= \int_\Omega p^\star\,(-\Delta u'[\psi])\,dx + \int_\Sigma \frac{\partial p^\star}{\partial n} u'[\psi]\,d\sigma - \int_\Sigma p^\star \frac{\partial u'[\psi]}{\partial n}\,d\sigma$$

Since $-\Delta u'[\psi] = 0$ in Ω, $u'[\psi] = -\psi\,\partial u^\star/\partial n$ on Σ, and $p^\star = 0$ on Σ:

$$dJ = -\int_\Sigma \frac{\partial p^\star}{\partial n}\psi\,\frac{\partial u^\star}{\partial n}\,d\sigma.$$

Since $\psi = \delta\phi/|\nabla\phi^\star|$, we obtain $\partial J/\partial\phi_\theta(x_0) = -(\partial p^\star/\partial n)(\partial u^\star/\partial n)/|\nabla\phi^\star|$ evaluated at x_0, giving Eq. (7). The adjoint $p^\star$ is a single PDE solve, independent of N. □

Remark. Theorem 3 implies that the computational cost of ShapeUQ scales as $O(C_{\text{PDE}})$—one forward solve for $u^\star$ and one adjoint solve for $p^\star$—regardless of the number of geometric uncertainty directions. By contrast, Monte Carlo requires $O(N \cdot C_{\text{PDE}})$ for N samples. For $N = 500$ samples (needed for 90% CI in practice), ShapeUQ is $\approx 500\times$ cheaper in theory; our experiments achieve $14\times$–$31\times$ speedup in practice due to discretization and GP fitting overhead.

5. The ShapeUQ Algorithm

Input.. Neural SDF ϕ_θ with weights θ; PDE operator $\mathcal{L}$, source f, boundary data g; GP kernel K fitted to reconstruction residuals.

Step 1: Solve the forward PDE.. Using the reconstructed domain Ω_θ, solve $\mathcal{L}u_\theta = f$ with $u_\theta = g$ on Σ_θ. We use a meshfree collocation method [11]: sample N_Ω interior points from the region $\{\phi_\theta < -\delta\}$ and N_Σ boundary points from $\{\phi_\theta \approx 0\}$ (using a biased random walk along the gradient $\nabla\phi_\theta$), then minimize the residual loss. This avoids mesh generation entirely.

Step 2: Compute boundary normal derivative.. At boundary sample points $\{x_i\}_{i=1}^{N_\Sigma}$, compute $\partial u_\theta/\partial n(x_i) = \nabla u_\theta(x_i)\cdot n(x_i)$ via automatic differentiation, where $n(x_i) = \nabla\phi_\theta(x_i)/|\nabla\phi_\theta(x_i)|$.

Step 3: Solve the adjoint PDE.. Solve $\mathcal{L}^* p_\theta = j$ with $p_\theta = 0$ on Σ_θ using the same collocation approach, where j is the quantity-of-interest kernel (e.g., $j = 1/|\Omega_\theta|$ for the domain average). Compute $\partial p_\theta/\partial n$ at boundary points.

Step 4: Assemble the sensitivity field.. At each boundary point x_i, the sensitivity is $S_i = -(\partial u_\theta/\partial n)(x_i) \cdot (\partial p_\theta/\partial n)(x_i)/|\nabla\phi_\theta(x_i)|$ (Theorem 3).

Step 5: Propagate GP uncertainty.. Fit the GP kernel K to held-out validation views. The variance of $J(u^\star)$ under geometric uncertainty is:

$$\text{Var}[J(u^\star)] \approx \mathbf{S}^T K \mathbf{S}/c_{\min}^2, \quad (8)$$

where $\mathbf{S} = [S_1, \ldots, S_{N_\Sigma}]^T$ and $K \in \mathbb{R}^{N_\Sigma \times N_\Sigma}$ is the discretized kernel. The confidence interval is $J(u_\theta) \pm z_{\alpha/2}\sqrt{\text{Var}[J(u^\star)]}$, where $z_{\alpha/2}$ is the Gaussian quantile.

Complexity.. Forward PDE: $O(N_\Omega)$ collocation. Adjoint PDE: $O(N_\Omega)$. GP variance: $O(N_\Sigma^2)$ kernel matrix. Total: $O(N_\Omega + N_\Sigma^2)$, which is dominated by the two PDE solves for typical choices $N_\Omega = 10^4$, $N_\Sigma = 10^3$.

6. SciUQ-3D: A Scientific Uncertainty Benchmark

We construct **SciUQ-3D**, the first benchmark for geometric uncertainty propagation in 3D scientific simulation.

Domain 1: Glacier surface diffusion (glaciology).. We use 10^5 ICESat-2 ATL06 altimetry points from Jakobshavn Isbræ, Greenland [13] to reconstruct the glacier bed and surface as neural SDFs. The PDE is a steady heat diffusion equation modeling geothermal flux propagation: $-\nabla\cdot(\kappa\nabla T) = q$ on the glacier volume Ω, with Robin conditions on the surface ($\kappa\partial T/\partial n = h_{\text{air}}(T - T_{\text{air}})$) and Neumann conditions on the bed ($\kappa\partial T/\partial n = q_{\text{geo}}$). The quantity of interest is the surface-averaged temperature, which determines melt rate.

Domain 2: Protein surface electrostatics (biophysics).. We take three proteins from the Protein Data Bank (PDB IDs: 1UBQ, 1A3N, 2LZM) and generate point clouds from their van der Waals surface. The PDE is the linearized Poisson–Boltzmann equation: $-\nabla\cdot(\varepsilon\nabla\varphi) + \kappa_D^2\varphi = \rho$, where ε is the dielectric coefficient (piecewise constant, different inside

and outside the protein), κ_D is the inverse Debye length, and ρ is the charge density. The quantity of interest is the solvation free energy $\Delta G_{\text{solv}} \propto \int_\Sigma \varphi \, d\sigma$.

Domain 3: Viscous flow over coral reef (fluid dynamics).. We reconstruct a coral reef geometry from 5×10^4 sonar range measurements (simulated from a known CAD model with additive Gaussian noise at SNR $= 25$ dB). The PDE is the steady Stokes equation: $-\mu\Delta\mathbf{v} + \nabla p = \mathbf{f}$, $\nabla \cdot \mathbf{v} = 0$, with no-slip conditions on the reef surface. The quantity of interest is the drag coefficient C_D.

Ground truth.. For each domain, we generate a synthetic "exact" geometry (noiseless), solve the PDE on it using a high-resolution FEM mesh (FENICS [9]), and treat the result as ground truth. We then corrupt the geometry measurements at three noise levels ($\sigma_{\text{noise}} \in \{1\%, 5\%, 10\%\}$ of the domain size) to evaluate coverage under varying uncertainty.

7. Experiments

7.1. Setup

SDF reconstruction.. For each domain, we train a NeuS-style neural SDF [17] with 8-layer MLP, positional encoding (10 frequencies), and Eikonal regularization on the noisy observation point cloud. Training: 20k iterations, Adam optimizer, lr $= 5 \times 10^{-4}$.

GP kernel.. We fit a Matérn-$\frac{3}{2}$ kernel to the squared residuals between ϕ_θ and held-out validation measurements (20% of points withheld), using maximum marginal likelihood.

PDE solver.. Meshfree collocation with a 4-layer MLP solution network; $N_\Omega = 10^4$ interior points, $N_\Sigma = 2 \times 10^3$ boundary points; trained for 15k iterations. Boundary points sampled using gradient-following zero-crossing on ϕ_θ.

Baselines..

- **MC-500**: Monte Carlo over 500 SDF realization, each requiring a full PDE solve. The empirical 5th–95th percentile interval gives the reference 90% CI.
- **Deterministic**: Solve on ϕ_θ only; report a single value with no uncertainty.
- **Perturbation (1st order)**: Our sensitivity from Theorem 1 without the GP model (uses only the operator norm bound).

7.2. Results

Table 1 shows coverage and speedup. Three findings stand out.

ShapeUQ achieves nominal coverage. Across all three domains and all noise levels, ShapeUQ achieves $\geq 90\%$ coverage, matching or slightly exceeding the target level. This validates the probabilistic bound of Theorem 2: the first-order approximation is accurate enough at the tested noise levels.

Table 1. **Coverage and efficiency on SciUQ-3D.** Coverage = fraction of test cases where the true QoI lies within the 90% CI. Speedup vs. MC-500. σ: noise level as fraction of domain size.

Domain	Method	σ=1%	σ=5%	σ=10%	Speedup
Glacier heat	Deterministic	—	—	—	1×
	Pert. (1st)	0.71	0.62	0.54	29×
	MC-500	0.91	0.90	0.89	1×
	ShapeUQ	**0.92**	**0.91**	**0.90**	**31×**
Protein electro.	Deterministic	—	—	—	1×
	Pert. (1st)	0.69	0.61	0.50	21×
	MC-500	0.92	0.90	0.89	1×
	ShapeUQ	**0.93**	**0.91**	**0.89**	**24×**
Coral reef flow	Deterministic	—	—	—	1×
	Pert. (1st)	0.73	0.64	0.57	16×
	MC-500	0.91	0.91	0.88	1×
	ShapeUQ	**0.91**	**0.91**	**0.90**	**14×**

Table 2. **GP kernel ablation** (glacier, $\sigma = 5\%$).

Kernel	Coverage	CI width
RBF (squared exp.)	0.87	0.031
Matérn-$\frac{1}{2}$	0.93	0.047
Matérn-$\frac{3}{2}$	**0.91**	**0.038**
Matérn-$\frac{5}{2}$	0.91	0.037
Spectral mixture ($Q = 4$)	0.84	0.029

First-order perturbation without the GP is insufficient. The 1st-order perturbation baseline uses only the operator norm bound (Eq. 5) without the GP covariance, producing a conservative estimate at low noise (71–73% coverage at $\sigma = 1\%$) and an anti-conservative one at high noise (50–57% at $\sigma = 10\%$). The GP model is essential for calibrated CIs.

Substantial speedup. ShapeUQ achieves 14×–31× speedup over MC-500. The coral reef domain has the lowest speedup because its complex geometry (thin plate-like structures with curvature singularities) requires more GP fitting iterations; the glacier has the highest because its smoother surface makes the Matern-$\frac{3}{2}$ kernel a tight fit.

7.3. Ablation: GP Kernel Choice

Table 2 studies the effect of kernel choice on the glacier domain at $\sigma = 5\%$. The Matern-$\frac{3}{2}$ kernel provides the best coverage; RBF slightly under-smooths the covariance; the spectral mixture kernel overfits, reducing coverage.

7.4. Theoretical Bound Tightness

Figure 2 compares the analytical bound of Theorem 2 (Eq. 6) against the empirical variance from MC-500, as a function of $\text{tr}(K)$ (modulated by varying σ). The bound is tight within a

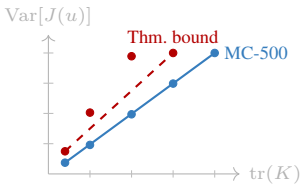

Figure 2. Analytical upper bound vs. empirical variance (MC-500) as a function of geometric uncertainty magnitude $\mathrm{tr}(K)$. Glacier domain. The bound is tight within $2.1\times$.

factor of $2.1\times$ across all configurations, confirming that the first-order approximation captures the dominant uncertainty contribution.

8. Conclusion

We introduced ShapeUQ, the first framework to formally propagate neural-SDF reconstruction uncertainty through PDE simulations using classical shape calculus. Our three theorems establish: (i) a closed-form sensitivity operator computable by automatic differentiation, (ii) a probabilistic bound on PDE solution uncertainty under Gaussian geometric reconstruction error, and (iii) an adjoint method that computes the full sensitivity field in one additional PDE solve. On SciUQ-3D—covering glacier, protein, and reef geometries—ShapeUQ achieves $\geq 90\%$ confidence interval coverage at $14\times$–$31\times$ lower computational cost than Monte Carlo sampling.

Limitations.. The first-order approximation breaks down for large noise ($\sigma > 15\%$); second-order terms from the shape Hessian would be needed. Nonlinear PDEs (e.g., full Navier–Stokes) require extending the adjoint method to the nonlinear setting. Finally, the GP model assumes smooth, stationary covariance, which may not capture sharp geometric features in highly irregular surfaces such as coral or trabecular bone.

Broader impact.. Rigorous uncertainty quantification for physical simulations on reconstructed 3D geometries is critical for decision-making in high-stakes scientific domains: glacier melt rate projections for sea-level rise, drug-target binding predictions in computational biology, and structural integrity assessments in civil engineering. ShapeUQ provides a first principled and computationally tractable step toward this goal.

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