High-accuracy numerical models of Brownian thermal noise in thin mirror coatings

Nils L. Fischer , 1, * Samuel Rodriguez , 2, 3 Tom Wlodarczyk , 1 Geoffrey Lovelace , 2 Harald P. Pfeiffer , 1 Gabriel S. Bonilla , 2 Nils Deppe , 4 François Hébert , 4 Lawrence E. Kidder , 5 Jordan Moxon , 4 and William Throwe

1 Max Planck Institute for Gravitational Physics (Albert Einstein Institute), Am Mühlenberg 1, Potsdam 14476, Germany

2 Nicholas and Lee Begovich Center for Gravitational-Wave Physics and Astronomy,
California State University, Fullerton, Fullerton, California 92831, USA

3 Department of Physics and Astronomy, University of Mississippi, University, Mississippi 38677, USA

4 Theoretical Astrophysics, Walter Burke Institute for Theoretical Physics,
California Institute of Technology, Pasadena, California 91125, USA

5 Cornell Center for Astrophysics and Planetary Science, Cornell University, Ithaca, New York 14853, USA

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Brownian coating thermal noise in detector test masses is limiting the sensitivity of current gravitational-wave detectors on Earth. Therefore, accurate numerical models can inform the ongoing effort to minimize Brownian coating thermal noise in current and future gravitational-wave detectors. Such numerical models typically require significant computational resources and time, and often involve closed-source commercial codes. In contrast, open-source codes give complete visibility and control of the simulated physics and enable direct assessment of the numerical accuracy. In this article, we use the open-source Spectre numerical-relativity code and adopt a novel discontinuous Galerkin numerical method to model Brownian coating thermal noise. We demonstrate that Spectre achieves significantly higher accuracy than a previous approach at a fraction of the computational cost. Furthermore, we numerically model Brownian coating thermal noise in multiple sub-wavelength crystalline coating layers for the first time. Our new numerical method has the potential to enable fast exploration of realistic mirror configurations, and hence to guide the search for optimal mirror geometries, beam shapes and coating materials for gravitational-wave detectors.

I. INTRODUCTION

Brownian coating thermal noise is the limiting noise source for current-generation, ground-based gravitational-wave detectors in their most sensitive frequency bands. For instance, following the A+ upgrade anticipated for completion in the mid 2020s, the Laser Intererometer Gravitational-Wave Observatory (LIGO) detector noise is dominated by Brownian coating thermal noise at frequencies $f \sim 100\,\mathrm{Hz}$ [1]. This noise arises from thermal fluctuations in the reflective coatings of the detectors' test masses [2].

Therefore, a reduction of the Brownian coating thermal noise directly increases a detector's sensitivity and thus its astronomical reach. Theoretical models of Brownian coating thermal noise are important for working toward this goal. Thermal noise modeling typically follow the approach pioneered by Levin [3], which computes the thermal noise in terms of an auxiliary elasticity calculation using the fluctuation-dissipation theorem [4–6]. While an approximate analytic solution is well known in the limit where coating thickness and edge effects can be neglected, numerical calculations of thermal noise are necessary to study effects that arise from the finite testmass size, the finite coating thickness, and from crystalline materials.

In this article we calculate Brownian coating thermal noise by numerically solving the auxiliary linear elasticity problem. Such numerical simulations typically adopt a conventional finite-element approach, as some of the authors did in Ref. [7]. These methods are widely used, but achieving high accuracy with them can require significant computational resources and time, because of their relatively slow rates of convergence.

For the first time to our knowledge, we apply a discontinuous Galerkin (DG) method to model Brownian coating thermal noise. In particular, we implement the relevant elastostatic equations in Spectre [8], an opensource, next-generation numerical-relativity code. While Spectre's primary aim is to model merging neutron stars and black holes, the elliptic solver needed to construct initial data for such simulations is also very well positioned to solve the elastostatics equations for thermalnoise modeling [9, 10]. As an open-source code, our approach has advantages compared to the closed-source and commercial solutions that are often adopted: we can directly control the physics incorporated in the calculation, and we can assess the accuracy and convergence rate of our simulations in a straightforward way. Our code also benefits from SpECTRE's task-based parallelism approach, implemented using the Charm++ [11] library, enabling our code to efficiently scale to large numbers of compute cores [12].

This article is organized as follows. Section II summarizes the elastic problem to be solved and presents the discontinuous Galerkin approach which we adopt. We use this approach to model thermal noise for cylindrical mirrors in Section III. We discuss our results and future work in Section IV.

^{*} nils.fischer@aei.mpg.de

II. METHODS

In this section, we formulate the auxiliary elasticity problem based on Refs. [3, 7], discretize it with the discontinuous Galerkin scheme developed in Ref. [10], and outline the numerical method we employ to solve the discretized problem with the Spectre code [9]. Section IIB3 details a novel extension of this method to handle discontinuous material properties at layer interfaces.

A. Auxiliary elasticity problem

We consider a gravitational-wave detector that measures the position of a test mass with a laser beam with a Gaussian intensity profile

$$p(r) = \frac{1}{\pi r_0^2} e^{-r^2/r_0^2}. (1)$$

Here, r is the cylindrical radial coordinate from the center of the beam with width r_0 . The intensity profile is normalized so that

$$\int_0^{2\pi} d\phi \int_0^{\infty} dr \, r p(r) = 1. \tag{2}$$

The laser beam effectively measures a weighted average q of the displacement Z of the test mass surface,

$$q(t) = \int_0^{2\pi} d\phi \int_0^R dr \, r p(r, \phi) Z(r, \phi, t). \tag{3}$$

As shown by Levin [3], Brownian thermal noise can be calculated from the energy dissipated in an auxiliary elastic problem. Specifically, to compute the thermal noise at frequency f, one applies an oscillating pressure to the face of the mirror with frequency f, with a pressure distribution profile p(r) equal to the beam intensity, and with an amplitude F_0 . In this auxiliary problem, energy $W_{\rm diss}$ will be dissipated in each cycle of the oscillation. The fluctuation-dissipation theorem relates this dissipated energy $W_{\rm diss}$ to the thermal noise, specifically to the power spectral density S_q associated with q, 1

$$S_q = \frac{2k_{\rm B}T}{\pi^2 f^2} \frac{W_{\rm diss}}{F_0^2},\tag{4}$$

where T is the mirror temperature and $k_{\rm B}$ is Boltzmann's constant. Because $W_{\rm diss} \propto F_0^2$, it follows that S_q does not depend on the overall amplitude F_0 .

For frequencies $f \sim 100\,\mathrm{Hz}$ much lower than the resonant frequencies $f \sim 10^4\mathrm{Hz}$ of the test-mass materials, the dissipated power can be computed using the quasistatic approximation. In this approximation, a static

pressure is applied to the mirror with amplitude F_0 and profile p(r), and the dissipated energy can be written as

$$W_{\rm diss} = U\phi, \tag{5}$$

where U is the potential energy stored in the deformation of the test-mass and ϕ is the material's loss angle determined by the material's imaginary, dissipative elastic moduli.

Therefore, our goal in this article is to solve the equations of elastostatics for the deformation of the test mass,

$$\nabla_i T^{ij} = f^j(\boldsymbol{x}),\tag{6}$$

when its surface is subjected to an applied pressure with profile p(r). Here, T^{ij} is the *stress* and we adopt the Einstein summation convention so that repeated tensor indices are summed over. f^j is the force density acting on each volume-element of the mirror as a function of position \boldsymbol{x} , which vanishes in our situation, $f^j = 0$. The pressure acting on the external surface of the test-mass will be reflected in suitable boundary conditions.

Eq. (6) is an equation for the displacement vector field $u^{i}(\boldsymbol{x})$, which describes the deformation of the elastic material as a function of the undeformed coordinates. The symmetric part of the gradient of the displacement vector field is the *strain*

$$S_{kl} = \nabla_{(k} u_{l)}. \tag{7}$$

For sufficiently small F_0 , the strain is proportional to the applied stress,

$$T^{ij} = -Y^{ijkl}S_{kl}, (8)$$

where the constitutive relation $Y^{ijkl}(\boldsymbol{x})$ captures the elastic properties of the material in the linear regime. The constitutive relation is symmetric on its first two indices, on its last two indices, and under exchange of the first pair of indices with the second pair of indices.

Inserting Eqs. (7) and (8) into Eq. (6) yields the equations of linear elasticity,

$$-\nabla_i Y^{ijkl} \nabla_{(k} u_{l)} = f^j(\boldsymbol{x}), \tag{9}$$

which we will solve numerically.

We consider amorphous and cubic-crystalline constitutive relations. The amorphous constitutive relation is isotropic and homogeneous,

$$Y^{ijkl} = \lambda \delta^{ij} \delta^{kl} + \mu \left(\delta^{ik} \delta^{jl} + \delta^{il} \delta^{jk} \right), \tag{10}$$

with Lamé parameter λ and shear modulus μ .² A cubiccrystalline material is characterized by the constitutive

¹ See e.g. Eq. (11.90) in Ref. [13].

² The Lamé parameter can also be replaced by the bulk modulus $K=\lambda+2\mu/3$. Alternatively, the two parameters can be replaced by the Young's modulus $Y=9K\mu/(3K+\mu)=\mu(3\lambda+2\mu)/(\lambda+\mu)$ and the Poisson ratio $\sigma=(3K-2\mu)/(2(3K+\mu))=\lambda/(2(\lambda+\mu))$.

relation

$$Y^{ijkl} = \begin{cases} c_{11} & \text{for } i = j = k = l \\ c_{12} & \text{for } i = j, k = l, i \neq k \\ c_{44} & \text{for } i = k, j = l, i \neq j \text{ or } i = l, j = k, i \neq j \end{cases}$$
(11)

where c_{11} , c_{12} and c_{44} are three independent material parameters.

After solving Eq. (9), the potential energy is finally evaluated by an integral over the volume of the test-mass,

$$U = -\frac{1}{2} \int_{V} dV S_{ij} T^{ij}. \tag{12}$$

The constitutive relation Y^{ijkl} can be discontinuous, representing a mirror composed of different materials, for instance thin coating layers. For a test-mass with a thin, reflective coating with different elastic properties than the substrate, the dissipated energy (5) decomposes as [14]

$$W_{\rm diss} = U_{\rm sub} \,\phi_{\rm sub} + U_{\rm coat} \,\phi_{\rm coat},\tag{13}$$

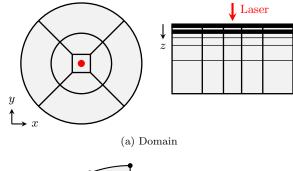
where $U_{\rm sub}$ and $\phi_{\rm sub}$ are the potential energy and loss angle of the substrate, respectively, while $U_{\rm coat}$ and $\phi_{\rm coat}$ are the potential energy and the loss angle of the coating. Note that a material can also have different loss angles associated with the different independent elastic moduli of a material. We do not consider further decompositions of the elastic potential energy in this article, but note that such quantities can straightforwardly be extracted from our simulations.

An approximate analytic solution exists for amorphous materials in the limit where the coating thickness d is small compared to both the size of the mirror and the width r_0 of the pressure profile. The approximate coating thermal noise is 3

$$S_q^{\text{coat}} = \frac{k_{\text{B}}T}{\pi^2 f} \frac{1 - \sigma_{\text{sub}}^2}{r_0 Y_{\text{sub}}} \frac{d}{r_0} \frac{\phi_{\text{coat}}}{Y_{\text{sub}} Y_{\text{coat}} (1 - \sigma_{\text{coat}}^2) (1 - \sigma_{\text{sub}}^2)} \times (Y_{\text{coat}}^2 (1 + \sigma_{\text{sub}})^2 (1 - 2\sigma_{\text{sub}})^2 + (14) Y_{\text{sub}}^2 (1 + \sigma_{\text{coat}})^2 (1 - 2\sigma_{\text{coat}}).$$

B. Numerical scheme

We employ the discontinuous Galerkin (DG) scheme detailed in Ref. [10] to discretize the elasticity problem, Eq. (9). We summarize the discretization scheme in this section, and extend it here to problems with discontinuous material properties.



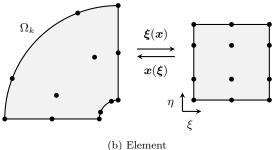


FIG. 1. Top: Geometry of our layered cylindrical domain, with the laser beam indicated in red. Four wedge-shaped elements envelop a cuboid. Another set of wedges extends to the outer radius of the cylinder. In z-direction the cylinder is partitioned into layers that can have different material properties (black and gray). The substrate layer has a logarithmic coordinate map in z-direction and is split in two twice in this example (thin lines). Bottom: The coordinate transformation $\boldsymbol{\xi}(\boldsymbol{x})$ maps an element to a reference cube $[-1,1]^3$. with logical coordinate-axes $\boldsymbol{\xi}=(\xi,\eta,\zeta)$. In this example we chose $N_{k,\xi}=3$ and $N_{k,\eta}=4$ Legendre-Gauss-Lobatto collocation points along ξ and η , respectively.

1. Domain decomposition

Our goal is to simulate a three-dimensional cylindrical mirror with radius R and height H. The cylinder axis coincides with the z-axis of our coordinates, and the plane z=0 represents the surface of the mirror on which the external pressure p(r) is applied. We decompose the cylindrical domain $\Omega=[0,R]\times[0,2\pi)\times[0,H]$ into a set of non-overlapping elements $\Omega_k\subset\Omega$ shaped like deformed cubes, as illustrated in Fig. 1a (h-refinement). Each element carries a coordinate map from the Cartesian coordinates $\boldsymbol{x}\in\Omega_k$, in which the elasticity equations (9) are formulated, to logical coordinates $\boldsymbol{\xi}\in[-1,1]^3$ representing the reference cube, as illustrated in Fig. 1b. The coordinate map to the reference cube is characterized by its Jacobian,

$$J_j^i = \frac{\partial x^i}{\partial \mathcal{E}^j} \tag{15}$$

with determinant J and inverse $(J^{-1})_i^j = \partial \xi^j / \partial x^i$. On the reference cube we choose a set of $N_{k,i}$ Legendre-Gauss-Lobatto (LGL) collocation points in each dimension i (p-refinement).

³ See Eq. (22) in Ref. [14], where $w=\sqrt{2}\,r_0,\,\phi_\parallel=\phi_\phi=\phi_{\rm coat},$ and we consider only the coating contribution.

Fields are represented numerically by their values at the collocation points. We denote the set of discrete field values within an element Ω_k as $\underline{u}^{(k)} = (u_1, \dots, u_{N_k})$, and the collection of discrete field values over *all* elements as \underline{u} . The field values at the collocation points within an element define a three-dimensional Lagrange interpolation,

$$u^{(k)}(\boldsymbol{x}) \coloneqq \sum_{p=1}^{N_k} u_p \psi_p(\boldsymbol{\xi}(\boldsymbol{x})) \quad \text{with} \quad \boldsymbol{x} \in \Omega_k,$$
 (16)

where the basis functions $\psi_p(\boldsymbol{\xi})$ are products of Lagrange polynomials,

$$\psi_p(\boldsymbol{\xi}) := \prod_{i=1}^3 \ell_{p_i}(\xi^i) \quad \text{with} \quad \boldsymbol{\xi} \in [-1, 1]^3. \tag{17}$$

based on the collocation points in dimension i of the element. Since Eqs. (16) and (17) are local to each element, fields over the entire domain are discontinuous across element boundaries.

2. DG residuals

To formulate the elasticity equations in first-order form for the DG discretization, we use the symmetric strain S_{kl} as auxiliary variable. According to Ref. [10], we first compute the discrete auxiliary variables on the computational grid as

$$S_{kl} = D_{(k} \cdot u_{l)} + L \cdot ((n_{(k}u_{l)})^* - n_{(k}u_{l)}), \tag{18}$$

where we make use of the discrete differentiation matrix $D_i := M^{-1}MD_i$, the mass matrix

$$M_{pq} = \int_{[-1,1]^3} \psi_p(\xi) \psi_q(\xi) \, \mathrm{J} \, \mathrm{d}^3 \xi, \tag{19}$$

the stiffness matrix

$$MD_{i,pq} = \int_{[-1,1]^3} \psi_p(\boldsymbol{\xi}) \, \frac{\partial \psi_q}{\partial \xi^j} (\boldsymbol{\xi}) \, (\mathbf{J}^{-1})_i^j \, \mathbf{J} \, \mathbf{d}^3 \boldsymbol{\xi}, \qquad (20)$$

the lifting operator

$$ML_{pq} = \int_{[-1,1]^2} \psi_p(\boldsymbol{\xi}) \psi_q(\boldsymbol{\xi}) J^{\Sigma} d^2 \xi, \qquad (21)$$

and $L := M^{-1}ML$ on the element Ω_k [10]. The integral in Eq. (21) is over the boundary of the element, $\partial\Omega_k$, where n_i is the outward-pointing unit normal one-form and J^{Σ} is the surface Jacobian. The operation \cdot denotes matrix multiplication with the field values over the computational grid of an element. In a second step, we compute the DG residuals in strong form [10],

$$-MD_{i} \cdot Y^{ijkl} S_{kl} - ML \cdot ((n_{i} Y^{ijkl} S_{kl})^{*}$$
$$-n_{i} Y^{ijkl} S_{kl}) = M \cdot f^{j}(\boldsymbol{x}), \tag{22}$$

which represent the set of algebraic equations for the values of the displacement vector field on the computational grid that we solve numerically.

3. Numerical flux

The quantities $(n_{(k}u_{l)})^*$ and $(n_iY^{ijkl}S_{kl})^*$ in Eq. (22) denote a numerical flux that couples grid points across nearest-neighbor element boundaries. We employ the generalized internal-penalty numerical flux developed in Ref. [10], with one notable extension. Contrary to Ref. [10] we allow neighboring elements to define different constitutive relations, meaning $Y^{ijkl}(\boldsymbol{x})$ can be double-valued on shared element boundaries.⁴ Therefore, we define the quantity

$$Y_*^{ijkl} = \frac{1}{2} \left(Y_{\text{int}}^{ijkl} + Y_{\text{ext}}^{ijkl} \right), \tag{23}$$

where "int" denotes the *interior* side of an element's shared boundary with a neighbor, and "ext" denotes the *exterior* side, i.e. the neighbor's side. With this quantity we can define the numerical flux

$$(n_{(k}u_{l)})^{*} = \frac{1}{2} \left[n_{(k}^{\text{int}} u_{l)}^{\text{int}} - n_{(k}^{\text{ext}} u_{l)}^{\text{ext}} \right],$$
(24a)

$$(n_{i}Y^{ijkl} S_{kl})^{*} = \frac{1}{2} \left[n_{i}^{\text{int}} Y_{\text{int}}^{ijkl} \partial_{(k} u_{l)}^{\text{int}} - n_{i}^{\text{ext}} Y_{\text{ext}}^{ijkl} \partial_{(k} u_{l)}^{\text{ext}} \right]$$

$$-\sigma \left[n_{i}^{\text{int}} Y_{*}^{ijkl} n_{(k}^{\text{int}} u_{l)}^{\text{int}} - n_{i}^{\text{ext}} Y_{*}^{ijkl} n_{(k}^{\text{ext}} u_{l)}^{\text{ext}} \right],$$
(24b)

where $n_i^{\rm ext} = -n_i^{\rm int}$ for the purpose of this article. Equation (24) is the generalized internal-penalty numerical flux defined in Ref. [10], with a choice between $Y_{\rm int}^{ijkl}$, $Y_{\rm ext}^{ijkl}$ and Y_*^{ijkl} for every occurrence of the constitutive relation. The particular choice in Eq. (24) ensures that the numerical flux remains consistent, meaning that $(n_iY^{ijkl}S_{kl})^* = -n_i^{\rm int}T^{ij}$ when both $n_i^{\rm int}Y_{\rm int}^{ijkl}\partial_{(k}u_{l)}^{\rm int} = -n_i^{\rm ext}Y_{\rm ext}^{ijkl}\partial_{(k}u_{l)}^{\rm ext} =: -n_i^{\rm int}T^{ij}$ and $n_{(k}^{\rm int}u_{l)}^{\rm int} = -n_{(k}^{\rm ext}u_{l)}^{\rm ext}$. In particular, note that the penalty term in Eq. (24b) vanishes when the displacement is continuous across the boundary, and that the numerical flux admits solutions where the stress is continuous across the boundary but the strain is not. Such solutions may arise in a layered material under stress, because the layers remain "glued together" but each layer responds to the stress differently.

The penalty function in Eq. (24b) is

$$\sigma = C \frac{(\max(p^{\text{int}}, p^{\text{ext}}) + 1)^2}{\min(h^{\text{int}}, h^{\text{ext}})}, \tag{25}$$

where we make use of the polynomial degree p and a measure of the element size, h, orthogonal to the element boundary on either side of the interface, as detailed in Ref. [10]. We choose C=100 in this article.

⁴ In the language of Ref. [10] we allow the fluxes $\mathcal{F}_{\alpha}{}^{i}[u_{A}, v_{A}; \boldsymbol{x}]$ to be double-valued on shared element boundaries.

4. Boundary conditions

We impose boundary conditions through fluxes, i.e. by a choice of exterior quantities in the numerical flux (24). Specifically, on external boundaries we set

$$(n_{(k}u_{l)})^{\text{ext}} = (n_{(k}u_{l)})^{\text{int}} - 2n_{(k}^{\text{int}}u_{l)}^{\text{b}}$$
 and (26a)

$$(n_i Y^{ijkl} S_{kl})^{\text{ext}} = (n_i Y^{ijkl} S_{kl})^{\text{int}} + 2n_i^{\text{int}} T_{\text{b}}^{ij}, \quad (26b)$$

where we choose either $u_{\rm b}^i$ to impose Dirichlet boundary conditions, or $n_i^{\rm int}T_{\rm b}^{ij}$ to impose Neumann boundary conditions, and set the respective other quantity to its interior value.

For the thermal noise problem we impose the pressure induced by the laser beam,

$$n_i^{\text{int}} T_b^{ij} = -n^j p(r), \tag{27}$$

as Neumann boundary condition on the z=0 side of the cylindrical mirror, where p(r) is the laser beam profile given in Eq. (1). On the side of the mirror facing away from the laser we impose

$$u_{\rm b}^i = 0 \quad (\text{``fixed''}) \tag{28}$$

as Dirichlet boundary condition, and on the mantle we impose

$$n_i^{\text{int}} T_{\text{b}}^{ij} = 0 \quad (\text{"free"}) \tag{29}$$

as Neumann boundary condition. Equation (28) means that the back of the mirror is held in place, whereas Eq. (29) implies no pressure on the sides, which however, are free to deform in response to the pressure applied to the front.

C. SpECTRE elliptic solver

Since the DG residuals (22) are linear algebraic equations for the discrete primal field values \underline{u}^i on all elements and grid points in the computational domain, Eq. (22) defines a matrix equation

$$\mathcal{A}\underline{u} = \underline{b}.\tag{30}$$

We solve the matrix equation (30) with the elliptic solver component of the open-source Spectre code, detailed in Ref. [9]. It employs a GMRES linear solver with a Multigrid-Schwarz preconditioner to solve Eq. (30) to the requested precision, and a task-based parallelization paradigm to distribute the computation across a computing cluster.

III. RESULTS

Our simulations with Spectre were performed on one or more 16-core compute nodes, each with 64 GB of memory and two eight-core Intel Haswell E5-2630v3 processors clocked at 2.40 GHz, connected with an Intel Omni-Path network. We distribute the elements that compose

the computational domain evenly among cores, leaving one core per node free to perform communications.

We compare our results with SpECTRE to previous work using an open-source finite-element code to calculate the Brownian coating thermal noise for amorphous and crystalline materials. Its methods are described in detail in Secs. 2.4–2.6 of Ref. [7]. The code was built using the deal.ii [15, 16] finite-element framework and we henceforth refer to it as deal.ii. It adopted a standard weak form of the elastostatic equations, discretized them using a conventional finite-element approach, and solved them using deal.ii with the PETSc [17] conjugate gradient linear solver and the ParaSAILS preconditioner in the hypre [18] package. The deal.ii code relies on the Message Passing Interface (MPI) for parallelization.

A. Single-coating comparison

First, we consider the single-coating scenario investigated in Ref. [7] and demonstrate the superior performance of our new approach. We choose the parameters listed in Ref. [7], Table 1 for a cylindrical mirror of radius $R=12.5\,\mathrm{mm}$ with a single $d=6.83\,\mathrm{\mu m}$ thin effective-isotropic AlGaAs coating. We simulate the scenario both with the deal.ii approach employed in Ref. [7] and with our new approach with the Spectre code.

Figure 2 presents the numerical precision and computational cost of both approaches. To assess the numerical precision we successively increase the resolution in both codes. In Spectre we increase the resolution by incrementing the number of grid points in all dimensions of all elements in the domain by one, and in deal.ii we employ an adaptive mesh-refinement scheme [7]. We compute the error in the elastic potential energy relative to a high-resolution reference simulation. We use a reference configuration simulated in Spectre where we have split all elements in two along all three dimensions, relative to the highest-resolution configuration included in Fig. 2.

We find that both codes converge to the same solution, but our new approach in SpECTRE achieves about four orders of magnitude higher accuracy than the <code>deal.ii</code> approach using the same number of grid points. Furthermore, our new approach simulates this scenario with sub-percent error in only 30 s on 15 cores, for which the <code>deal.ii</code> approach required multiple hours on 324 cores. Our new approach also achieves a fractional error below 10^{-5} in only half a core-hour, or two minutes of real time, which was prohibitively expensive with the <code>deal.ii</code> approach.

B. Accuracy of the approximate analytic solution

Second, we study the accuracy of the approximate analytic solution for the single-coating thermal noise, Eq. (14), using the superior numerical precision we can now achieve over the results presented in Ref. [7]. The

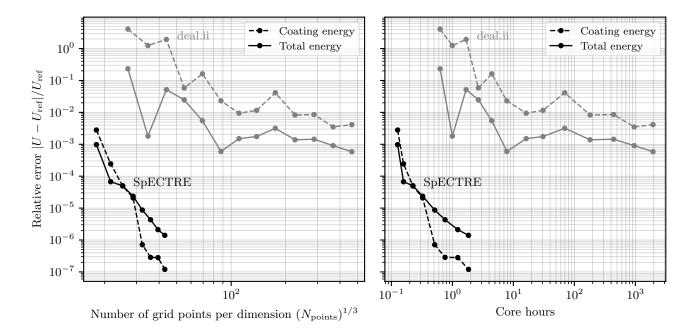


FIG. 2. Relative error of the potential energy in a single amorphous coating layer (dashed lines) and in the full mirror (solid lines). Left: Spectre, with our discontinuous Galerkin method, resolves the coating layer at high precision using only a fraction of the number of grid points needed by the deal.ii approach. Right: Spectre solves the elliptic problem using only a fraction of the computational resources needed by the deal.ii approach.

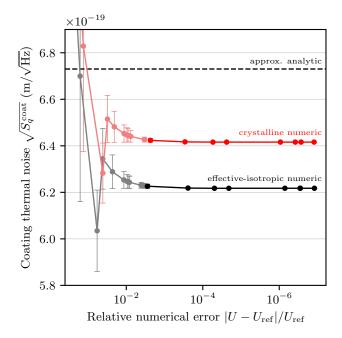


FIG. 3. Thermal noise in an AlGaAs-coated mirror computed from the approximate analytic solution (14) and from our numerical simulations. The effective-isotropic simulation (black) retains the amorphous approximation for the material, but includes finite-size effects. The crystalline simulation (red) eliminates this approximation. Previous simulations with the deal.ii approach are shown in lighter colors to the left.

approximate solution holds for a thin coating, $d/r_0 \ll 1$, a semi-infinite mirror, $r_0/R \ll 1$ and $d/R \ll 1$, and for isotropic-homogeneous materials. Therefore, it does not capture the finite-size effects included in our simulations, and approximates the crystalline AlGaAs coating as an amorphous material.

To assess the magnitude of the finite-size effects, we employ the simulations detailed in Section III A, which use the same effective-isotropic model for the AlGaAs coating that underpins the approximate analytic solution. Figure 3 presents both the thermal noise computed from the simulations and the approximate analytic solution (black). Error bars are computed as $\Delta\sqrt{S_q^{\rm coat}}/\sqrt{S_q^{\rm coat}}=1/2\,\Delta U_{\rm coat}/U_{\rm coat}$ from the relative numerical error in the elastic potential energy. While Ref. [7] estimated the magnitude of finite-size effects for this problem to 7%, we can now report that their simulations captured the effect to 7.5(2)%. With our new numerical method, we can make this statement more precise and report a finite-size effect of 7.616 649(6)%.

To assess the magnitude of the amorphous approximation to the crystalline coating material, we repeat the simulations with a crystalline constitutive relation. The thermal noise computed from these simulations is presented in Fig. 3 as well (red). We refine the estimate of 4% from Ref. [7] to 4.5(2)%, and report 4.667990(6)% using our new numerical method.

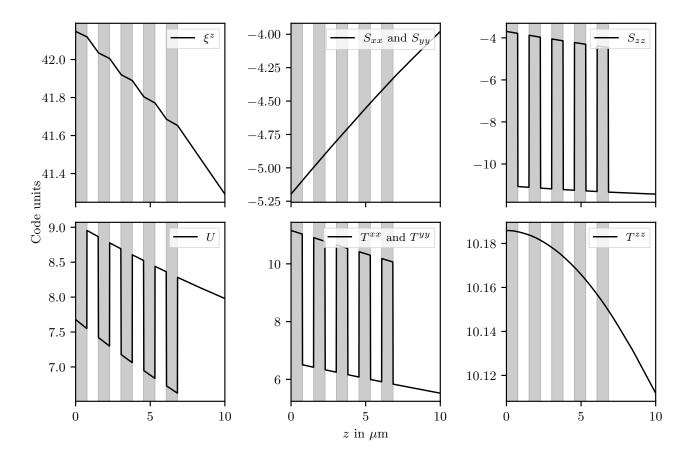


FIG. 4. Elastic variables along the z-axis for a mirror with multiple thin coating layers, simulated with Spectre. Gray layers are crystalline AlGaAs, and white regions are fused silica. The nine coating layers have a combined thickness of $6.83 \, \mu m$ and the material extends to $z = 12.5 \, mm$.

C. Multiple sub-wavelength crystalline coatings

Finally, we apply our new computational approach to a scenario that presents many of the challenges we expect for applications to realistic mirror configurations. We simulate a cylindrical mirror of the same radius $R=12.5\,\mathrm{mm}$ as before, but split the $d=6.83\,\mathrm{\mu m}$ thin coating into nine layers, so the thickness of each coating layer is below the typical 1 $\mathrm{\mu m}$ wavelength of the laser. The coating layers alternate between fused silica and crystalline AlGaAs, with the elastic moduli c_{11}, c_{12} and c_{44} listed in Ref. [7], Table 1. Neither sub-wavelength coatings nor multiple layers were simulated in Ref. [7], but our new computational approach in SpECTRE achieves both.

Figure 4 presents our numerical solution of this scenario. Our new computational approach based on discontinuous Galerkin methods resolves the thin coating layers at high accuracy without spurious oscillations. Figure 5 presents the numerical precision of the solution. We increase the resolution by incrementing the number of grid points per element and dimension and compute the relative error to a high-resolution reference configuration, as

we did in Section III A.

IV. DISCUSSION

We have presented a new numerical method to model Brownian thermal noise in thin mirror coatings based on a discontinuous Galerkin (DG) discretization. With our new method, we model thermal noise in a one-inch cylindrical mirror with a microns-thick coating at unprecedented accuracy at a fraction of the time needed in a previous, conventional finite-element approach [7]. Using these high-accuracy simulations, we find that a commonly-used approximate analytic solution overestimates the coating thermal noise for this problem by 7.6 % when taking only finite-size effects into account, and by 4.7% when modeling it as a crystalline material, which refines a previous estimate in Ref. [7]. We also demonstrate that, unlike the approach in Ref. [7], our new method is capable of resolving multiple sub-wavelength coatings, including coatings of a cubic-crystalline material. Our new numerical method is implemented in the open-source Spectre code and the results presented in this article are reproducible with the supplemental input-

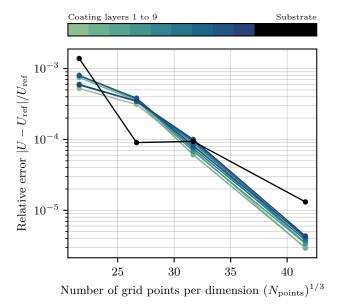


FIG. 5. Convergence test of the elastic potential energy in each coating layer, and in the substrate. Our new numerical method achieves exponential convergence despite the discontinuous material properties.

file configurations.

We found that it is crucial for the success of our new method that the interfaces between layers of different materials coincide with element boundaries in our computational domain. Then, our discontinuous Galerkin discretization with a suitable choice of numerical flux converges exponentially, achieving high accuracy with a small number of grid points. The scheme can potentially be improved in future work. Most notably, an adaptive mesh-refinement (AMR) algorithm that distributes the resolution in the computational domain to regions and dimensions where it is most needed would have great potential to further improve the accuracy and efficiency of the scheme.

Furthermore, the elliptic solver in the Spectre code that we employ to solve the discretized problem numerically can be improved to accelerate thermal-noise calculations. The calculations we have presented in this article require a few hundred solver-iterations to converge, or up to ~ 1400 for our highest-resolution simulation with multiple sub-wavelength crystalline coatings. While simple configurations complete in seconds or minutes of real-time on 15 cores, where the previous approach needed hours on 324 cores, the more challenging configurations, which were prohibitively expensive with the previous approach, solve in about an hour on 45 cores.

We expect additional speedup with further improvements to the elliptic solver algorithm in Spectre. In particular, improvements to its multigrid preconditioner

have great potential to speed up the simulations. The multigrid algorithm relies on solving the problem approximately on coarser grids to resolve large-scale modes in the solution. It currently cannot coarsen the grid any further than the size of each coating layer because the layers define the material properties. To accelerate the calculations, we intend to let the multigrid algorithm combine layers with different materials into fiducial coarse layers with effective material properties. This approach is possible because the partitioning of the domain into layers is necessary only to define material properties, not to define the geometry of the domain. Reference [9] shows that the multigrid algorithm can achieve resolution-independent iteration counts when the domain can be coarsened sufficiently.

Our numerical models of thermal noise have the potential to inform upgrades that increase the sensitivity of gravitational-wave detectors, using the advanced computational technology that we develop for numericalrelativity simulations in the Spectre code. In the future, we intend to apply our new numerical method to simulate Brownian thermal noise in more realistic mirror configurations and materials that are under consideration for current and future gravitational-wave detectors, such as the optimized configuration found in Ref. [19]. While approximate analytic solutions can provide useful estimates, only numerical models can precisely quantify the finite-size effects of changing the mirror geometry. In particular, finite-size effects are more important for real gravitational-wave detectors than for tabletop experiments measuring thermal noise. Tabletop experiments often use small beam sizes to enlarge the thermal noise and hence make it easier to measure, whereas gravitational-wave detectors prefer large beam sizes to minimize thermal noise. Therefore, we plan to employ our new numerical method to explore realistic mirror configurations, with the goal of finding configurations that minimize Brownian coating thermal noise.

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