SAND2014-20580C

Optimization–Based Coupling of Nonlocal and Local Diffusion Models

Marta D'Elia[1] and Pavel B. Bochev[1]
[1]Sandia National Laboratories [2] , Computer Science Research Institute,
P.O. Box 5800, Albuquerque, NM 87185-1320

ABSTRACT

In this work we introduce an optimization–based method for the coupling of nonlocal and local diffusion problems. Our approach is formulated as a control problem where the states are the solutions of the nonlocal and local equations, the controls are the nonlocal volume constraint and the local boundary condition, and the objective of the optimization is a matching functional for the state variables in the intersection of the nonlocal and local domains. For finite element discretizations we present numerical results in a one–dimensional setting; though preliminary, our tests show the consistency and efficacy of the method, and provide the basis for realistic simulations.

INTRODUCTION

Nonlocal continuum models are used in many scientific and engineering applications where the material response and dynamics depend on the micro–structure. Such models differ from the classical, local, models in the fact that interactions between points can occur at distance, without contact; for this reason they are used to accurately resolve small scale features such as crack tips or dislocations that can affect the global material behavior. However, nonlocal models are often computationally too expensive, sometimes even intractable (see Figure 1 where we report the pattern of the finite element (FE) stiffness matrices of a nonlocal diffusion problem for increasing values of the radius of nonlocal interactions), especially when compared to partial differential equations for which efficient numerical solvers are available.

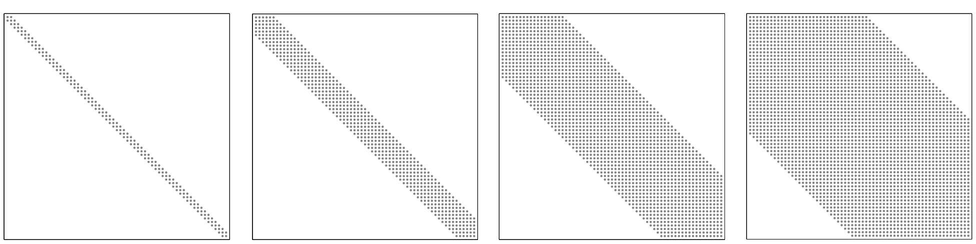

Figure 1: Pattern of FE stiffness matrices of a one–dimensional nonlocal diffusion problem in $\Omega = (-1, 1)$ for increasing values of the radius of nonlocal interactions. From left to right, the matrices corresponding to the local case, $\varepsilon = 0.1$, $\varepsilon = 0.5$, $\varepsilon = 1$.

Therefore, methods for the coupling of nonlocal and local models have been proposed for efficiently obtaining accurate solutions; these methods employ nonlocal models in small parts of the domain and local, macroscopic, models elsewhere.

[2]Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DEAC0494AL85000.

We propose an optimization–based coupling method for nonlocal diffusion problems; we split the problem domain in a nonlocal and local domain such that they feature a non–zero intersection and we minimize the difference between the nonlocal and local solutions in the overlapping regions tuning their values on the common boundaries and volumes.

THEORY

We introduce the nonlocal and local diffusion models and describe the coupling strategy. We define the nonlocal diffusion operator as

$$\mathcal{L}u(\boldsymbol{x}) := 2\int_{\mathbb{R}^d} \big(u(\boldsymbol{y}) - u(\boldsymbol{x})\big)\,\gamma(\boldsymbol{x},\boldsymbol{y})\,d\boldsymbol{y}, \tag{1}$$

where $u(\boldsymbol{x})\colon \mathbb{R}^d \to \mathbb{R}$ and $\gamma(\boldsymbol{x},\boldsymbol{y})\colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a symmetric non–negative kernel such that $\gamma(\boldsymbol{x},\boldsymbol{y}) = 0,\ \forall\,\boldsymbol{y} : |\boldsymbol{x}-\boldsymbol{y}| \geq \varepsilon$. We refer to ε as the interaction radius. For an open bounded region $\Omega \in \mathbb{R}^d$ we define the interaction domain as a layer of thickness ε that surrounds Ω, i.e.

$$\widetilde{\Omega} = \{\boldsymbol{y} \in \mathbb{R}^d \setminus \Omega :\ |\boldsymbol{y}-\boldsymbol{x}| < \varepsilon,\ \boldsymbol{x} \in \Omega\}. \tag{2}$$

We formulate the nonlocal and local diffusion problems in $\Omega_n \subset \mathbb{R}^d$ and $\Omega_l \subset \mathbb{R}^d$ as follows

$$\text{(NL)}\quad \begin{cases} -\mathcal{L}u_n = f_n & \boldsymbol{x} \in \Omega_n \\ \quad u_n = \sigma_n & \boldsymbol{x} \in \widetilde{\Omega}_n, \end{cases} \qquad\qquad \text{(L)}\quad \begin{cases} -\Delta u_l = f_l & \boldsymbol{x} \in \Omega_l \\ \quad u_l = \sigma_l & \boldsymbol{x} \in \partial\Omega_l, \end{cases} \tag{3}$$

where f_n, f_l are square integrable functions and σ_n, σ_l are the volume constraint (the nonlocal counterpart of a Dirichlet condition) for (NL) and the Dirichlet boundary condition for (L).

Given a diffusion problem whose solution features discontinuities or irregularities (due to e.g. discontinuous forcing terms) only in a part of the domain, we want to use the accurate nonlocal model (NL) in that region and the macroscopic local model (L) in the remaining part, coupling (NL) and (L) on the common boundaries or volumes.

The coupling method

Let $\Omega^+ = \Omega \cup \widetilde{\Omega}$ be an open bounded domain in $\mathbb{R}^d$. We partition Ω^+ into a nonlocal subdomain Ω_n with interaction volume $\widetilde{\Omega}_n$ and a local subdomain Ω_l, such that $\Omega_n^+ := \Omega_n \cup \widetilde{\Omega}_n \subset \Omega^+$ and $\Omega_b = \Omega_n^+ \cap \Omega_l \neq \emptyset$; we partition $\widetilde{\Omega}_n$ and $\partial\Omega_l$ as in Figure 2.

The idea of our coupling approach is to tune the values of the nonlocal and local solutions, u_n and u_l, on the control regions $\widetilde{\Omega}_c$ and Γ_c so that they are as close as possible on the overlap domain Ω_b. The optimization–based coupling is formulated as a control problem where we minimize the mismatch between the u_n and u_l in Ω_b subject to the nonlocal and local equations; the control variables, denoted by θ_n and θ_l, are the values of the nonlocal volume constraint on $\widetilde{\Omega}_c$ and the local boundary condition on Γ_c. Formally, we solve the following problem

$$\min_{u_n,u_l,\theta_n,\theta_l} J(u_n,u_l) = \frac{1}{2}\int_{\Omega_b} (u_n - u_l)^2\,d\boldsymbol{x}$$
$$\text{s.t.}\quad \begin{cases} -\mathcal{L}u_n = f_n & \boldsymbol{x} \in \Omega_n \\ \quad u_n = \theta_n & \boldsymbol{x} \in \widetilde{\Omega}_c \\ \quad u_n = 0 & \boldsymbol{x} \in \widetilde{\Omega}_i \end{cases} \quad \text{and} \quad \begin{cases} -\Delta u_l = f_l & \boldsymbol{x} \in \Omega_l \\ \quad u_l = \theta_l & \boldsymbol{x} \in \Gamma_c \\ \quad u_l = 0 & \boldsymbol{x} \in \Gamma_i. \end{cases} \tag{4}$$

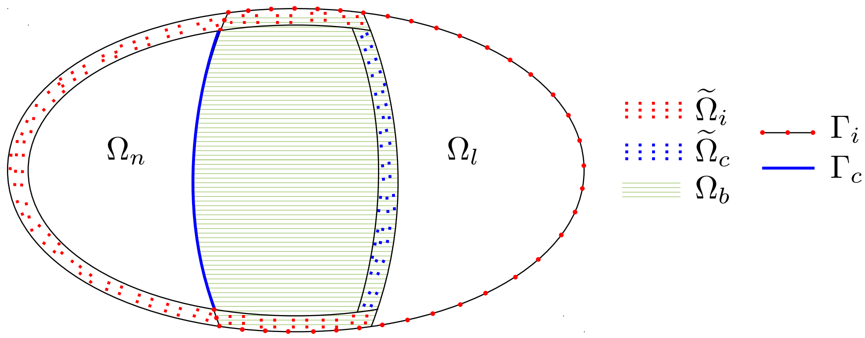

Figure 2: An example of domain configuration in two–dimensions.

We denote the optimal controls and the corresponding states by (θ_n^*, θ_l^*) and (u_n^*, u_l^*). We define the optimal "coupled" solution as $u^* = u_n^* \chi(\boldsymbol{x} \in \Omega_n^+) + u_l^* \chi(\boldsymbol{x} \in \Omega_l \setminus \Omega_b)$, where $\chi(\boldsymbol{x})$ is the indicator function.
In [1] this problem is treated in a variational form and analyzed using the nonlocal vector calculus (see e.g. [2]), a recently developed technique that allows us to study nonlocal diffusion problems as their local counterpart. There, one can find results such as the well–posedness and the analysis of the error of u^* with respect to the "true" solution, i.e. the solution of (NL) in Ω^+ with $\sigma_n = 0$.

Numerical approximation

For the numerical solution of problem (3) we consider the variational form of the state equations and we discretize it with the FE method (see e.g. [3] for an introduction to weak formulations and Galerkin discretizations).
Let $u_{nh}, u_{lh}, \theta_{nh}, \theta_{lh}$ be the discretized nonlocal and local states and controls; specifically, they are discontinuous (for nonlocal) and continuous (for local) piecewise polynomial approximations of the corresponding infinite dimensional variables $u_n, u_l, \theta_n, \theta_l$.
For the solution of the optimization problem we use an iterative gradient–based algorithm.

ALGORITHM 1.
Given an initial guess $(\theta_{nh}^0, \theta_{lh}^0)$, for $k = 0, 1, 2, \ldots$
1. solve the state equations to obtain (u_{nh}^k, u_{lh}^k) and compute $J(u_{nh}^k, u_{lh}^k)$
2. compute the gradient of the functional with respect to the controls and evaluate it at $(\theta_{nh}^k, \theta_{lh}^k)$:

$$\left.\frac{\mathrm{d}J}{\mathrm{d}(\theta_{nh}, \theta_{lh})}\right|_{(\theta_{nh}^k, \theta_{lh}^k)}$$

3. use **1.** and **2.** to compute the increments $\delta(\theta_{nh}^k)$ and $\delta(\theta_{lh}^k)$
4. set $\theta_{nh}^{k+1} = \theta_{nh}^k + \delta(\theta_{nh}^k)$ and $\theta_{lh}^{k+1} = \theta_{lh}^k + \delta(\theta_{lh}^k)$.

In **3.** one can use any optimization algorithm such as Conjugate Gradient, Newton methods, Inexact Newton methods, etc. In this work we adopt the BFGS method [4]. [1] shows that for each k, we only need one solve for the nonlocal and local states.

RESULTS

We report the numerical results of one–dimensional numerical tests; though preliminary, these results prove the robustness of the method and provide the ground for realistic simulations. We refer to the configuration in Figure 3.

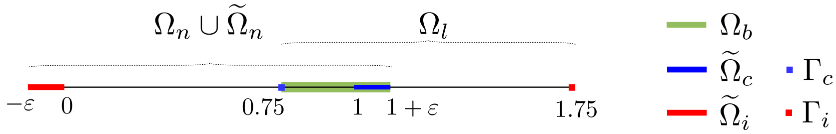

Figure 3: One–dimensional domain configuration used in the numerical tests.

We consider the kernel

$$\gamma(x, y) = \frac{1}{\varepsilon^2 |x - y|} \chi(x - \varepsilon, x + \varepsilon), \tag{5}$$

which is often used in the literature, e.g. in a linearized peridynamics model for solid mechanics [5]. We use discontinuous piecewise linear FE spaces for u_{nh} and θ_{nh} and continuous piecewise linear FE spaces for u_{lh}; θ_{lh} is a scalar as we consider a one–dimensional setting. We use uniform grids on both Ω_n^+ and Ω_l with the same grid size h.

Patch Test We utilize the following data set: $u_n = u_l = x$, $u_n|_{\widetilde{\Omega}_i} = x$, $u_l(1.75) = 1.75$, $f_n = f_l = 0$. Using linear FE spaces the optimal discretized solutions (u_{nh}^*, u_{lh}^*) are exact; this test proves the consistency of our method. In Figure 4, on the left, we report the optimal solutions (u_{nh}^*, u_{lh}^*) and their initial guesses (u_{nh}^0, u_{lh}^0).

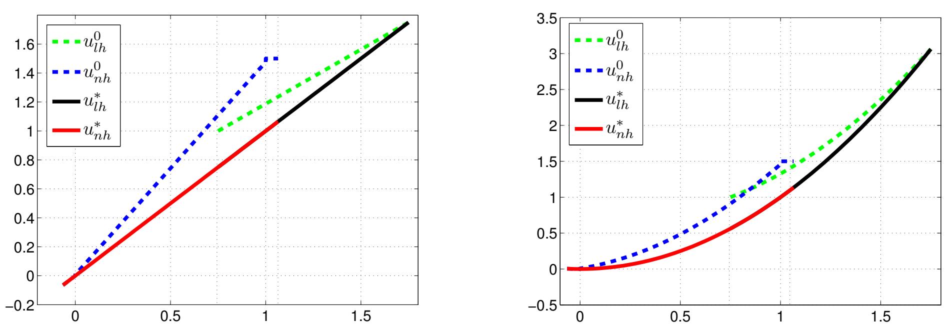

Figure 4: (u_{nh}^*, u_{lh}^*) and (u_{nh}^0, u_{lh}^0) for the *Patch Test* (left) and for *Test 1.* (right).

Test 1. We utilize the following data set: $u_n = u_l = x^2$, $u_n|_{\widetilde{\Omega}_i} = x^2$, $u_l(1.75) = 1.75^2$, $f_n = f_l = -2$. In correspondence of quadratic functions the nonlocal and local operators are equivalent; this can be appreciated in Figure 4, on the right, where the optimal solutions accurately approximate x^2 over $\Omega^+ = [-\varepsilon, 1.75]$.

Test 2. The purpose of this test is to illustrate the coupling method in cases where the nonlocal model is required in a part of the domain to capture irregular behavior, whereas the local model provides adequate resolution in the rest of the domain. This situation arises when, for example, the forcing term features discontinuities only in a part of the domain and it is smooth elsewhere. In Figure 5, on the left, we report the right hand side over Ω^+. We prescribe homogeneous

Dirichlet conditions on $\widetilde{\Omega}_i$ and Γ_i. In Figure 5, on the right, we report the optimal solutions and their initial guesses.

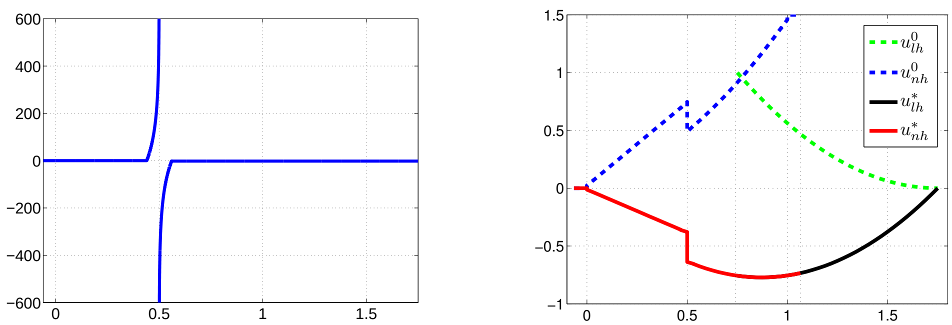

Figure 5: On the left, for <u>*Test 2.*</u> the forcing term with an infinite discontinuity. On the right, the corresponding (u_{nh}^*, u_{lh}^*) and the initial guess (u_{nh}^0, u_{lh}^0).

CONCLUSIONS

We introduced a robust, accurate and efficient method for coupling nonlocal and local diffusion models and we illustrated its properties with several one–dimensional tests. The generalization of our approach to more complex models (involving e.g. transport, reaction, or nonlinear terms) is straightforward and the preliminary results presented in the previous section are promising. An extensive mathematical and numerical analysis can be found in [1] as well as other numerical tests illustrating the theoretical results. Our current work is focused on the application of the coupling method to three–dimensional test cases and to nonlocal continuum mechanics models such as peridynamics.

ACKNOWLEDGMENTS

Part of this research was carried under the auspices of the Collaboratory on Mathematics for Mesoscopic Modeling of Materials (CM4).

REFERENCES

1. M. D'Elia and P. B. Bochev, *Sandia technical report*, no. SAND2014-17373J (2014).
2. Q. Du, M. Gunzburger, R. B. Lehoucq and K. Zhou, *SIAM Rev*, **54**,4, 667–696 (2012).
3. C. Johnson, *Numerical Solution of Partial Differential Equations by the Finite Element Method*, (Courier Dover Publications, New York, 2009).
4. J. Nocedal and S. Wright, *Numerical Optimization*, 2nd ed. (Springer, New York, 2006).
5. S. A. Silling, R. B. Lehoucq, *Advances in applied mechanics*, **44**, 73–168 (2010).