Using Reduced Order Modeling to Solve Nonlocal and Anomalous Diffusion Problems

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Introduction

Anomalous diffusion problems include such applications as flow through a porous media, where the diffusion rate is not necessarily linear with respect to time. Nonlocal approaches have been shown to be prime candidates for solving these types of diffusion problems. These nonlocal methods rely on the concept of a horizon, or radius in which surrounding particles interact with one another. Due to the increase in interactions for a given particle in a defined system, as well as the use of discontinuous basis functions, the computational cost for such problems can balloon significantly.

Reduced Order Modeling (ROM) is a widely used class of methods used to reduce the computational cost of solving differential equations using standard techniques like the Finite Element Method (FEM) among others. The ROM method that we will use in this research is called the Proper Orthogonal Decomposition (POD) and makes use of the Singular Value Decomposition (SVD) to develop an intelligent set of reduced basis functions.

This research will demonstrate the viability of using ROM coupled with a nonlocal approach to solving nonlocal problems. Specifically we would like to apply this method to solutions with discontinuities. In order to construct our reduced order nonlocal solution we will follow the provided steps:

1. Solve the nonlocal problem a set number of times with respect to a parameter sample set to understand how the solution behaves with respect to a given set of inputs. This is called collecting snapshots.
2. Use SVD on the snapshot set to form a reduced set of basis functions that intelligently capture the major features and trends of the solution with respect to the parameter inputs.
3. Construct the reduced order solution to the nonlocal problem using as few reduced basis functions as it takes to accurately represent the solution to the differential equation.

We will attempt to follow these general steps in order to construct a reduced order solution to our one dimensional time dependent nonlocal equation.

Finally, we wish to apply this work to a two-dimensional diffusion problem in order to extend the applicability of this work. We will include some preliminary results at the end of this poster.

Solving the Non-Local problem

S. A. Silling first introduced the nonlocal approach as a way to solve mechanics problems with the objective of focusing on problems with discontinuities. What resulted, was an integro-differential equation that depends on a horizon where only particles within some radius are allowed to interact, or "see" one another. By applying his theories and methodology, it can be shown that one can form the following integro-differential equation:

$$\rho\ddot{u}(\mathbf{x},t) = \int_{H_x} c\frac{(\mathbf{x}'-\mathbf{x})\otimes(\mathbf{x}'-\mathbf{x})}{|\mathbf{x}'-\mathbf{x}|^3}(\mathbf{u}(\mathbf{x}',t)-\mathbf{u}(\mathbf{x},t))dV_x + \mathbf{f}(\mathbf{x},t)$$

where ρ is the mass density in the reference configuration, $\boldsymbol{x}$ and $\boldsymbol{x'}$ are the different locations of the two particles within our reference frame (H_x), c is a constant accounting for material properties and spatial dimensions and $\mathbf{f(x,t)}$ is a given body force density. Finally we must add in a temporal derivative to make this a time-dependent problem:

$$\begin{cases} a_1\dfrac{du(x,t)}{dt} + a_2\dfrac{1}{\delta^2}\displaystyle\int_{x-\delta}^{x+\delta}\frac{u(x,t)-u(x',t)}{|x-x'|}dx' = f(x,t), & x\in\Omega \\ u(x) = g(x) & x\in\Gamma \end{cases} \quad [1]$$

where a_1 and a_2 are problem specific constants and δ is the horizon length.

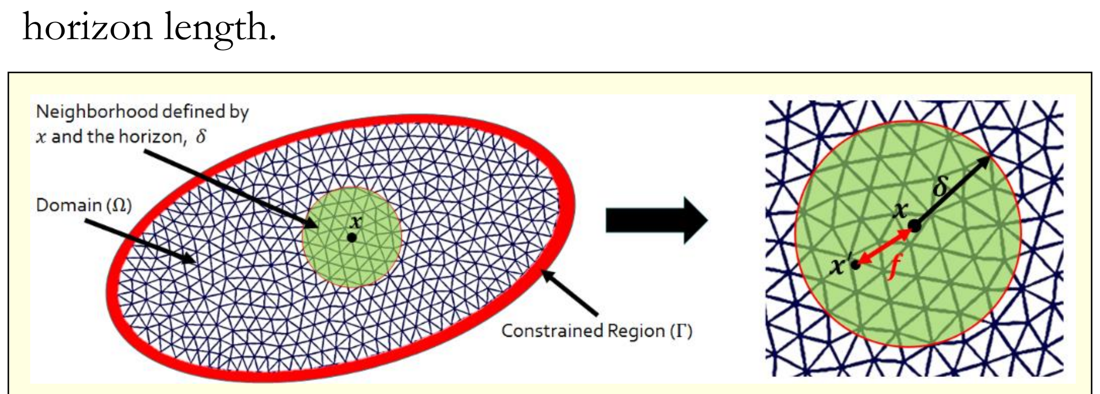


Figure 1. Nonlocal methods allow for more information to be factored into the computation of a solution at a given node, via the definition of the horizon.

Non-Local cont.

Under the assumption that γ and β represent the left and right hand sides of our domain respectively, we can define the domains as:

$$\begin{aligned} \Omega &= (\gamma,\beta), \\ \Omega' &= (\gamma-\delta,\beta+\delta) \\ \Gamma &= \Omega'\backslash\Omega = [\gamma-\delta,\gamma]\cup[\beta+\delta,\beta] \end{aligned} \quad [2]$$

where, Γ is known as the volume constraint and Ω contains the solution space.

Then by applying a Galerkin finite element approach, we can discretize the problem and define the solution as a linear combination of a set of basis functions and unknown vector. Additionally, if we account for the volume constraint, approximate the time derivative with backwards difference and modify the nonlocal term to remain stable in a quadrature routine, we get:

$$\begin{aligned} &\frac{a_1}{\Delta t}\sum^{\Omega} C_j^k \int_{\Omega}\phi_j(x)\phi_i(x)dx + \frac{a_2}{2\delta^2}\sum^{\Omega} C_j^k\int_{\Omega}\int_{x-\delta}^{x+\delta}\frac{\phi_j(x)-\phi_j(x')}{|x-x'|}(\phi_i(x)-\phi_i(x'))dx'dx \\ &= \int_{\Omega'} f(x,t)\phi_i(x)dx + \frac{a_1}{\Delta t}\sum^{\Omega} C_j^{k-1}\int_{\Omega}\phi_j(x)\phi_i(x)dx \\ &-\frac{a_2}{2\delta^2}\sum^{\Gamma} g(x,t)\int_{\Omega}\int_{x-\delta}^{x+\delta}\frac{\phi_j(x)-\phi_j(x')}{|x-x'|}(\phi_i(x)-\phi_i(x'))dx'dx \end{aligned} \quad [3]$$

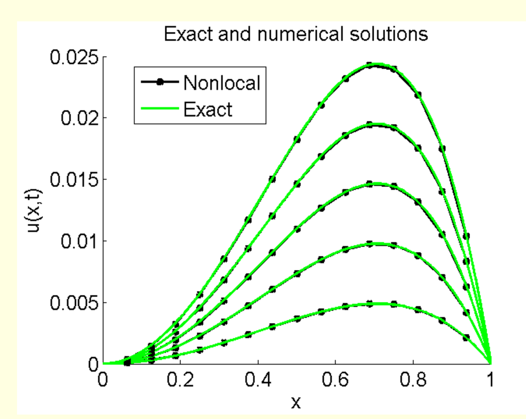


Figure 2. Solution to nonlocal problem at various time steps via method of manufactured solutions where: $u_{exact} = (x^2(1-x^2))\sin(t)$

Discontinuous problem

One stated goal of this research is to be able to effectively solve reduced order nonlocal problems with discontinuities in the solutions. Due to the fact that nonlocal methodologies do not have any spatial derivatives, they are ideal methods for finding solutions with discontinuities.

In order to accurately approximate solutions with discontinuities, we need to redefine our set of basis functions. Previously, we used continuous piecewise linear basis functions to solve the nonlocal problem. This approach would not work for a solution with a discontinuity, so we propose using discontinuous linear basis functions. One can define these basis functions as:

$$\phi_{2j}(x) = \begin{cases} \frac{x_j - x}{x_j - x_{j-1}}, & \text{for } x\in(x_{j-1},x_j) \\ 0, & \text{Everywhere else} \end{cases}$$

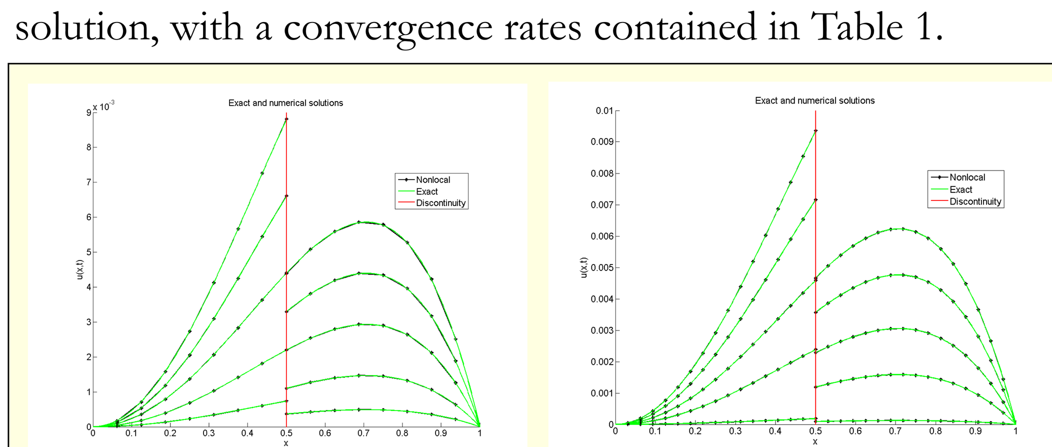
and,

$$\phi_{2j}(x) = \begin{cases} \frac{x_j - x}{x_j - x_{j-1}}, & \text{for } x\in(x_{j-1},x_j) \\ 0, & \text{Everywhere else} \end{cases}$$

By this definition of our basis functions, it is clear that the linear system size is going to double compared to the continuous piecewise linear case. This makes ROM all the more relevant. So if we solve a sample problem with our exact solution defined as:

$$u(x,t) = \begin{cases} tx^2(1-x^2), & \text{for } 0\le x<\frac{1}{2} \\ \frac{1}{2}tx^2(1-x^2), & \text{for } \frac{1}{2}<x\le 1 \end{cases}$$

Figures 3 and 4 depict the nonlocal approximation to this solution, with a convergence rates contained in Table 1.



Figures [3]-[4]. Nonlocal approximation of solution with discontinuity using discontinuous basis functions

h	Euclidean distance Error	Rate
0.25	6.348301e-004	
0.125	1.553428e-004	2.030915
0.0625	3.852442e-005	2.011610
0.03125	9.702576e-006	1.989334

Table [1]. Convergence rate for nonlocal approximation to solution with discontinuity

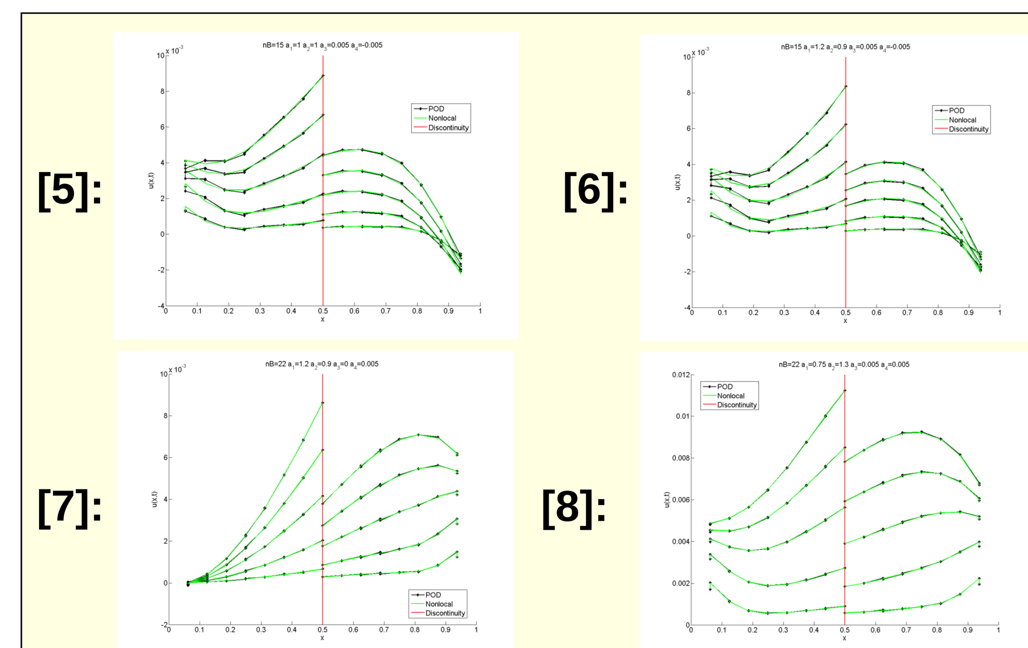
Reduced Order Modeling

Using the steps defined in the introduction to formulate our ROM, we are finally ready to reconstruct a reduced order solution. To start off, we will define our reduced order solution as a linear combination of a set of unknowns and the reduced basis functions which are in turn, a linear combination of the basis vector values and the nonlocal basis functions:

$$u_{ROM}(x,t_k) = \sum\sigma_j^k\Psi_j(x) \text{ where } \Psi_j(x) = \sum C_i^k\phi_i(x)$$

where σ^k is the set of unknown values that we will solve for and Ψ are the reduced basis functions themselves.

Although the concept of reconstructing the reduced order nonlocal problem is straightforward, there are a few minor complexities. One such complexity involves using a particular solution when we have inhomogeneous Dirichlet boundary conditions. By including a particular solution to control the ROM boundary conditions, we can add in parameters: a_1 and a_2 to bring our total parameter count to 4. For this work, we use a Latin Hypercube method to sample the four parameters for collecting a total of 250 snapshots.

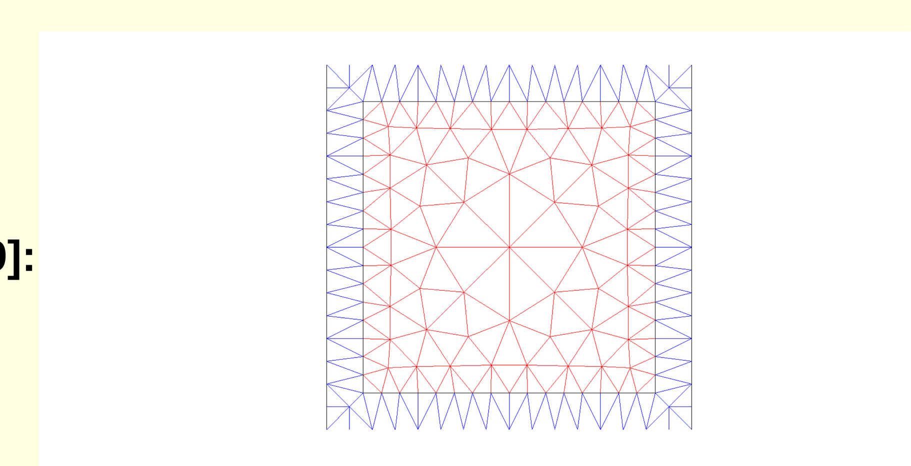


Figures [5],[6]: Sample ROM plots at 15 basis functions
Figures [7],[8]: Sample ROM plots at 22 basis functions
All: ROM plots at various parameter samples

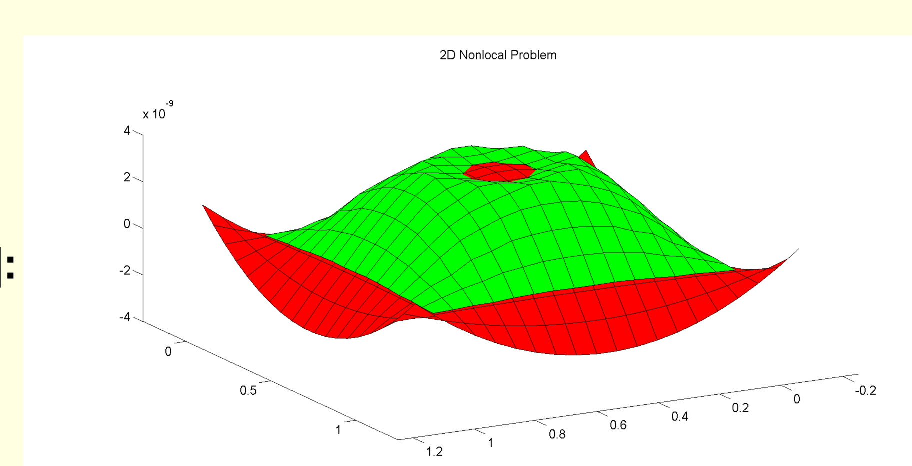
Preliminary 2D Results

One of the ultimate goals of this research is to apply ROM to a two-dimensional nonlocal problem with a discontinuity. Before applying ROM, we must first understand how the nonlocal problem in two dimensions works. For the anomalous diffusion case, the equations are effectively the same with some minor changes for the kernel function. Figures 9 and 10 shows an example unstructured triangular mesh created using the MATLAB Mesh2d package and a preliminary nonlocal result .

[9]:



[10]:



Bibliography and Acknowledgement

1. Xi Chen and Max Gunzburger. Continuous and discontinuous finite element methods for a peridynamics model of mechanics. *Computer Methods in Applied Mechanics and Engineering*, 200(9):1237–1250, 2011.
2. Stewart A Silling. Reformulation of elasticity theory for discontinuities and long-range forces. *Journal of the Mechanics and Physics of Solids*, 48(1):175-209, 2000.

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