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Localized Method Of Approximate Particular Solutions For Solving Optimal Control Problems Governed By PDES

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LOCALIZED METHOD OF APPROXIMATE PARTICULAR SOLUTIONS FOR
SOLVING OPTIMAL CONTROL PROBLEMS GOVERNED BY PDES

by

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A Thesis
Submitted to the Graduate School,
the College of Arts and Sciences
and the School of Mathematics and Natural Sciences
of The University of Southern Mississippi
in Partial Fulfillment of the Requirements
for the Degree of Masters of Science

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2019

ABSTRACT

In this thesis, the method of approximate particular solutions(MAPS) and localized method of approximate particular solutions(LMAPS) with polynomial basis, and radial basis functions are proposed and applied on the optimal control problems(OCPs) governed by partial differential equations(PDEs).

This study proceeds in several steps. First, polynomial basis and radial basis functions are used to globally approximate solutions for the PDEs which have been combined into a single matrix system numerically from the optimality conditions of the OCPs. Secondly, polynomial and radial basis functions are used to locally approximate particular solutions for the same matrix system numerically. We use these approaches to two types of problems, a smooth and singular problem. The first example numerically experiments on a square domain and the second example on an L-shaped disc domain. These approaches are tested and compared. The results show our proposed method for solving optimal control problems governed by partial differential equations works.

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LIST OF ABBREVIATIONS

| | | |
|--------------|---|------------------------------------------------------|
| RBF | - | Radial Basis Function |
| MQ | - | Multiquadrics |
| OCP | - | Optimal Control Problems |
| RMSE | - | Root Mean Square Error |
| IMQ | - | Inverse Multiquadrics |
| PDE | - | Partial Differential Equation |
| MAPS | - | Method of Approximate Particular Solutions |
| LMAPS | - | Localized Method of Approximate Particular Solutions |
| FEM | - | Finite Element Method |
| FDM | - | Finite Difference Method |

NOTATION AND GLOSSARY

General Usage and Terminology

The several notation used in this thesis represents fairly standard mathematical and computational usage. The methods used in this study have interdisciplinary applications, and in this particular study is being centered around partial differential equations. In several cases these fields tend to use different preferred notation to indicate the same idea. While it would be convenient to utilize a standard nomenclature for this important symbol, the many alternatives currently in the published literature will continue to be utilized.

These blackboard fonts are used to denote standard sets of numbers: \mathbb{R} for the field of real numbers. The capital letters, A, P, L, F, \dots are used to denote matrices in the global method. Boldface capital letter P represents polynomial space. Also, capital boldfaced greek letters, e.g., Θ, Ψ for matrices in the local method. Functions which are denoted in boldface type typically represent vector valued functions, and real valued functions usually are set in lower case roman letters e.g., f, g . Caligraphic letters \mathcal{L}, \mathcal{B} are used to denote partial differential operators. Again, lower case roman letters e.g., k, n, s, j are used to denote indices.

Vectors and matrices are typeset in square brackets, e.g., $[\cdot]$, and parenthesis, e.g., (\cdot) . In general the norms are typeset using double pairs of lines, e.g., $\|\cdot\|$.

Chapter 1

BACKGROUND

1.1 Introduction

The use of differential equation applications has become rampant in various fields in the world like engineering, biology, physics, computational mathematics, and economics. Due to this, it has become necessary to solve these differential equations analytically but most of these differential equations problems cannot be solved analytically. Therefore, it has become expedient to find other ways to solve these kinds of equations. Researchers found several methods of numerically solving these problems by approximating their solutions.

In this thesis, we focus is on optimal control problems governed by PDEs. Optimal control theory was developed by Lev Semenovic Pontryagin and his colleagues in the late 1950s, which generalizes the calculus of variations. This optimal control for finite dimensional problems is derived by using the Pontryagin's maximum principle which is governed by ordinary differential equations [10,14,16]. J. L. Lions developed the optimal control system theory governed by PDEs [10,13]. Pontryagin's maximum principles are used to help characterize an optimal control problem via an optimality system, which includes the state and adjoint system. When the optimal controls and its state variables are given, there are adjoint variables, which satisfy the system. With this concept, the source terms of the adjoint PDEs equal the partial derivatives of the integrand of the objective function with respect to the state variables [10,26]. For some decades now optimal control problems governed by partial differential equations have become an area of interest by researchers because of its application to real-world problems. Some of these applications include optimizing the cooling process of hot steel [8,12], pollutant control in a river [5,8] and magnetic drug targeting [6,8].

This chapter will introduce us to the optimal control problem in this study. This chapter will also discuss some of the works that have been done on this problem over the years and the aim of this study.

1.2 Optimal Control Problems

In this section, we discuss optimal control problems in detail but the kind of partial differential equation we will discuss in this research is the Poisson equation. Poisson equations are

elliptic partial differential equation problems and have the form

$$\Delta u = u_{xx} + u_{yy} = f(x, y). \quad (1.1)$$

In [11], the paper mentions two of the problems. These problems are the distributive control problem and boundary control problem. The distributive control problem means the controlling is being done in the domain. While the boundary control problem means the controlling is being done only on the boundary. This study focuses just on the distributed control problem. Optimizing a quantity with Poisson equation as a constraint, one can call it a Poisson control problem. This is one of the most commonly PDE-constrained optimization problems researched.

The problem we consider in this study is of the form

$$\min_{y, u} \frac{1}{2} \|y - \hat{y}\|_{L_2(\Omega)}^2 + \frac{\beta}{2} \|u\|_{L_2(\Omega)}^2 \quad (1.2)$$

such that

$$\begin{aligned} -\Delta y &= u, \quad \text{in } \Omega, \\ y &= f, \quad \text{on } \partial\Omega, \end{aligned}$$

for some penalty constant $\beta > 0$. β 's value is very important, so if it is small, then y being far away from \hat{y} is penalized heavily [11]. If β is large, it is very important u has small $L_2(\Omega)$. We define y to be the *state variable* and u to be the *control variable* in the entire domain(Ω) and \hat{y} is the optimality state. Ω is a two dimension bounded domain. y and u are continuous functions, $y \in H^1(\Omega)$ and $u \in L_2(\Omega)$ [11]. To solve this problem (1.2), there are two approaches, which are the discretize-then-optimize formulation and the optimize-then-discretize formulation of the distributed control problem in [11]. We use the optimize-then-discretize formulation idea in [11]. The importance of using this approach is to come up with a Lagrangian on the continuous space, get optimality conditions and discretize it finally. The Lagrangian $L = L(y, u, p_1, p_2)$ on the continuous space is

$$L = \frac{1}{2} \|y - \hat{y}\|_{L_2(\Omega)}^2 + \frac{\beta}{2} \|u\|_{L_2(\Omega)}^2 + \int_{\Omega} (-\Delta y - u) p_1 d\Omega + \int_{\partial\Omega} y p_2 ds, \quad (1.3)$$

where, p_1 represents continuous adjoint variable in the domain(Ω), p_2 represents the continuous adjoint variable on the boundary($\partial\Omega$). Take note that p in general denotes the continuous adjoint variable and also performs the same role as the Lagrange multipliers in section 3.1 of Pearson's paper [11,18].

The Lagrangian(1.3) is differentiated with respect to the continuous variables u, y and p . This results in getting the optimality conditions, which are, the **State equation**:

$$\begin{aligned} -\Delta y &= u, \text{ in } \Omega, \\ y &= f, \text{ on } \partial\Omega, \end{aligned} \tag{1.4}$$

the **Gradient equation**:

$$\begin{aligned} \beta u - p &= 0, \text{ in } \Omega, \\ u &= 0, \text{ on } \partial\Omega, \end{aligned} \tag{1.5}$$

the **Adjoint equation**:

$$\begin{aligned} -\Delta p &= \hat{y} - y, \text{ in } \Omega, \\ p &= 0, \text{ on } \partial\Omega. \end{aligned} \tag{1.6}$$

For a full understanding of this derivation of these conditions, one should refer to [11,18,23]. These optimality conditions are discretized in section 2.2 for the global method and section 3.2 for the local method to form a system of a matrix.

1.3 A Brief Literature Review

For some years now several methods have been used to solve optimal control problems due to its various applications in the aerodynamic, medical, biological, finance and engineering fields. Distributed control problems governed by PDEs are generally difficult to obtain their analytical solution [15]. Sometimes the exact solutions of these problems are not available, therefore, the applications of many traditional numerical procedures, for example, finite element method (FEM), finite difference method (FDM) are used to approximate their solutions. In [19], they transformed the control problem into a two boundary problem. They also, integrated the generalized orthogonal polynomials to get an operational matrix and then used Taylor series, lots of orthogonal polynomials to obtain the optimal control, by using only the cross-product Legendre vectors. Apel et. al [21], solves an optimal control problem for a two-dimensional elliptic equation with point wise control constraints and the domain used is assumed to be a polygon but non-convex. They treat the corner

singularities by prior mesh grading and the approximations of the solutions are constructed by a projection of the discrete adjoint state. They again prove that the approximations have a convergence order of h^2 . In [24], they solved a Dirichlet boundary control problem by using a Mixed finite element method. This paper [25] uses a convergent adaptive finite element method for elliptic Dirichlet boundary control problems. Pearson's article uses a radial basis function method to solve PDE-constrained problems (that is Poisson equations), he derives new collocation-type methods to solve distributed control problems that have Dirichlet boundary conditions and also extends it to Neumann boundary conditions problem. Again he proves the results pertaining to invertibility of the matrix he generates. These methods are implemented using MATLAB and produce numerical results to exhibit the capability of the method in his article [11]. For Darehmiraqi's paper, he presents a reproducing kernel Hilbert spaces method to get numerical solutions for the optimal control problem. He approximated the solution by truncating the series form of the analytical solution in the reproducing kernel space [15]. In this paper [25] uses a convergent adaptive finite element method for elliptic Dirichlet boundary control problems. This paper [7] proposes a nonconforming finite element method to solve an optimal control problem governed by the bilinear state equation. They approximate the state and adjoint equation by using a nonconforming EQ_1^{rot} element, and the control is approximated by orthogonal projection through the state and adjoint state. Superconvergence and super close properties are obtained by full use of the characters of this EQ_1^{rot} element and the consistency error is one order higher than its interpolation error. Guan et. al in [8], uses two meshless scheme for solving Dirichlet boundary optimal control problems governed by elliptic equations. They use a radial basis function collocation method for both state and adjoint state equations in the first scheme, and in the second scheme, they employ the method of fundamental solutions for the state equation when it has a zero source term, and radial basis function collocation method for the adjoint state equation.

1.4 Aim of this Study

This study will solve the optimal control problem (1.4) with Dirichlet boundary conditions on a square domain and L-shape disc domain by using global and localized method of approximate solutions with radial basis functions and polynomial basis. This study was motivated by Pearson's paper [11], who used Global Kansas Method with RBFs and also Compact Supported RBFs. Based on the method he used, I considered MAPS and LMAPS.

Chapter 2

GLOBAL METHOD OF APPROXIMATE PARTICULAR SOLUTIONS

There are several methods of numerically solving partial differential equations. One of the methods discussed in this chapter is the method of approximate particular solutions with the use of radial basis functions (RBFs) and polynomial basis. This is a meshless method used to solve the large size of partial differential equations in engineering and the sciences. Radial basis functions used in solving partial differential equations are simple and can be applied to various PDEs. It is effective in dealing with high dimensions problems with sophisticated geometries. Polynomial basis, on the other hand, can be used to approximate solutions to PDEs because sometimes it is not convenient to choose a shape parameter in RBF functions for finding a particular solution for a differential operator governing an equation.

In this chapter we will introduce MAPS for Poisson equation, MAPS solutions scheme for Optimal Control Problems and then talk about the numerical experiments.

2.1 Introduction of Method of Approximated Particular Solutions For Poisson Equation

This section, we will lay more emphasis on the basis and the method we are going to use to approximate the particular solution for a differential operator (\mathcal{L}). We define RBFs as: let \mathbb{R}^d with d being the dimensional Euclidean space. A function $h: \mathbb{R}^d \rightarrow \mathbb{R}$ is a radial when there exist a univariate function $\phi: [0, \infty) \rightarrow \mathbb{R}$ such that

$$h(x) = \phi(r),$$

where r is the Euclidean norm of x , that is $r = \|x\|$. The table below shows some commonly used RBFs.

Table 2.1: Commonly used RBF's.

| RBF's Names | Formulations |
|----------------------------|------------------------------------------------|
| linear | $\phi(r) = r$ |
| cubic | $\phi(r) = r^3$ |
| Gaussian | $\phi(r) = e^{-cr^2}, c > 0$ |
| Multiquadrics(MQ) | $\phi(r) = \sqrt{r^2c^2 + 1}, c > 0$ |
| Inverse Multiquadrics(IMQ) | $\phi(r) = \frac{1}{\sqrt{r^2c^2 + 1}}, c > 0$ |
| Thine-plate spline (TPD) | $\phi(r) = r^2 \ln(r)$ |

For MAPS, a solution, $\Phi(r)$, for a particular differential equation is to be known:

$$\mathcal{L}\Phi(r) = \phi(r).$$

Table 2.2 shows the closed forms of solutions used as basis functions to approximate solutions of the given PDE under study, and the RBF used is Multiquadrics(MQ). The positive constant c in Table 2.1 and Table 2.2 denotes the shape parameter of the RBF.

Table 2.2: The Particular Solution of MQ RBF for the Laplace operator in this study.

$$\Phi(r) = \frac{2c^2}{\sqrt{c^2r^2 + 1}} - \frac{c^4r^2}{(\sqrt{c^2r^2 + 1})^3}$$

The use of polynomial basis function as particular solutions for a differential operator equation is unstable as the degree of the polynomial is being increased. It is unstable because the resultant matrix becomes ill-conditioned due to how dense the matrix is. Therefore, polynomial basis functions for approximating our closed-form particular solutions are not good for a global approach unless there is a proper treatment of our matrix resulting from our formulation. There are several types of preconditioning treatments for the matrix but the one used in this thesis is called the multi-scale technique. It is used to reduce the condition number of the method of approximated particular solutions resultant matrix. For a standard polynomial basis for a 2D case, finding the particular solutions for a differential operator(\mathcal{L}) of an equation, we choose a sequence of polynomials

$$\mathbf{p}_n(x, y) = x^{i-j}y^j, \quad 0 \leq j \leq i, \quad 0 \leq i \leq k, \quad 1 \leq n \leq w, \quad \forall (x, y) \in \mathbb{R}^2.$$

This sequence forms a basis for the polynomial space \mathbf{P}_k^r , the set r-variate polynomials of degree $\leq k$, and $r = 2$. The dimension of the polynomial space \mathbf{P}_k^r is $w = \frac{(k+1)(k+2)}{2}$. From Thir Raj Dungal's dissertation in 2017[22], a simple example was used to find the particular solution. A conclusion was drawn that the procedure used for finding the particular solution can be extended to find the particular solution for the polynomial functions for any general differential operator.

Theorem 2.1.1. *Consider a general form second-order linear partial differential equation in two variables with constant coefficients:*

$$a_1 \frac{\partial^2 u_p}{\partial x^2} + a_2 \frac{\partial^2 u_p}{\partial x \partial y} + a_3 \frac{\partial^2 u_p}{\partial y^2} + a_4 \frac{\partial u_p}{\partial x} + a_5 \frac{\partial u_p}{\partial y} + a_6 u_p = x^m y^n, \quad (2.1)$$

where $\{a_i\}_{i=1}^6$ are real constants, $a_6 \neq 0$ and m and n are positive integers. Then the polynomial particular solution of (2.1) is given by

$$u_p = \frac{1}{a_6} \sum_{k=0}^N \left(\frac{-1}{a_6} \right)^k \mathcal{L}^k(x^m y^n), \quad (2.2)$$

where $N = m + n$ and

$$\mathcal{L} = a_1 \frac{\partial^2}{\partial x^2} + a_2 \frac{\partial^2}{\partial x \partial y} + a_3 \frac{\partial^2}{\partial y^2} + a_4 \frac{\partial}{\partial x} + a_5 \frac{\partial}{\partial y}.$$

The proof of this theorem can be again found in Thir Raj Dungal's dissertation in 2017[22].

Now that we done talking about ways of getting the particular solutions, we consider a PDE, which in this paper is a Poisson equation but we would like to use a general differential operator.

$$\mathcal{L}u(x) = f(x), \quad x \in \Omega, \quad (2.3)$$

$$u(x) = g(x), \quad x \in \partial\Omega. \quad (2.4)$$

We then use the two discussed particular solutions above to solve this problem by generalizing this particular solution to fit for both types of particular solution. The approximation \tilde{u} to the exact solution u in (2.3) and (2.4) is

$$u(x) \approx \tilde{u}(x) = \sum_{k=1}^N \alpha_k \Phi_k, \quad (2.5)$$

where Φ denotes the closed form solutions used as basis functions to approximate solutions of the given PDEs for RBF or polynomial basis i.e $\mathcal{L}\Phi(r) = \phi(r)$ and below is some notations we need to know.

- $\{x_k\}_1^N$ the set of all collocation points.
- $\{x_k\}_1^{N_i}$ the set of interior points.
- $\{x_k\}_{N_i+1}^{N_i+N_b}$ the set of boundary points.

and $N = N_i + N_b$. Next we substitute (2.5) into (2.3) and (2.4):

$$\mathcal{L}\tilde{u}(x) = \sum_{k=1}^N \alpha_k \mathcal{L}\Phi_k = f(x), \quad x \in \Omega, \quad (2.6)$$

$$\tilde{u}(x) = \sum_{k=1}^N \alpha_k \Phi_k = g(x), \quad x \in \partial\Omega. \quad (2.7)$$

Then linear system (2.6) and (2.7) is discretized on collocation points to form a system of matrices with a coefficient α :

$$A\alpha = C, \quad (2.8)$$

where $\alpha = [\alpha_1, \alpha_2 \cdots \alpha_N]^T$, and the matrix A and C denotes

$$A = \begin{pmatrix} L_{N_i \times N} \\ B_{N_b \times N} \end{pmatrix}_{N \times N}, \quad C = \begin{pmatrix} F_{N_i \times 1} \\ G_{N_b \times 1} \end{pmatrix}_{N \times 1},$$

where L, B, F and G are defined as

$$L = \mathcal{L}\Phi = \phi, \quad B = \Phi, \quad F = f(x_k), \quad G = g(x_k).$$

2.2 Method of Approximated Particular Solutions Scheme for Optimal Control Problems

In this section, we use MAPS scheme for solving the optimality conditions which is the systems in (1.4), (1.5) and (1.6), to which we use RBFs and Polynomial basis to approximate solutions to both Poisson equations for the state(1.4) and adjoint equations(1.6). We let X be a set of collocation point on the boundary and in the domain, such that $\{x_i\}_1^{N_i}$ and $\{x_i\}_1^{N_b}$ represents the set of interior and boundary collocation points respectively. The entire set of collocation points which is $\{x_i\}_1^N$ with $N := N_i + N_b$ is used to approximate the exact solution. We seek to use RBF and Polynomial basis:

$$\tilde{y} = \sum_{j=1}^N \alpha_j \Phi_j, \quad \tilde{p} = \sum_{j=1}^N \tau_j \Phi_j, \quad (2.9)$$

where Φ , is a known solution for a chosen radial basis function or a polynomial basis function, α_j and τ_j are unknown coefficients of either the RBF or polynomial basis functions. So discretizing the **adjoint equation**(1.6), we have

$$-\sum_{j=1}^N \tau_j \nabla^2 \Phi_j + \sum_{j=1}^N \alpha_j \Phi_j = \hat{y}, \text{ in } \Omega, \quad (2.10)$$

$$\sum_{j=1}^N \tau_j \Phi_j = 0, \text{ on } \partial\Omega. \quad (2.11)$$

We then move on to discretize the **state equation**(1.4) and we have

$$-\sum_{j=1}^N \alpha_j \nabla^2 \Phi_j - \frac{1}{\beta} \sum_{j=1}^N \tau_j \Phi_j = 0, \text{ in } \Omega, \quad (2.12)$$

$$\sum_{j=1}^N \alpha_j \Phi_j = f, \text{ on } \partial\Omega. \quad (2.13)$$

The above systems define a linear system with unknown variables α and τ . For simplicity, we can write it into a matrix form:

$$A \begin{bmatrix} \tau \\ \alpha \end{bmatrix} = F, \quad (2.14)$$

where

$\tau = [\tau_1, \tau_2 \cdots \tau_N]^T$, $\alpha = [\alpha_1, \alpha_2 \cdots \alpha_N]^T$, and the matrix A and F denotes

$$A = \begin{bmatrix} \begin{bmatrix} -L \\ P_b \end{bmatrix}_{(N_i+N_b) \times N} & \begin{bmatrix} P_i \\ 0 \end{bmatrix}_{(N_i+N_b) \times N} \\ \begin{bmatrix} -\frac{P_i}{\beta} \\ 0 \end{bmatrix}_{(N_i+N_b) \times N} & \begin{bmatrix} -L \\ P_b \end{bmatrix}_{(N_i+N_b) \times N} \end{bmatrix}, F = \begin{bmatrix} \hat{y}_{N_i \times 1} \\ 0_{N_b \times 1} \\ 0_{N_i \times 1} \\ f_{N_b \times 1} \end{bmatrix},$$

where L, P_i, P_b, \hat{y} and f are defined as follows:

$$L = [\Delta \Phi = \phi]_{N_i \times N},$$

$$P_i = [\Phi]_{N_i \times N}, P_b = [\Phi]_{N_b \times N},$$

$$\hat{y} = [\hat{y}(x_i)]_{N_i \times 1}, f = [f(x_i)]_{N_b \times 1}.$$

2.3 Numerical experiments

We consider two numerical examples in this section. The meshfree scheme in section 2.2 is applied to the examples and we consider both multiquadric(MQ) RBF $\phi(x) = \sqrt{r^2 + c^2}$, c and polynomial basis in the numerical experiments. The LOOCV technique used in getting a good shape parameter in this thesis is a borrowed idea from [3,4,9]. To measure errors and convergence rates of the method use in this paper, we compute the root mean square error (RMSE) between the numerical state \tilde{y} and exact solution y , numerical control \tilde{u} and exact solution u and also the numerical adjoint \tilde{p} and exact solution p , if known at all collocation points, that is,

$$E_y = \sqrt{\frac{1}{N} \sum_{j=1}^N (\tilde{y}(x_j) - y(x_j))^2} ,$$

$$E_p = \sqrt{\frac{1}{N} \sum_{j=1}^N (\tilde{p}(x_j) - p(x_j))^2} ,$$

$$E_u = \sqrt{\frac{1}{N} \sum_{j=1}^N (\tilde{u}(x_j) - u(x_j))^2} .$$

Figure 2.1 and Figure 2.2 shows the two domains of the two examples we will be dealing with in this study.

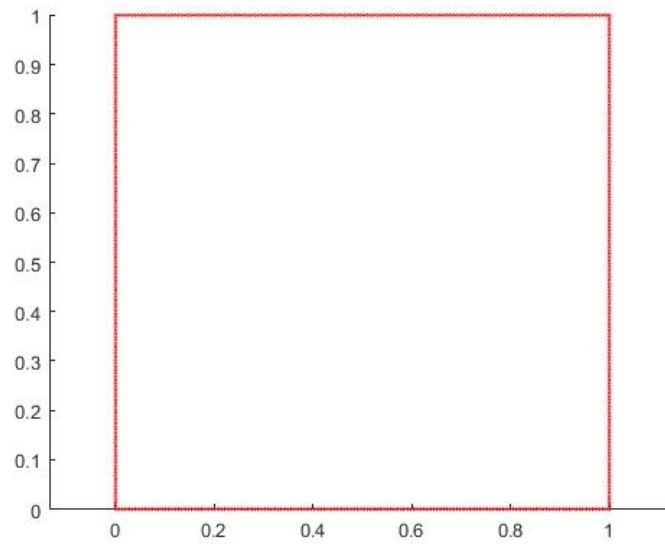


Figure 2.1: Square Domain

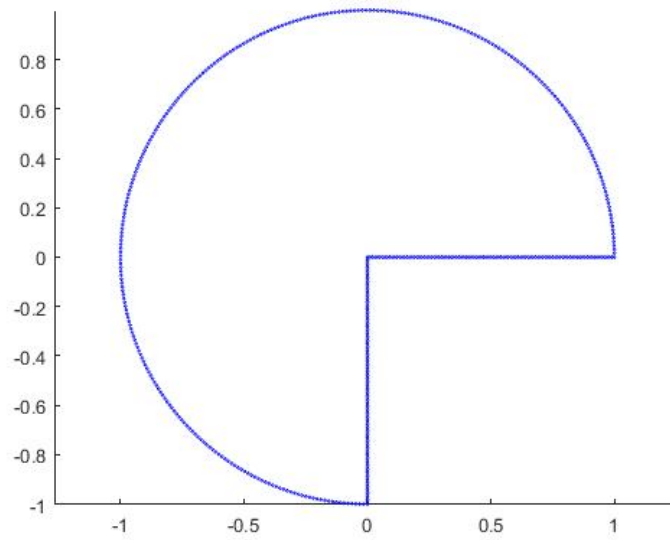


Figure 2.2: L-shaped Disc Domain

Example 1: This is a distributive Poisson control problem

$$\min_{y,u} \frac{1}{2} \|y - \hat{y}\|_{L_2(\Omega)}^2 + \frac{\beta}{2} \|u\|_{L_2(\Omega)}^2,$$

such that

$$\begin{aligned} -\nabla^2 y &= u, \quad x \in \Omega, \\ y &= f, \quad x \in \partial\Omega, \end{aligned}$$

where $\Omega = [0, 1]^2$, $\beta = 1$, and

$$\begin{aligned} \hat{y} &= \sin(\pi x_1) \sin(\pi x_2), \quad x \in \Omega, \\ f &= 0. \end{aligned}$$

This particular problem results in continuous optimality conditions with the following exact solution:

$$y = \frac{1}{1 + 4\beta\pi^4} \sin(\pi x_1) \sin(\pi x_2), \quad u = \frac{2\pi^2}{1 + 4\beta\pi^4} \sin(\pi x_1) \sin(\pi x_2).$$

In this example, the numerical solutions are computed on the number of collocation points $N = 16, 64, 256, 1024$ and the figure below shows 16×16 square domain grid that the numerical solution was computed on.

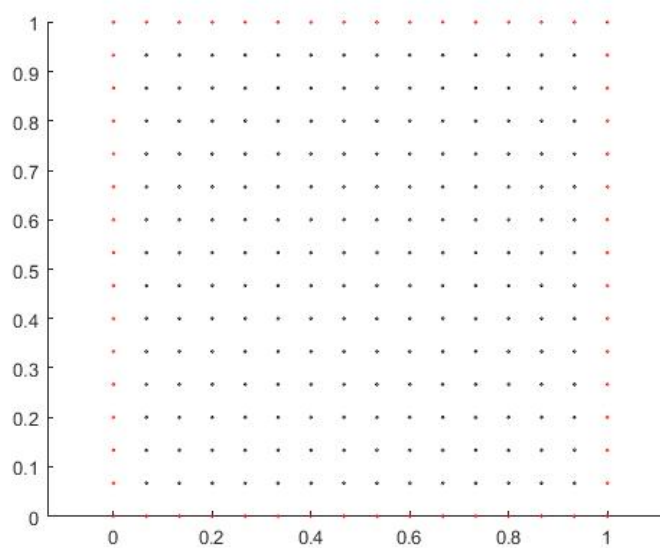


Figure 2.3: 16×16 square domain

The numerical results in Table 2.3 and 2.4 exhibits the errors of RBF and Polynomial basis of order 15 respectively. These solutions show a high order of convergence due to the

smoothness of the analytical solutions. Polynomial basis of order 10 and 12 was also used in this study, but order 15 showed the fastest convergence to the true solution and that is why it was selected. From figure(2.4), we realize that the errors of MAPS using a polynomial basis for the E_y converges faster than MAPS using RBFs even though at $N = 1024$ the error becomes smaller slightly. For E_u , using a polynomial basis of order 15 converges very faster than RBFs. Therefore, we recommend the MAPS with a polynomial basis for problems like this. Also, using the LOOCV technique our shape parameter was selected from the interval $[0,2]$.

Table 2.3: Root Mean Square Errors of \tilde{y} and \tilde{u} for using RBFs.

| | Multiquadric RBF | | c |
|------|------------------|--------------|----------|
| N | E_y | E_u | $[0, 2]$ |
| 16 | 5.579757e-02 | 1.684177e-01 | 0.0050 |
| 64 | 6.386032e-07 | 6.504844e-06 | 0.4934 |
| 256 | 3.565571e-09 | 2.903432e-08 | 0.9894 |
| 1024 | 4.343409e-08 | 1.076788e-07 | 1.5217 |

Table 2.4: Root Mean Square Errors of \tilde{y} and \tilde{u} for using Polynomial Basis.

| | Polynomial basis | | Polynomial order=15 |
|------|------------------|--------------|---------------------|
| N | E_y | E_u | |
| 16 | 4.781535e-04 | 5.267579e-03 | |
| 64 | 9.843530e-07 | 1.784064e-05 | |
| 256 | 1.258398e-09 | 1.701334e-08 | |
| 1024 | 1.853949e-08 | 8.291085e-08 | |

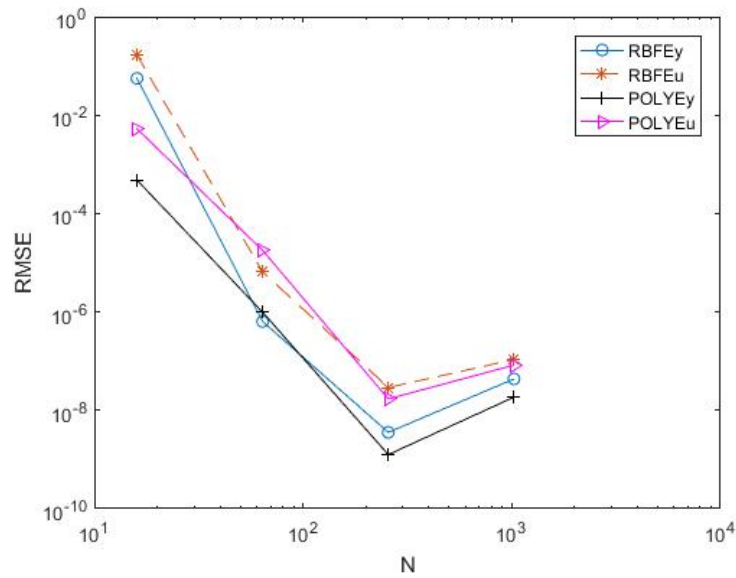


Figure 2.4: RMSE errors of \tilde{y} and \tilde{u} of MAPS with both RBFs and Polynomial basis.

Example 2: We consider the OCP with the following optimality conditions:

$$\begin{aligned} -\Delta y + y &= u + f, \quad x \in \Omega, \\ y &= 0, \quad x \in \partial\Omega, \end{aligned}$$

$$\begin{aligned} -\Delta p + p &= y - y_d, \quad x \in \Omega, \\ p &= 0, \quad x \in \partial\Omega, \end{aligned}$$

$$u = \left(-\frac{1}{v}p \right), \quad x \in \Omega,$$

with homogeneous Dirichlet boundary conditions for y and p . The data $f = \mathcal{L}\tilde{y} - \tilde{u}$ and $y_d = \tilde{y} - \mathcal{L}\tilde{p}$ are chosen such that the functions

$$\begin{aligned} \tilde{y}(r, \varphi) &= (r^\lambda - r^\alpha) \sin \lambda \varphi, \\ \tilde{p}(r, \varphi) &= v(r^\lambda - r^\beta) \sin \lambda \varphi, \end{aligned}$$

with $\lambda = \frac{2}{3}$ and $\alpha = \beta = \frac{5}{2}$ solve the optimal control problem exactly. Note that these functions have the typical singularity near the corner. The control \tilde{u} is defined above where $v = 1$.

In this example 2, the numerical solutions are computed on a L-shaped disc and the number of collocation points for calculating the numerical solution are $N = 64, 229, 859, 1889$.

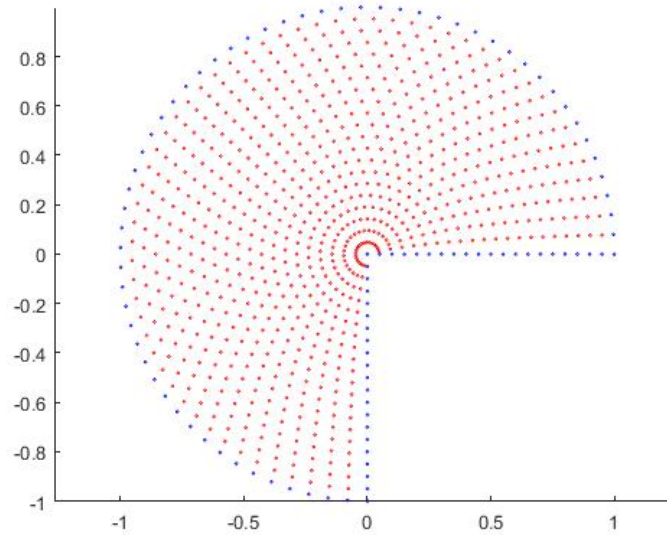


Figure 2.5: 860 collocation points on a L-shape disc domain

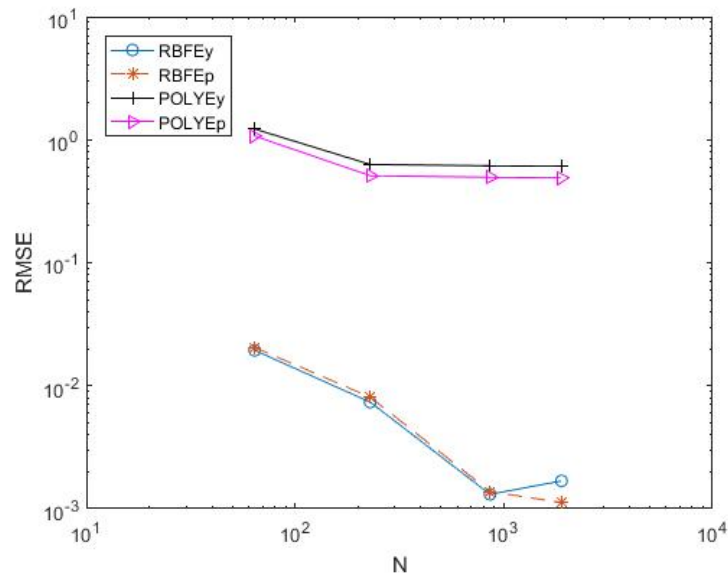
The numerical results in Table 2.5 and 2.6 show the errors of RBF and Polynomial basis of order 15 respectively. Again, polynomial order 15 was chosen because polynomial order 10 and 12 did not give good errors. We notice that using MAPS with multiquadric RBF on this problem, it converges faster to the exact solution than using MAPS with polynomial basis, which converges very slow for both E_y and E_p . This observation happens as N is being increased. Therefore, further research in MAPS with RBFs or polynomial basis for OCPs governed by PDEs with singularities should be considered in the future. For this problem our shape parameter was selected from the interval $[1,10]$ using the LOOCV technique.

Table 2.5: Root Mean Square Errors of \tilde{y} and \tilde{p} for using RBFs.

| | Multiquadric RBF | | c |
|------|------------------|--------------|---------|
| N | E_y | E_p | [1, 10] |
| 64 | 1.939667e-02 | 2.049829e-02 | 1.2107 |
| 229 | 7.356244e-03 | 8.082736e-03 | 2.0779 |
| 859 | 1.309311e-03 | 1.379941e-03 | 4.1193 |
| 1889 | 1.683642e-03 | 1.121649e-03 | 5.4946 |

Table 2.6: Root Mean Square Errors of \tilde{y} and \tilde{p} for using Polynomial Basis.

| | Polynomial basis | | Polynomial order=15 |
|------|------------------|--------------|---------------------|
| N | E_y | E_p | |
| 64 | 1.222977e+00 | 1.071309e+00 | |
| 229 | 6.291747e-01 | 5.100166e-01 | |
| 859 | 6.138518e-01 | 4.949926e-01 | |
| 1889 | 6.072540e-01 | 4.894141e-01 | |

Figure 2.6: RMSE errors of \tilde{y} and \tilde{p} of MAPS with both RBFs and Polynomial basis.

Chapter 3

LOCALIZED METHOD OF APPROXIMATE PARTICULAR SOLUTIONS

In this chapter, we will be discussing how to generate the numerical scheme for the OCP using LMAPS. In MAPS, RBFs and polynomial basis are used to get the closed form solution. These solutions are used as a basis function for an approximated solution to the PDE being treated. The MAPS is very effective and simple but in approximations, it makes use of all the collocation points in the domain which makes it unstable. This happens due to how dense the matrices become. This results in it being increasingly ill-conditioned. When this happens it makes it more complicated to use MAPS to solve large scale problems. There are several methods to prevent this difficulty but we will concentrate on the localized formulations.

The localized formulations reduce the ill-conditioning of the coefficient matrix resulted from dense and large matrices. In local RBFs, MQ or IMQ's shape parameter slightly affects the numerical results. When it comes to accuracy MQ is considered as one of the best RBFs. Another advantage of the localized formulations is that it is computationally efficient. This does not affect the accuracy of the methods. Our main emphasis is on when a localized formulation is applied to MAPS which makes it a localized method of approximate particular solutions. LMAPS uses the same procedure as finding the approximations for MAPS, but it does not use all the collocation points, instead, a local domain is found for each collocation point. There are n nearest neighbors at that point in the local domain. This local domain is used to approximate the solution at each point and this turns the dense matrix in MAPS into sparse in LMAPS.

In this study, we will introduce LMAPS for Poisson equations, discuss the LMAPS scheme for OCPs and discuss the numerical results.

3.1 Introduction of Local Method of Approximated Particular Solutions For Poisson Equation

We will be dealing with poisson equations as the PDE but we will generalize it to cover other PDEs by using the differential operator \mathcal{L} . We take a look at this PDE

$$\mathcal{L}u(x) = f(x), \quad x \in \Omega, \quad (3.1)$$

$$\mathcal{B}u(x) = g(x), \quad x \in \partial\Omega. \quad (3.2)$$

$\{x_i\}_1^N$ is the set of collocation points and the interior points are denoted by $\{x\}_1^{N_i}$. Also, $\{x\}_{N_i+1}^N$ represents the collocation points on the boundary. Where, N here is the summation of $N_i + N_b$. We will like to use Yao's notation in her dissertation[27] for showing a local domain for a collocation point x_s as $x_k^{[s]}$, where $k = 1, 2, \dots, n$ and n is number of nearest neighbors around x_s . So all the $x_k^{[s]}$ with the same s value depict being part of the same local domain Ω_s for x_s , with k being the particular nearest neighbor. Also, we have to bare in mind that the local domains of different collocation points can overlap other local domains.

In the local domain Ω_s of an interior point x_s , with $s = 1, 2, \dots, N_i$ and the function values in u in (3.1) and (3.2) can be approximated by a generalized equation for local RBFs or Polynomial basis:

$$u(x_s) \approx \tilde{u}(x_s) = \sum_{k=1}^n \alpha_k^{[s]} \Phi_k^{[s]}. \quad (3.3)$$

Applying the collocation method within Ω_s , this gives us a linear system below,

$$\begin{bmatrix} \tilde{u}(x_1^{[s]}) \\ \tilde{u}(x_2^{[s]}) \\ \vdots \\ \tilde{u}(x_n^{[s]}) \end{bmatrix} = \begin{bmatrix} \Phi_{11} & \Phi_{12} & \dots & \Phi_{1n} \\ \Phi_{21} & \Phi_{22} & \dots & \Phi_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ \Phi_{n1} & \Phi_{n2} & \dots & \Phi_{nm} \end{bmatrix} \begin{bmatrix} \alpha_1^{[s]} \\ \alpha_2^{[s]} \\ \vdots \\ \alpha_n^{[s]} \end{bmatrix}. \quad (3.4)$$

Φ here represents the solution for a differential operator for a given RBF($\phi(r)$) (i.e $\mathcal{L}\Phi = \phi$) or Polynomial basis. We can re-write (3.4) as,

$$U^{[s]} = P_{nm} \alpha^{[s]},$$

where

$$U^{[s]} = [\tilde{u}(x_1^{[s]}), \tilde{u}(x_2^{[s]}) \dots \tilde{u}(x_n^{[s]})]^T, \quad P_{nn} = [\Phi_{ij}], \quad \alpha^{[s]} = [\alpha_1^{[s]}, \alpha_2^{[s]} \dots \alpha_n^{[s]}]^T.$$

Note that P_{nn} is non-singular and realize,

$$\alpha^{[s]} = P_{nn}^{-1} U^{[s]}. \quad (3.5)$$

Now, we apply the differential operators \mathcal{L} and \mathcal{B} on both (3.1) and (3.2) respectively.

$$\begin{aligned} \mathcal{L}\tilde{u}(x_s) &= \sum_{k=1}^n \mathcal{L}\alpha_k^{[s]}\Phi_k^{[s]} \\ &= \mathcal{L}\Phi^{[s]}P_{nn}^{-1}U^{[s]} \\ &= \Psi^{[s]}U^{[s]}, \end{aligned}$$

where

$$\Psi^{[s]} = \mathcal{L}\Phi^{[s]}P_{nn}^{-1}.$$

We have to know that $\Psi(x_s)$ consist of all $\Psi^{[s]}$ obtained by stuffing this local vector with zeros. Also, the differential operator affects just $\Phi^{[s]}$ and this is part of the vector $\Psi^{[s]}$. Therefore, we have

$$\mathcal{L}\tilde{u}(x_s) = \Psi(x_s)U = f(x_s), \quad 1 \leq s \leq N_i, \quad (3.6)$$

This same procedure is applied on (3.2)

$$\begin{aligned} \mathcal{B}\tilde{u}(x_s) &= \sum_{k=1}^n \mathcal{B}\alpha_k^{[s]}\Phi_k^{[s]} \\ &= \mathcal{B}\Phi^{[s]}P_{nn}^{-1}U^{[s]} \\ &= \Theta^{[s]}U^{[s]}, \end{aligned}$$

where

$$\Theta^{[s]} = \mathcal{B}\Phi^{[s]}P_{nn}^{-1}.$$

Again, we have to know that $\Theta(x_s)$ consist of all $\Theta^{[s]}$ obtained by stuffing this local vector with zeros and also the differential operator(\mathcal{B}) affects just $\Phi^{[s]}$ and this is part of the vector $\Theta^{[s]}$. Therefore we get

$$\mathcal{B}\tilde{u}(x_s) = \Theta(x_s)U = g(x_s), \quad N_i + 1 \leq s \leq N. \quad (3.7)$$

Adding (3.6) and (3.7) we form a sparse system of equations

$$\begin{bmatrix} \Psi(x_1) \\ \Psi(x_2) \\ \vdots \\ \Psi(x_{N_i}) \\ \Theta(x_{N_i+1}) \\ \vdots \\ \Theta(x_N) \end{bmatrix} = \begin{bmatrix} U(x_1) \\ U(x_2) \\ \vdots \\ U(x_{N_i}) \\ U(x_{N_i+1}) \\ \vdots \\ U(x_N) \end{bmatrix} = \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{N_i}) \\ g(x_{N_i+1}) \\ \vdots \\ g(x_N) \end{bmatrix}. \quad (3.8)$$

So solving this sparse of system of equation, getting the approximations of u , we use all the given nodes ($\tilde{u}(x_s)$), with $s = 1, 2, 3 \dots N$.

3.2 Localized Method of Approximate Particular Solutions Scheme for Optimal Control Problems

In this section, we show the numerical scheme of the optimality conditions of the optimal control problems. Both RBFs and Polynomial basis are used to approximate the solutions of the optimality conditions which comprises the state(1.4) and adjoint Poisson equations(1.6). For the purpose of this study, we generalize the numerical scheme to fit for RBFs and Polynomial basis. Local particular solutions are defined as follows:

$$\tilde{y}(x_s) = \sum_{j=1}^n \alpha_j^{[s]} \Phi_j, \quad \tilde{p}(x_s) = \sum_{j=1}^n \tau_j^{[s]} \Phi_j, \quad (3.9)$$

where Φ denotes the solution for the Poisson equation for a radial basis function($\phi(r)$) or a polynomial basis function. So discretizing the **adjoint equation**(1.6), we have

$$-\sum_{j=1}^n \tau_j \Delta \Phi_j + \sum_{j=1}^n \alpha_j \Phi_j = \hat{y}, \quad \text{in } \Omega_s, \quad (3.10)$$

$$\tilde{p}(x_k) = p(x_i), \quad (3.11)$$

for any x_i on the boundary $\partial\Omega$. Then we discretize the state equation(1.4) as well

$$-\sum_{j=1}^n \alpha_j \Delta \Phi_j - \frac{1}{\beta} \sum_{j=1}^n \tau_j \Phi_j = 0, \text{ in } \Omega_s, \quad (3.12)$$

$$\tilde{y}(x_k) = y(x_i), \quad (3.13)$$

for any x_i on the boundary $\partial\Omega$. From the above equation, we derive a matrix system for State equation(1.4)

$$\begin{bmatrix} -A_{N_i \times N} \\ I_{N_b \times N} \end{bmatrix} \begin{bmatrix} \tilde{y}_{N \times 1} \\ \tilde{p}_{N \times 1} \end{bmatrix} - \begin{bmatrix} \frac{1}{\beta} I_{N_i \times N} \\ 0_{N_b \times N} \end{bmatrix} \begin{bmatrix} \tilde{p}_{N \times 1} \\ \tilde{y}_{N \times 1} \end{bmatrix} = \begin{bmatrix} 0_{N_i \times 1} \\ f_{N_b \times 1} \end{bmatrix}. \quad (3.14)$$

Also we derive a matrix system for Adjoint equation(1.6)

$$\begin{bmatrix} -A_{N_i \times N} \\ I_{N_b \times N} \end{bmatrix} \begin{bmatrix} \tilde{p}_{N \times 1} \\ \tilde{y}_{N \times 1} \end{bmatrix} + \begin{bmatrix} I_{N_i \times N} \\ 0_{N_b \times N} \end{bmatrix} \begin{bmatrix} \hat{y}_{N_i \times 1} \\ 0_{N_b \times 1} \end{bmatrix} = \begin{bmatrix} \hat{y}_{N_i \times 1} \\ 0_{N_b \times 1} \end{bmatrix}. \quad (3.15)$$

We then add (3.14) and (3.15) to get a general matrix system

$$\begin{bmatrix} \begin{bmatrix} I_{N_i \times N} \\ 0_{N_b \times N} \end{bmatrix}_{(N_i+N_b) \times 2N} & \begin{bmatrix} -A_{N_i \times N} \\ I_{N_b \times N} \end{bmatrix}_{(N_i+N_b) \times 2N} \\ \begin{bmatrix} -A_{N_i \times N} \\ I_{N_b \times N} \end{bmatrix}_{(N_i+N_b) \times 2N} & \begin{bmatrix} -\frac{1}{\beta} I_{N_i \times N} \\ 0_{N_b \times N} \end{bmatrix}_{(N_i+N_b) \times 2N} \end{bmatrix} \begin{bmatrix} \tilde{y}_{N \times 1} \\ \tilde{p}_{N \times 1} \end{bmatrix} = \begin{bmatrix} \hat{y}_{N_i \times 1} \\ 0_{N_b \times 1} \\ 0_{N_i \times 1} \\ f_{N_b \times 1} \end{bmatrix}, \quad (3.16)$$

where

$$P = [\Phi^{[s]}]_{nn}, \quad A = [\Delta \hat{\Phi}^{[s]} P_{nn}^{-1} = \phi P_{nn}^{-1}],$$

$$I = \text{identity matrix},$$

$$\hat{y} = [\hat{y}(x_s)], \quad f = [f(x_s)].$$

3.3 Numerical experiments

This LMAPS scheme is applied to two examples. We consider both multiquadric(MQ) RBF $\phi(x) = \sqrt{r^2 + c^2}$, $c > 0$ and polynomial basis in the numerical experiments. The LOOCV technique used in getting a good shape parameter in this thesis is a borrowed idea from [3,4,9]. To measure errors and convergence rates of the method used in this paper, we compute the root mean square error (RMSE) between the numerical state \tilde{y} and exact solution y , numerical control \tilde{u} and exact solution u and also the numerical adjoint \tilde{p} and

exact solution p , if known at all collocation points, that is,

$$E_y = \sqrt{\frac{1}{N} \sum_{j=1}^N (\tilde{y}(x_j) - y(x_j))^2} ,$$

$$E_u = \sqrt{\frac{1}{N} \sum_{j=1}^N (\tilde{u}(x_j) - u(x_j))^2} ,$$

$$E_p = \sqrt{\frac{1}{N} \sum_{j=1}^N (\tilde{p}(x_j) - p(x_j))^2} .$$

The domains in figure 2.1 and 2.2 are considered in this chapter.

Example 1: This is a distributed Poisson control problem

$$\min_{y,u} \frac{1}{2} \|y - \hat{y}\|_{L_2(\Omega)}^2 + \frac{\beta}{2} \|u\|_{L_2(\Omega)}^2 ,$$

such that

$$\begin{aligned} -\nabla^2 y &= u, \quad x \in \Omega, \\ y &= f, \quad x \in \partial\Omega, \end{aligned}$$

where $\Omega = [0, 1]^2$, $\beta = 1$, and

$$\begin{aligned} \hat{y} &= \sin(\pi x_1) \sin(\pi x_2), \quad x \in \Omega, \\ f &= 0. \end{aligned}$$

This particular problem results in continuous optimality conditions with the following exact solution:

$$y = \frac{1}{1 + 4\beta\pi^4} \sin(\pi x_1) \sin(\pi x_2), \quad u = \frac{2\pi^2}{1 + 4\beta\pi^4} \sin(\pi x_1) \sin(\pi x_2).$$

In this example 1, the numerical solutions are computed on the number of collocation points $N = 16, 64, 256, 1024$ and figure 2.3 is a square domain grid that the numerical solution was computed on.

The numerical results in Table 3.1 and 3.2 exhibit the errors of RBF and Polynomial basis of order 2 solutions show a high order of convergence due to the smoothness of the analytical solutions. Polynomial basis of order 3 and 4 was used but the convergence of the error was slow, so order 2 was preferred in this study. From figure 3.1, we observe LMAPS with polynomial basis and RBFs for E_y converges to the true solution steadily and fast as N increases, even though the error at $N = 16384$ for polynomial basis is bigger than that of RBF. On the other hand, for E_u , LMAPS with a polynomial basis converges faster than LMAPS with RBF as N increases. Also, note that the number of neighborhoods selected for each point is 9 for LMAPS with RBF and 6 for LMAPS with polynomial basis. The shape parameter(c) is selected in the interval $[0,5]$ and used for all collocation points and not just for a collocation point selected and its local neighborhood is created.

Table 3.1: Root Mean Square Errors of \tilde{y} and \tilde{u} for using RBFs.

| N | Multiquadric RBF | | c |
|-------|------------------|--------------|----------|
| | E_y | E_u | $[0, 5]$ |
| 256 | 7.012635e-06 | 6.912346e-05 | 0.297717 |
| 1024 | 1.311229e-06 | 1.291132e-05 | 0.618581 |
| 4096 | 2.861201e-07 | 2.816801e-06 | 1.254435 |
| 16384 | 2.072601e-07 | 2.040249e-06 | 2.755456 |

Table 3.2: Root Mean Square Errors of \tilde{y} and \tilde{u} for using Polynomial Basis.

| N | Polynomial basis | | Polynomial order=2 |
|-------|------------------|--------------|--------------------|
| | E_y | E_u | |
| 256 | 1.004045e-05 | 9.865928e-05 | |
| 1024 | 2.260251e-06 | 2.224096e-05 | |
| 4096 | 5.377729e-07 | 5.293433e-06 | |
| 16384 | 1.312450e-07 | 1.291978e-06 | |

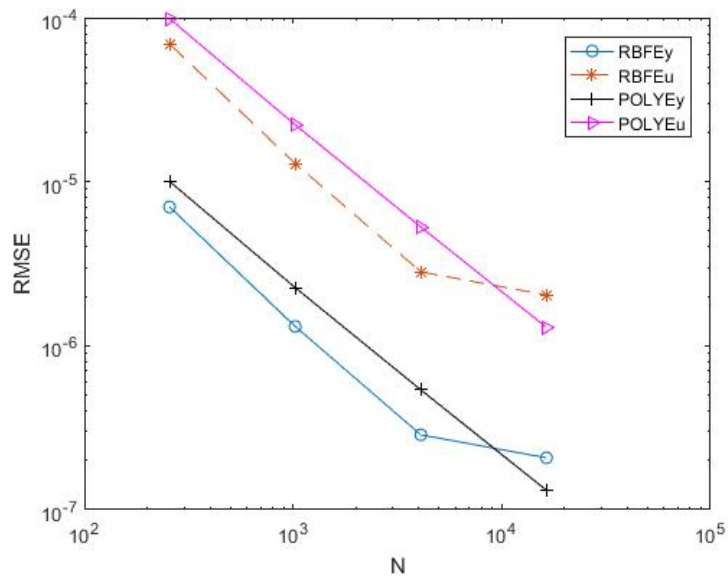


Figure 3.1: RMSE errors of \tilde{y} and \tilde{u} of LMAPS with both RBFs and Polynomial basis.

Example 2: We consider the OCP with the following optimality conditions:

$$-\Delta y + y = u + f, \quad x \in \Omega,$$

$$y = 0, \quad x \in \partial\Omega,$$

$$-\Delta p + p = y - y_d, \quad x \in \Omega,$$

$$p = 0, \quad x \in \partial\Omega,$$

$$u = \left(-\frac{1}{v}p \right), x \in \Omega,$$

with homogeneous Dirichlet boundary conditions for y and p . The data $f = \mathcal{L}\tilde{y} - \tilde{u}$ and $y_d = \tilde{y} - \mathcal{L}\tilde{p}$ are chosen such that the functions

$$\tilde{y}(r, \varphi) = (r^\lambda - r^\alpha) \sin \lambda \varphi,$$

$$\tilde{p}(r, \varphi) = v(r^\lambda - r^\beta) \sin \lambda \varphi,$$

with $\lambda = \frac{2}{3}$ and $\alpha = \beta = \frac{5}{2}$ solve the optimal control problem exactly. Note that these functions have the typical singularity near the corner. The control \tilde{u} is defined above where $v = 1$.

In this example, the numerical solutions are computed on a L-shaped disc (figure 2.5) and the number of collocation points for calculating the numerical solution are $N = 859, 1889, 3319, 5149$.

The numerical results in Table 3.3 and 3.4 display the errors of the multiquadric RBF and Polynomial basis of order 2. Again, the polynomial basis of order 3 and 4 was used but the errors given was not as good as order 2. The number of neighborhoods selected around each collocation point is 9 for LMAPS with RBF and 6 for LMAPS with polynomial basis. Considering this example the errors for LMAPS with RBFs depicts a fast convergence to the analytical solution as compared to LMAPS with polynomial basis as N becomes large. The shape parameter (c) is selected in the interval $[3, 10]$ and used for all collocation points and not just for a collocation point selected and its local neighborhood is created.

Table 3.3: Root Mean Square Errors \tilde{y} and \tilde{p} for using RBFs.

| N | Multiquadric RBF | | c |
|------|------------------|--------------|-----------|
| | E_y | E_p | $[3, 10]$ |
| 859 | 2.909685e-02 | 3.700834e-02 | 3.000615 |
| 1889 | 4.249532e-03 | 5.392278e-03 | 3.000468 |
| 3319 | 7.745670e-03 | 1.069875e-02 | 3.000583 |
| 5149 | 4.587839e-03 | 5.280697e-03 | 3.000583 |

Table 3.4: Root Mean Square Errors \tilde{y} and \tilde{p} for using Polynomial Basis.

| N | Polynomial basis | | Polynomial order=2 |
|------|------------------|--------------|--------------------|
| | E_y | E_p | |
| 859 | 7.263737e-01 | 6.099878e-01 | |
| 1889 | 5.783176e-01 | 4.731535e-01 | |
| 3319 | 4.994133e-01 | 6.651886e-01 | |
| 5149 | 5.585314e-01 | 4.653635e-01 | |

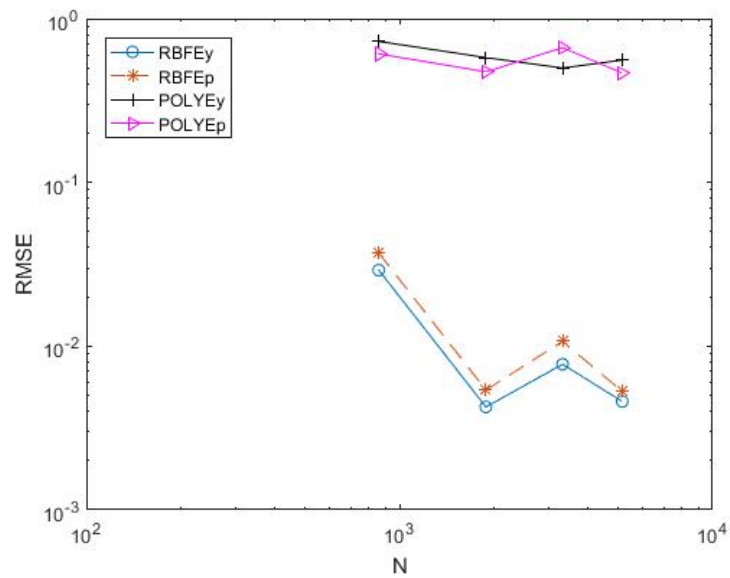


Figure 3.2: RMSE errors of \tilde{y} and \tilde{p} of LMAPS with both RBFs and Polynomial basis.

Chapter 4

CONCLUSIONS AND REMARKS

In this study we introduced MAPS and LMAPS for solving OCPs. On the basis of the numerical results obtained from chapter 2 and chapter 3 examples, we have come to the following conclusions and remarks:

- This is the first time MAPS and LMAPS is used to solve OCPs governed by PDEs.
- From the numerical results, we found that MAPS and LMAPS using RBFs works for OCPs governed by PDEs.
- It was also found that MAPS with polynomial basis and RBFs also works for smooth problems.
- From the study, it was also observed that further study is needed on LMAPS and MAPS using polynomial basis to solve OCPs governed by PDEs with singularities.
- In the future, I will consider the following:
 - Solving OCPs with other boundary conditions since we considered just Dirichlet boundary in this study.
 - Higher orders of differential equations.
 - The choice of the shape parameter.

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