FUNCTION SPACE NONLINEAR RESCALING METHODS FOR ELLIPTIC CONTROL PROBLEMS WITH POINT-WISE STATE AND CONTROL CONSTRAINTS

by

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A Dissertation
Submitted to the
Graduate Faculty
of
George Mason University
in Partial Fulfillment of
The Requirements for the Degree
of
Doctor of Philosophy
Computational Sciences and Informatics

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Acknowledgments

I would like to thank the following people, who are in truth a subset of those who assisted me in this process:

- My wife, Angela: Thank you for the love, encouragement, and support you provided, particularly during those first few years of late nights attending classes, doing homework, and beginning work on the research.
- My parents, Robert and Donna: Thank you for everything you did for us growing up. You helped lay the foundation for my drive to continue my education.
- Dr. Griva: Thank you for the guidance and help provided in developing this work.
- Drs. Yang, Camelli, and Seshaiyer: Thank you for serving on my committee and for your helpful comments.
- My colleagues: Thanks goes out to the many of you who have assisted in the process, by providing general support, putting up with me leaving early for classes on a regular basis, discussing the research, and for finding the topic of state constrained problems.

This work was supported by the Naval Surface Warfare Center, Dahlgren Division In-House Laboratory Independent Research Program.

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Abstract

FUNCTION SPACE NONLINEAR RESCALING METHODS FOR ELLIPTIC CONTROL PROBLEMS WITH POINT-WISE STATE AND CONTROL CONSTRAINTS

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State inequality constraints in PDE Constrained Optimization (PDECO) arise in many areas of science and engineering. Unfortunately these constraints, and the resulting Lagrange multipliers, are known to negatively influence the behavior of many existing optimization methods. In this work Nonlinear Rescaling based methods are used for the state and control constraints. In particular, a Nonlinear Rescaling-Primal Dual Augmented Lagrangian method is analyzed and proven to have linear convergence for state and control constrained problems. In addition, a Primal Dual Nonlinear Rescaling Augmented Lagrangian method is analyzed for control constraints and shown to have superlinear convergence properties. In each of the derived methods the Finite Element Method will be used to construct and solve the discretized version of the inner iteration.

Chapter 1: Introduction

The field of optimization for problems with Partial Differential Equation (PDE) constraints has been an active area of research for many decades, which has been documented within works by Lions [26], Biegler et.al. [9], and Hinze et.al. [23] and the references contained within. The difficulty of these PDE Constrained Optimization (PDECO) problems arises from two primary sources.

One of these sources of difficulty lies with the PDE constraint itself. The level of difficulty involved depends on a number of factors, including the specific PDE(s) being solved and the domain on which they are solved. Decades of research have gone into developing methods for solving just the PDE systems themselves, focusing on things such as the discretization methods, nonlinear solver techniques, and efficient preconditioners for the resulting linear systems and their respective solvers. The resulting size of these linear systems has also been increasing. Discretized PDEs with millions of degrees of freedom are now common, and problems with billions of degrees of freedom are now also being solved.

The second source of difficulty in solving PDECO problems is in reality a result of two factors. One factor is that even under a relatively simple, linear PDE constraint the resulting optimality condition system of equations which must be solved may be nonlinear, and therefore PDECO problems with the simple PDE constraint become nonlinear optimization problems. The other factor is related to the size of the optimization problem, which relates back to the size of the discretized PDE system itself. An example demonstrating this issue could be a simple optimal control problem governed by an elliptic PDE, where the control is distributed throughout the domain. If the problem's state variable, control variable, and the Lagrange multiplier associated with the PDE constraint are discretized in the same method then there can be an equal number of discretized degrees of freedom for all three variables. Furthermore, for each point-wise inequality imposed on the PDECO an additional Lagrange multiplier would be added. Therefore a PDECO problem with point-wise inequality constraints both the state and control leads to 5 times the number of discretized degrees of freedom than just the PDE alone. One additional detail is that efficient solvers may exist for finding the solution to the discretized PDE, and linear systems that may arise from the optimization problem are often more complex, requiring different preconditioning and solution strategies.

PDECO problems which contain point-wise inequality constraints on the state variables pose additional problems. These constraints cause their associated Lagrange multipliers to be highly irregular [12, 13, 7] which cause problems both in the theoretical convergence of the method as well as with implementations of the method. The irregularity and the issues which ensue will be discussed in Chapter 2.

Many methods for solving state constrained problems have been proposed and investigated over the last few decades. Standard optimization methods such as Sequential Quadratic Programming (SQP) [10], Augmented Lagrangian [5, 24], and Interior Point [4, 39, 38] have been applied to state constrained problems. Among the more recent methods over the last 10-15 years for solving state constrained optimization problems have focused on the use of Semi-Smooth versions of Newton's Method and Moreau-Yosida regularization of the state constraint [4, 6, 21, 22, 14].

As an alternative to these, the work described here uses is based on Nonlinear Rescaling. The Nonlinear Rescaling (NR) principal was introduced by Polyak [30] in the early 1990's as a method for handling inequality constraints for finite dimensional optimization. NR methods, unlike classical barrier methods, do not require the barrier parameter to approach infinity to guarantee convergence, which is the cause of ill-conditioning of the Hessian in most other barrier methods such as the Interior Point method. Goldfarb, et.al. [16] modified the NR based methods to include equality constraints through the augmented Lagrangian (AL). These Nonlinear Rescaling Augmented Lagrangian (NRAL) methods are the basis for the methods examined here, and these methods will be introduced in Chapter 3.

All previous work in NR-based methods has been done in the $\mathbb{R}^n$ space, whereas the target application space of this research is in the solution of PDECO problems, which are infinite dimensional in nature. It is possible to recast these infinite dimensional problems as finite dimensional problems in $\mathbb{R}^n$, which can often then be solved using existing, well established nonlinear optimization methods.

But there are a number of disadvantages to this technique, primarily related to the fact that one is solving an approximation to the problem instead of the problem itself. Specific optimality conditions, interpretation of norms and their meaning from one iteration to the next, and the solution itself is dependent on the discretization of the problem. This dependence is both on the discretization method (finite difference, finite element, etc.) and the specific triangularization of the domain of interest. Changing the discretization, either by method or resolution of the triangularization, results is modified optimality conditions.

This is an important point given that many modern discretization methods, in particular the Finite Element Method, can employ adaptive meshing capability to both reduce the time required to solve the problem and potentially increase the fidelity of the solution. In the case where a discretized optimization problem is solved using a method that employs adaptive meshing one must take extra care in using previous solution information. But in an infinite dimensional method solution information remains valid from one mesh to the next, provided the mesh is sufficiently resolved.

Each method presented and analyzed in this document is done so in its infinite dimensional form. Within the implementation of the example problem one does, at some point need to discretize a system of equations, since in general these systems of equations do not have analytical solutions. In the implementations described here the only system of equations discretized are the linearized operators solved within the inner most iteration. The Finite Element Method [35] is chosen as the discretization and solution methods for solving the infinite dimensional systems.

Chapter 2: Elliptic Optimization with State- and Control-Constraints

2.1 Problem Statement and Notation

The general optimization problem examined here is a stationary optimal control problem with an elliptic PDE constraint, with independent inequality constraints on the state and control variables. Optimization problems with elliptic constraints are very frequently analyzed throughout optimization and control research, for two primary reasons. Many physical, mathematical, and financial phenomena are governed by elliptic constraints, and therefore optimization problems do often arise with these PDE constraints. Elliptic constraints are also more amenable for analysis due to the well behaved and well studied qualities of the elliptic PDE.

Let $J(u, q)$ be the functional being minimized, where u is the state variable and q is the control variable of the problem. Let Ω be a convex, bounded domain in $\mathbb{R}^n$ for $n = 1, 2, 3$. The state variable is in the Sobolev space $\mathcal{W} = H^2(\Omega) \cap H_0^1(\Omega)$, where $H_0^1(\Omega)$ is defined as a H^1 space over Ω such that $u = 0$ on $\partial\Omega$ (the boundary of Ω) for all $u \in H^1(\Omega)$.

Define A to be a second-order uniformly elliptic operator of the form

$$A(\cdot) = \sum_{i,j=1}^{n} \frac{\partial}{\partial x_i} \left(a_{ij}(x) \frac{\partial}{\partial x_j} (\cdot) \right) \tag{2.1}$$

where there exists some constant θ such that

$$\sum_{i,j=1}^{n} a_{ij}(x)\xi_i\xi_j \geq \theta|\xi|^2 \tag{2.2}$$

for all $\xi \in \mathbb{R}^n$ and $x \in \Omega$. Additionally, the coefficients a_{ij} of A are defined to be bounded and continuously differentiable. Finally, define the operators $(\cdot,\cdot)_L^2(\Omega)$ and $\|\cdot\|_L^2(\Omega)$ are the L^2 inner product and norm, respectively, over the domain Ω. The more general form of $(\cdot,\cdot)$ and $\|\cdot\|$ will imply these operators over Ω unless a different space is specified.

$$\begin{aligned}
&\text{minimize } J(u,q) = \frac{1}{2}\|u - u_d\|^2 + \frac{\alpha}{2}\|q\|^2 \\
&\text{subject to } Au = q \text{ in } \Omega \\
&\eta_u \geq u \geq \eta_l \text{ a.e. in } \Omega \\
&\beta_u \geq q \geq \beta_l \text{ a.e. in } \Omega
\end{aligned} \tag{2.3}$$

where $u \in \mathcal{W}$, and $A : \mathcal{W} \to L^2(\Omega)$, and $q, u_d, \eta_u, \eta_l, \beta_u$and β_l are all in $L^2(\Omega)$. Note that while there are no boundary conditions directly specified in the problem statement, placing $u \in \mathcal{W}$ includes the requirement that $u = 0$ on $\partial\Omega$.

Problem (2.3) is assumed to satisfy strict complementarity. Furthermore, the strong convexity of $\mathcal{J}(u,q)$ allows one to assume that the second order optimality conditions are satisfied.

The regions P_η and P_β will be defined to be the passive regions $P_\eta = \{x \in \Omega \mid \eta_u > u > \eta_l\}$ and $P_\beta = \{x \in \Omega \mid \beta_u > q > \beta_l\}$, respectively. Similarly, $A_{i\eta}$ and $A_{i\beta}$ are the active regions $A_{i\eta} = \{x \in \Omega \mid u = \eta_i\}$ and $A_{i\beta} = \{x \in \Omega \mid q = \beta_i\}$, for $i = \{u, l\}$ respectively.

2.2 Optimality Conditions

The first order optimality conditions of problems similar to Problem 2.3 have been considered in a number of texts [12, 6, 7] . The following analysis follows the material presented by Bergounioux and Kunisch [7], but generalized to include bounds on the control, modifying the state constraint to be include both an upper and lower bound, and replacing the Laplacian in the PDE constraint with a more generic elliptic operator.

Theorem 2.2.1. *Let $A : \mathcal{W} \to L^2$ be an elliptic operator and Ω be a convex domain in $\mathbb{R}^n$, $n = 1, 2, 3$. The variables $(u^*, q^*) \in \mathcal{W} \times L^2$ is the solution to Problem* (2.3) *if* *and only if there exists a* $\lambda^* \in L^2$, $\sigma_u^*, \sigma_l^* \in \mathcal{C}^*$, *and* $\chi_u^*, \chi_l^* \in L^2$ *such that*

$$(\lambda^*, Au) + \langle \sigma_u^*, u\rangle_{\mathcal{C}^*,\mathcal{C}} - \langle \sigma_l^*, u\rangle_{\mathcal{C}^*,\mathcal{C}} + (u^* - u_d, u) = 0 \;\; \forall u \in \mathcal{C} \text{ such that } \eta_u \geq u \geq \eta_l \tag{2.4a}$$

$$A(u^*) = q^* \tag{2.4b}$$

$$\alpha q^* + \chi_u^* - \chi_l^* - \lambda^* = 0 \tag{2.4c}$$

$$\langle \sigma_u^*, u - u^*\rangle_{\mathcal{C}^*,\mathcal{C}} \leq 0 \;\; \forall u \in \mathcal{C} \text{ such that } u \leq \eta_u \tag{2.4d}$$

$$u^* \leq \eta_u \tag{2.4e}$$

$$\langle \sigma_l^*, u^* - u\rangle_{\mathcal{C}^*,\mathcal{C}} \leq 0 \;\; \forall u \in \mathcal{C} \text{ such that } u \geq \eta_l \tag{2.4f}$$

$$u^* \geq \eta_l \tag{2.4g}$$

$$\chi_u^* \geq 0, \; q^* \leq \beta_u, \; (\chi_u^*, \beta_u - q^*) \geq 0 \tag{2.4h}$$

$$\chi_l^* \geq 0, \; q^* \geq \beta_l, \; (\chi_l^*, q^* - \beta_l) \geq 0 \tag{2.4i}$$

Proof. In order to derive the optimality conditions for (2.3) some additional notation is required. Define $\mathcal{T} : L^2 \to \mathcal{C}$ as the operator that maps a function $q \in L^2$ to $u(q) \in \mathcal{W}$, which is the solution to the state equation $Au = q$. Additionally define the sets K_{us}, K_{ls}, K_{uc}, and K_{lc} as

$$K_{us} = \{u \in \mathcal{W} \subset \mathcal{C}(\Omega) \mid u \leq \eta_u\} \tag{2.5a}$$

$$K_{ls} = \{u \in \mathcal{W} \subset \mathcal{C}(\Omega) \mid u \geq \eta_l\} \tag{2.5b}$$

$$K_{uc} = \left\{q \in L^2 \subset \mathcal{C}(\Omega) \mid q \leq \beta_u\right\} \tag{2.5c}$$

$$K_{lc} = \left\{q \in L^2 \subset \mathcal{C}(\Omega) \mid q \geq \beta_l\right\} \tag{2.5d}$$

and define indicator functions over these sets.

$$I_U = \begin{cases} 0 \text{ for } u \in K_U \\ +\infty \text{ for } u \notin K_U \end{cases} \tag{2.6}$$

for $U = us, ls, uc,$ and lc.

Using the convexity of these indicator functions, and the functional being minimized, the standard properties of subdifferential calculus [37] imply that (u^*, q^*) will be the solution to Problem (2.3) if and only if

$$0 \in \partial\left(\frac{1}{2}\|\mathcal{T}q^* - u_d\|^2 + \frac{\alpha}{2}\|q^*\|^2 + I_{us}(\mathcal{T}q^*) + I_{ls}(\mathcal{T}q^*) + I_{uc}(q^*) + I_{lc}(q^*)\right) \tag{2.7}$$

Convexity of the operator (2.7) implies that the following statement is equivalent.

$$\begin{aligned} 0 \in \partial\left(\frac{1}{2}\|\mathcal{T}q^* - u_d\|^2 + \frac{\alpha}{2}\|q^*\|^2\right) &+ \mathcal{T}^\dagger\partial\left(I_{us}(\mathcal{T}q^*)\right) + \mathcal{T}^\dagger\partial\left(I_{ls}(\mathcal{T}q^*)\right) \\ &+ \partial\left(I_{uc}(q^*)\right) + \partial\left(I_{lc}(q^*)\right) \end{aligned} \tag{2.8}$$

Define σ_u^*, σ_l^*, χ_u^* and χ_l^* to be the elements within indicator functions I_{us}, I_{ls}, I_{uc}, and I_{lc}.

$$\sigma_u^* \in \partial I_{us}(\mathcal{T} q^*) \tag{2.9a}$$

$$\sigma_l^* \in \partial I_{ls}(\mathcal{T} q^*) \tag{2.9b}$$

$$\chi_u^* \in \partial I_{uc}(q^*) \tag{2.9c}$$

$$\chi_l^* \in \partial I_{lc}(q^*) \tag{2.9d}$$

Using (2.9a), (2.9b), (2.9c) and (2.9d) we see that (2.8) is equivalent to

$$0 \in \partial\left(\frac{1}{2}\|\mathcal{T} q^* - u_d\|^2 + \frac{\alpha}{2}\|q^*\|^2\right) + \mathcal{T}^\dagger \sigma_u^* + \mathcal{T}^\dagger \sigma_l^* + \chi_u^* + \chi_l^*. \tag{2.10}$$

This equation may be expressed as

$$0 =(\mathcal{T} q^* - u_d, \mathcal{T} q - \mathcal{T} q^*) + \alpha(q^*, q - q^*) + (\mathcal{T}^\dagger \sigma_u^*, q - q^*) - (\mathcal{T}^\dagger \sigma_l^*, q - q^*) \tag{2.11}$$

$$+ (\chi^*, q - q^*) - (\chi^*, q - q^*) \tag{2.12}$$

$$=(\mathcal{T}^\dagger(\mathcal{T} q^* - u_d) + \mathcal{T}^\dagger \sigma_u^* - \mathcal{T}^\dagger \sigma_l^* + \alpha q^* + \chi_u^* - \chi_l^*, q - q^*) \tag{2.13}$$

$$=(-\lambda^* + \alpha q^* + \chi_u^* - \chi_l^*, q - q^*) \tag{2.14}$$

for all $q \in \mathcal{C}$, and where

$$\lambda^* = -\mathcal{T}^\dagger(\mathcal{T} q^* - u_d) - \mathcal{T}^\dagger \sigma_u^* + \mathcal{T}^\dagger \sigma_l^*. \tag{2.15}$$

Equation (2.15) can be analyzed in its weak form, by multiplying through by a $q \in L^2$.

$$\begin{aligned} 0 &= (\lambda^*, q) + \langle \mathcal{T}^\dagger \mathcal{T} q^* - u_d), q\rangle + \langle \mathcal{T}^\dagger \sigma_u^*, q\rangle - \langle \mathcal{T}^\dagger \sigma_l^*, q\rangle \\ &= (\lambda^*, q) + \langle \mathcal{T} q^* - u_d), \mathcal{T} q\rangle + \langle \sigma_u^*, \mathcal{T} q\rangle - \langle \sigma_l^*, \mathcal{T} q\rangle \end{aligned} \tag{2.16}$$

The definition of $\mathcal{T}$ then provides the following result.

$$(\lambda^*, Au) + \langle \sigma_u^*, u\rangle_{\mathcal{C}^*,\mathcal{C}} - \langle \sigma_l^*, u\rangle_{\mathcal{C}^*,\mathcal{C}} + (u^* - u_d, u) = 0 \ \ \forall u \in \mathcal{C}, \eta_u \geq u \geq \eta_l \tag{2.17}$$

and

$$A(u) = q \tag{2.18}$$

which satisfies (2.4a) and (2.4b). Equation (2.14) is true for all q, and therefore can be simplified as

$$\alpha q^* + \chi_u^* - \chi_l^* - \lambda^* = 0 \tag{2.19}$$

which satisfies (2.4c).

The remaining optimality conditions to be proven require additional analysis of (2.9a), (2.9b), (2.9c), and (2.9d), which require understanding the definition of an element in a subdifferential. First define $f : \mathcal{U} \to \mathbb{R}$ be a convex function, and let x be in $\mathcal{U}$. Let ϕ be in the dual space $\mathcal{U}^*$. Element ϕ is defined to be a subgradient of f at x if

$$f(y) - f(x) \geq \langle \phi, y - x\rangle_{\mathcal{U}^*,\mathcal{U}} \quad \forall y \in \mathcal{U} \tag{2.20}$$

The subdifferential $\partial f(x)$ is the set of all subgradients of f at x. Using this and the definition of $\mathcal{T}$ we know that (2.9a) is equivalent the following inequality, which holds for all $u^* \in K_{us}$.

$$I_{us}(u) - I_{us}(u^*) \geq \langle \sigma_u^*, u - u^* \rangle_{\mathcal{C}^*,\mathcal{C}} \quad \forall u \in K_{us} \tag{2.21}$$

Since both u and u^* must be in K_{us} we have that $I_{us}(u) = 0$ and $I_{us}(u^*)$=0, and therefore we arrive at

$$u^* \in K_{us} \text{ and } \langle \sigma_u^*, u - u^* \rangle_{\mathcal{C}^*,\mathcal{C}} \leq 0 \quad \forall u \in K_{us}. \tag{2.22}$$

which is equivalent to (2.4d). A similar analysis may be used to show that (2.9b), (2.9c), and (2.9d) are equivalent to

$$u^* \in K_{ls} \text{ and } \langle \sigma_u^*, u^* - u \rangle_{\mathcal{C}^*,\mathcal{C}} \leq 0 \quad \forall u \in K_{ls} \tag{2.23a}$$

$$q^* \in K_{uc} \text{ and } \langle \chi_u^*, q - q^* \rangle_{\mathcal{C}^*,\mathcal{C}} \leq 0 \quad \forall q \in K_{uc} \tag{2.23b}$$

$$q^* \in K_{lc} \text{ and } \langle \chi_l^*, q^* - q \rangle_{\mathcal{C}^*,\mathcal{C}} \leq 0 \quad \forall q \in K_{lc} \tag{2.23c}$$

The Lagrange multipliers associated with control constraints are in $L^2(\Omega)$ [26]. Therefore q, q^*, χ_u^* and χ_l^* are in L^2 and

$$\langle \chi_u^*, q - q^* \rangle_{\mathcal{C}^*,\mathcal{C}} = (\chi_u^*, q - q^*)_{L^2} \leq 0 \quad \forall q \in L^2 \tag{2.24}$$

and similarly

$$\langle \chi_l^*, q^* - q \rangle_{\mathcal{C}^*,\mathcal{C}} = (\chi_l^*, q^* - q)_{L^2} \leq 0 \quad \forall q \in L^2. \tag{2.25}$$

Additional information may be derived for χ^* by examining it in regions Ω_{A_β} and Ω_{P_β}. Within Ω_{A_β} we know $\beta = q^*$, and by selecting any $q < \beta$ we see that $(\chi^*, q -$

$q^*)_{L^2(\Omega_{A_\beta})} \leq 0$ will be true if and only if $\chi^* > 0$. Similarly, within Ω_{P_β}, we know that $\beta > q^*$. By selecting $q = \beta$ we see that $(\chi^*, q - q^*)_{L^2(\Omega_{A_\beta})} \leq 0$ implies $\chi^* \leq 0$. By selecting any $q \leq \beta$ such that $q < q^*$ we see that $(\chi^*, q - q^*)_{L^2(\Omega_{A_\beta})} \leq 0$ implies $\chi^* \geq 0$. Thus for any $q \in L^2(\Omega_{K_\eta})$ we have that $\chi^* = 0$. Thus at the solution (u^*, q^*) we have

$$\chi^* \geq 0,\ \beta \geq q^*,\ (\chi^*, \beta - q^*) \geq 0 \tag{2.26}$$

which is the same as (2.4f), completing the proof. □

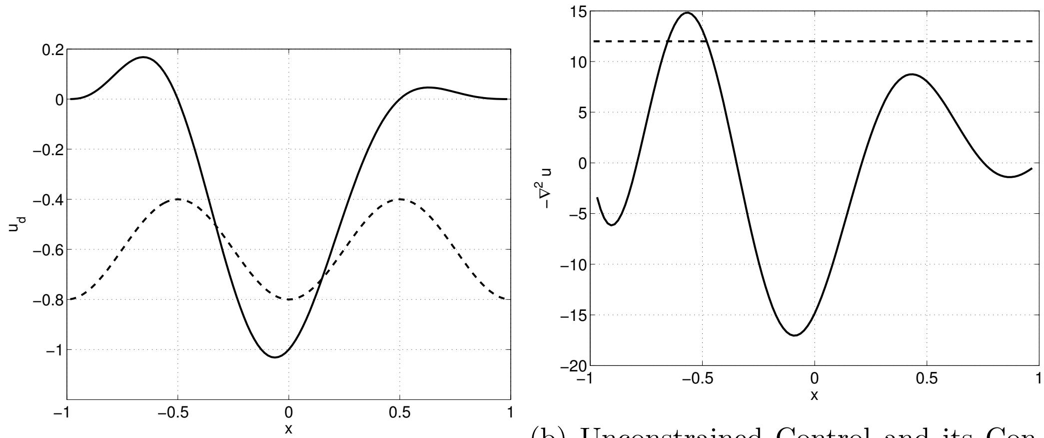
2.3 Example State Constrained Problem

Irregularity of the Lagrange multipliers associated with can easily be shown with the following 1D state constrained problem.

$$\begin{aligned}
\text{minimize } J(u,q) &= \frac{1}{2}\|u - u_d\|^2 + \frac{\alpha}{2}\|q\|^2 \\
\text{subject to } &-\nabla^2 u = q \text{ in } \Omega \\
&u(-1) = u(1) = 0 \\
&u \geq -\frac{3 + \cos(2\pi x)}{5} \text{ a.e. in } \Omega \\
&12 \geq q \text{ a.e. in} \Omega
\end{aligned} \tag{2.27}$$

where $\Omega = [-1, 1]$. Let the desired state, u_d, be defined as

$$u_d(x) = e^{-x} cos(\pi x)(x-1)^3(x+1)^3 \tag{2.28}$$



(a) Desired state u_d and State Constraint

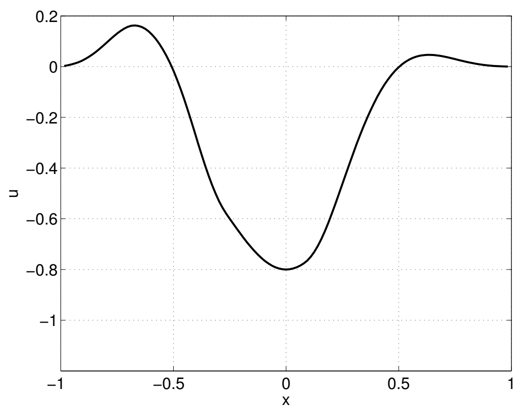
(b) Unconstrained Control and its Constraint

Figure 2.1: Idealized State and Control

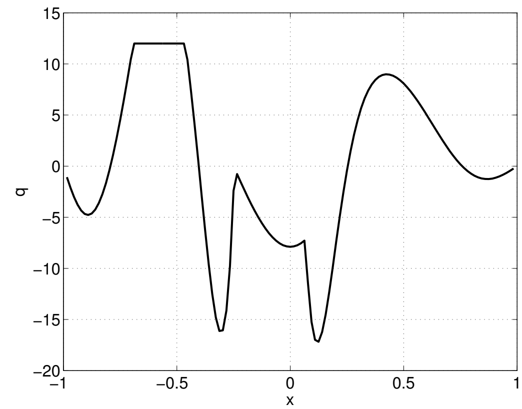
which can be seen in Figure 2.1a, along with the state constraint. Without either the state or control inequality constraint the solution would trivially be $q = -\nabla^2 u_d$, seen in Figure 2.1b. For this example the regularization parameter α is set to 10^{-5}.

This state constrained problem is small and simple enough that a number of existing solvers are able to find a solution, but yet is able to demonstrate the issues resulting from the state constraint. This problem was solved using the Interior Point method as implemented in the Optimization Toolbox™within MATLAB®[27]. The solution to Problem (2.27) is shown in Figure 2.2. The Lagrange multiplier associated with the control constraints is known to be in $L^2([-1,1])$, and can be seen in Figure 2.2d.

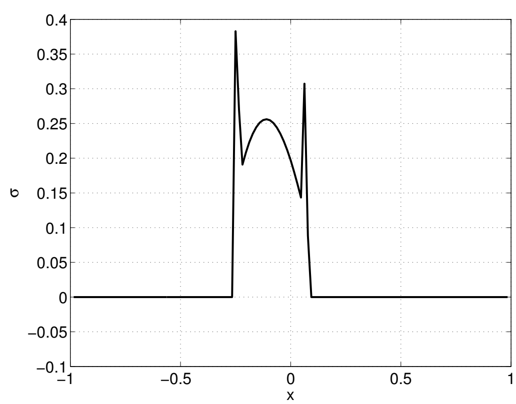
The Lagrange multiplier associated with the control constraint is a well behaved function, as expected of an L^2 function. The Lagrange multiplier associated with the state constraint, though, is not well behaved, which can be seen in 2.2c. In the passive region the multiplier is zero, and away from the boundary between the active and passive regions the multiplier is well behaved. But at the boundary a sharp discontinuity is formed.



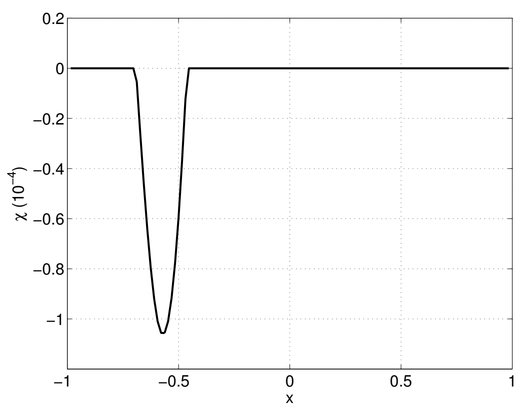
(a) State Variable



(b) Control Variable



(c) State Constraint Multiplier



(d) Control Constraint Multiplier

Figure 2.2: Solution to Example State Constrained Problem

Chapter 3: Nonlinear Rescaling Augmented Lagrangian Methods

The NRAL family of methods was first introduced in the late 1990's by Goldfarb et. al. [16]. In this work two separate methods were coupled to handle optimization problems with both equality and inequality constraints. The inequality constraints were used using the Nonlinear Rescaling (NR) method, which is described in Section 3.1. The Augmented Lagrangian (AL) method, described in Section 3.2, was used for the equality constraints.

In order to introduce the NRAL method both the NR and AL methods will be presented in their classic finite dimensional form. Let $F(x)$, $f_i(x)$, and $g_j(x)$ be $\mathcal{C}^2$ functions in $\mathbb{R}^n$, for $i = 1, \ldots, m$ and $j = 1, \ldots, r$. The generic problem used to describe these methods follows.

$$\begin{aligned} &\text{minimize } F(x) \\ &\text{subject to } f_i(x) \geq 0 \;\; i = 1, \ldots, m \\ &\qquad\qquad g_i(x) = 0 \;\; j = 1, \ldots, r \end{aligned} \tag{3.1}$$

Define $f(x) = \{f_i(x), i = 1, \cdots, m\}$ and $g(x) = \{g_j(x), i = 1, \cdots, r\}$.

3.1 Nonlinear Rescaling

The Nonlinear Rescaling method was introduced by Polyak in the early 1990's [30] as a method for constrained optimization problems with inequality constraints. The NR methods use barrier functions with appropriate properties to recast the inequality constrained problem into an equivalent problem. These barrier functions are similar to those in the Interior Point method [15, 42, 41, 11], but unlike the interior point method the barrier functions exist at the solutions, and therefore the NR method does not experience the ill-conditioning at each iteration seen in the Interior Point method.

The classic NR method is applied for problems with inequality constraints only. Therefore we drop the equality constraints from Problem (3.1).

$$\begin{aligned} &\text{minimize } F(x) \\ &\text{subject to } f_i(x) \geq 0 \;\; i = 1, \ldots, m \end{aligned} \tag{3.2}$$

Define the problem's Lagrangian, $L(x, \lambda)$, in the usual way, and let $\lambda \in \mathbb{R}^m$.

$$L(x, \lambda) = F(x) - \lambda \cdot f(x) \tag{3.3}$$

If $F(x)$ is convex and in $\mathcal{C}^2$, $f_i(x)$ is concave and in $\mathcal{C}^2$, and the Slater condition holds, then it is known [29] that there must exist a λ^* such that at the solution x^* the following Karush-Kuhn-Tucker (KKT) conditions hold.

$$\nabla_x L(x^*, \lambda_i^*) = \nabla F(x^*) - \sum_{i=1}^{m} \lambda_i^* \nabla_x f_i(x^*) = 0 \tag{3.4a}$$

$$f_i(x)\lambda_i = 0 \;\; i = 1, \cdots, m \tag{3.4b}$$

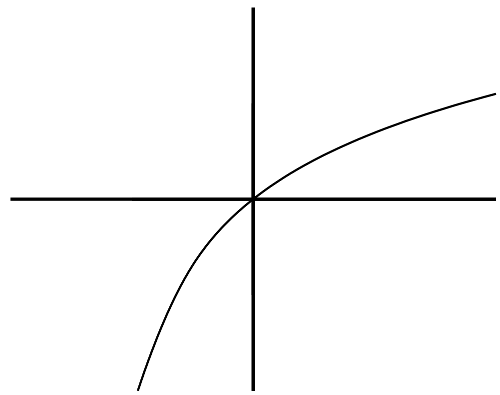


Figure 3.1: Example Rescaling Function Ψ

In the NR method, the inequalities in problem (3.1) are modified using a rescaling function $\Psi(t) : \mathbb{R} \to \mathbb{R}$. The rescaling function is a concave, $\mathcal{C}^2$, function and defined to have the following properties.

$$\Psi(0) = 0 \tag{3.5a}$$

$$\Psi'(t) > 0 \tag{3.5b}$$

$$\Psi'(0) = 1 \tag{3.5c}$$

$$\Psi''(t) < 0 \tag{3.5d}$$

The following additional requirements on $\Psi(t)$ are standard requirements used in the analysis of NR based methods. There exists a $a > 0$ and $b > 0$ such that

$$\Psi'(t) \leq \frac{a}{t+1} \tag{3.6a}$$

$$\Psi''(t) \geq -\frac{b}{(t+1)^2} \tag{3.6b}$$

for all $t \geq 0$. Finally, in support of the future analysis within this work one requires one additional bound on Ψ. In particular, for $c > 0$ there exists a small $\xi > 0$ such that for any $|t| < \xi$

$$|\Psi'''(t)| \leq c. \tag{3.7}$$

The new problem becomes

$$\begin{aligned} &\text{minimize } F(x) \\ &\text{subject to } \frac{1}{k}\Psi(kf_i(x)) \geq 0 \;\; i = 1, \ldots, m \end{aligned} \tag{3.8}$$

where k is some positive barrier parameter. The modified Lagrangian associated with this rescaled problem is

$$\mathcal{L}_{NR,k}(x, \lambda) = F(x) - \sum_{i=1}^{m} \frac{\lambda_i}{k} \Psi(kf_i(x)). \tag{3.9}$$

At the optimal pair (x^*, λ^*) we know that

$$\nabla_x \mathcal{L}_{NR,k}(x^*, \lambda^*) = \nabla_x F(x^*) - diag(\Psi'(\lambda^* k f(x^*)))\nabla_x f(x^*) = 0 \tag{3.10a}$$

Define $\hat{x}$ to be the minimizer for $\mathcal{L}_{NR,k}(x, \lambda_f)$ for a fixed λ_f. It can be shown [30] that under appropriate assumptions $\mathcal{L}_{NR,k}(x, u)$ is strongly convex near the solutions x^*, and that if $\hat{\lambda}_f$ is close enough to λ_f^* than $\hat{x}$ will be a good approximation to x^* if k is sufficiently large. This behavior can be more easily seen by defining the intermediate variable $\hat{\lambda}$ as

$$\hat{\lambda}_{fi} = \Psi'(k(f_i(\hat{x})))\lambda_{fi} \tag{3.11}$$

and inserting $\hat{\lambda}_f$ into (3.10a). Since $\hat{x}$ is the minimizer to $\nabla_x \mathcal{L}_{NR,k}(x, \lambda_f)$ we have

$$\nabla_x \mathcal{L}_{NR,k}(\hat{x}, \lambda_f) = \nabla_x F(\hat{x}) - \sum_{i=1}^{m} \nabla_x f_i(\hat{x})^T \hat{\lambda}_{fi} = 0. \tag{3.12}$$

We see that $\nabla_x \mathcal{L}_{NR,k}(\hat{x}, \lambda_f) = \nabla_x L(\hat{x}, \hat{\lambda}_f)$, and therefore we see that the minimizer is also a stationary point of the original problem's Lagrangian (3.3).

The primal NR method then uses this information to construct a Sequential Unconstrained Minimization Technique (SUMT) method. The minimization step is finding the $\hat{x}$ which minimizes $\mathcal{L}_{NR,k}(x, \lambda_f)$ under a constant λ_f. The second step then uses (3.11) as the update method to the Lagrange multiplier λ_f. This method has been shown [30] to have linear convergence with a constant barrier parameter k. The convergence of this method can be improved by simply increasing k as the method approaches the solution.

Simply increasing the barrier parameter k can have the unfortunate side effect of ill-conditioning that affects other barrier methods. To avoid this issue another modification has been made to the NR method. This modification involved converting the primal NR method described above to a primal-dual NR (PDNR) method [31, 17, 32]. In the PDNR methods the primal and dual variables are treated simultaneously by solving (3.11) and (3.12) as a coupled system of equations. These methods have been shown to have up to 1.5-q-superlinear convergence [17] when coupled with an appropriate update scheme for k.

3.2 Augmented Lagrangian

The classical Augmented Lagrangian as introduced by Hestenes [20] and Powell [34] have been used for equality and inequality constraints for over 40 years, but in this context it will only be used for the equality constraints. Now consider the following problem, which is simply (3.1) without the inequality constraints.

$$\begin{aligned} &\text{minimize } F(x) \\ &\text{subject to } g_i(x) = 0 \quad j = 1, \ldots, r \end{aligned} \tag{3.13}$$

The Lagrangian is defined in its usual way. Define $\lambda_g \in \mathbb{R}^r$, then the Lagrangian is

$$L(x, v) = F(x) - \lambda_g \cdot g(x) \tag{3.14}$$

At the optimal pair (x^*, λ_g^*) we have

$$\nabla L_x(x^*, \lambda_g^*) = \nabla_x F(x^*) - \sum_{j=1}^{r} \lambda_{gj}^* \nabla_x g_j(x^*) = 0 \tag{3.15}$$

In the classical Augmented Lagrangian method the original problem's Lagrangian is augmented with a penalty term, resulting in

$$\mathcal{L}_{AL,k}(x, \lambda_g) = F(x) - \lambda_g \cdot g(x) + \frac{k}{2}\left(g(x) \cdot g(x)\right) \tag{3.16}$$

At the solution pair (x^*, λ_g^*) we have that $\mathcal{L}_{AL,k}(x^*, \lambda_g^*) = 0$ and

$$\nabla_x \mathcal{L}_{AL,k}(x^*, \lambda_g^*) = \nabla_x F(x^*) - \lambda_g \cdot \nabla_x g(x) + k \nabla_x g(x^*) g(x^*) = 0 \tag{3.17}$$

and just like in the NR method we see that $\nabla_x \mathcal{L}_{AL,k}(x^*, \lambda_g^*) = \nabla_x L(x^*, \lambda_g^*) = 0$. Therefore the minimizer of $\mathcal{L}_{AL,k}$ is also a stationary point for $L(\hat{x}, \hat{\lambda}_g)$.

Define $\hat{x}$ to be the minimizer of $\mathcal{L}_{AL,k}(x, \lambda_g)$ for a fixed λ_g. It again can be shown [33] that under the appropriate assumptions $\mathcal{L}_{AL,k}(x, \lambda)$ is strongly convex near the solution x^*, that that if $\hat{\lambda}_g$ is close enough to λ_G^* than $\hat{x}$ will be a good approximation to x^* if k is sufficiently large. This behavior, like in the NR case, can be more readily seen by defining the intermediate variable

$$\hat{\lambda}_g = \lambda_g - kg(\hat{x}) \tag{3.18}$$

and inserting $\hat{\lambda}_g$ into $\nabla_x \mathcal{L}_{AL,k}(x, \hat{\lambda}_g)$. Since $\hat{x}$ is the minimizer to $\mathcal{L}_{AL,k}(x, \lambda_g)$

$$\nabla_x \mathcal{L}_{AL,k}(\hat{x}, \lambda_g) = \nabla_x F(\hat{x}) - \sum_{j=1}^{r} \hat{\lambda}_{gj} \nabla_x g_j(\hat{x}) = 0 \tag{3.19}$$

This fact, combined with strong convexity of $\mathcal{L}_{AL,k}$ [33] again indicates that with a constant λ_g we have that $\hat{x}$ is the minimizer for both $\mathcal{L}_{AL,k}(x, \lambda_g)$ and $L(x, \hat{\lambda}_g)$.

The primal AL, similar to the primal NR method, is a SUMT method. The first step of this method is to find the $\hat{x}$ which minimizes $\nabla_x \mathcal{L}_{AL,k}(x, \hat{\lambda}_g)$ under a constant $\hat{\lambda}_g$. The second step is to update the Lagrange multiplier λ_g using (3.18). The primal AL method has been shown to have linear convergence with a constant k, where the convergence constant is inversely proportional to the penalty parameter k [8]. The convergence rate may be improved to super-linear then with an appropriate sequence of k.

Simply increasing the penalty parameter k can, again, have the unfortunate side effect of ill-conditioning. A Primal-Dual AL (PDAL) method has also been introduced [33]. In this method, equations (3.19) and (3.18) are simultaneously solved for both the primal and dual variable. This method has been shown to have quadratic convergence [33].

3.3 Nonlinear Rescaling Augmented Lagrangian

The similarities of the NR and AL methods are striking. The classic, primal versions of these methods are simply variations on the Uzawa algorithm [36]; an unconstrained minimization followed by a prescribed update to the dual variables. In was recognized as early as the 1960's by Fiacco and McCormick [15] that penalty and barrier methods can be combined into a single method in order to handle optimization problems with both equality and inequality constraints.

A combination of the AL method for equality constraints and NR method for inequality constraints was introduced in the late 1990's by Goldfarb, et. al. [16]. Since both equality and inequality constraints are included the original problem (3.1) may now be considered.

The Lagrangian for problem (3.1) is

$$L(x, \lambda_f, \lambda_g) = F(x) - \lambda_f \cdot f(x) - \lambda_g \cdot g(x) \tag{3.20}$$

where $\lambda_g \in \mathbb{R}^m$ and $\lambda_f \in \mathbb{R}^r$ are the same Lagrange multipliers introduced in Sections 3.1 and 3.2. At the solution x^* we assume there exists λ_f^* and λ_g^* such that

$$\nabla_x L(x^*, \lambda_f^*, \lambda_g^*) = \nabla_x F(x) - \sum_{i=1}^{m} \lambda_{fi}^* \nabla_x f_i(x^*) - \sum_{j=1}^{r} \lambda_{gj} \nabla_x g_i(x^*) = 0. \tag{3.21}$$

This NRAL algorithm begins by rescaling the original problem's inequalities as done in the NR method, and applying an augmented Lagrangian penalty term to the Lagrangian.

$$\mathcal{L}_k(x, \lambda_g, \lambda_f) = F(x) - \sum_{i=1}^{m} \frac{\lambda_{fi}}{k} \Psi(kf_i(x)) - \lambda_g \cdot g(x) + \frac{k}{2} g(x) \cdot g(x) \tag{3.22}$$

At x^* it is known that $\mathcal{L}_k$ is strongly convex [16]. Define $\hat{x}$ to be the minimizer of $\mathcal{L}_k(x, \lambda_f, \lambda_g)$ with constant λ_f and λ_g close to λ_f^* and λ_g^*, respectively. Then the following must be true.

$$\begin{aligned} \nabla_x \mathcal{L}_k(\hat{x}, \lambda_f, \lambda_g) = \nabla_x F(\hat{x}) - \sum_{i=1}^{m} \lambda_{fi} \Psi'(kf_i(\hat{x})) \nabla_x f_i(\hat{x}) \\ - \sum_{j=1}^{r} (\lambda_{gj} \nabla_x g_j(\hat{x}) + k g_j(\hat{x}) \nabla_x g(\hat{x})) \\ = 0 \end{aligned} \tag{3.23}$$

The intermediate variables $\hat{\lambda}_f$ and $\hat{\lambda}_g$ remain as defined in the previous sections.

$$\hat{\lambda}_{fi} = \Psi'(kf_i(\hat{x}))\lambda_{fi} \tag{3.24}$$

$$\hat{\lambda}_g = \lambda_g - kg(\hat{x}) \tag{3.25}$$

Substituting $\hat{\lambda}_f$ and $\hat{\lambda}_g$ into (3.23) again shows that $\nabla_x \mathcal{L}_k(\hat{x}, \lambda_f, \lambda_g) = \nabla_x L(\hat{x}, \hat{\lambda}_g, \hat{\lambda}_f)$, and therefore the minimizer of $\mathcal{L}_k(x, \lambda_f, \lambda_g)$ remains a stationary point of $L(x, \hat{\lambda}_f, \hat{\lambda}_g)$.

Just as in the NR and AL methods, the primal NRAL method performs an unconstrained minimization of $\mathcal{L}(x, \lambda_f, \lambda_g)$ under constant λ_f and λ_g, followed by the

Lagrange multiplier updates (3.24). And just like the primal NR and AL methods, the primal NRAL method has been shown to have linear convergence when the barrier/penalty parameter k is held constant [16]. A primal-dual NRAL method, which incorporates a specific update strategy to k has been shown to have 1.5-q-superlinear convergence [18].

3.4 Function Space NRAL Methods

In the previous section the NRAL method were introduced in their classic finite dimensional form. Many of the mainline optimization methods (SQP, Interior Point, Augmented Lagrangian, etc.) have been used to solve PDECO problems in the finite dimensional form. In this method, commonly referred to as the Discretize-Than-Optimize (DTO), the original problem (2.3) is approximated with a new discretized version of itself. The space Ω is replaced with some triangularization $\Omega_h \subset \Omega$, and all functionals in the problem are discretized on the space Ω_h using a selected discretization method such as a Finite Difference or a Finite Element methods.

$$
\begin{aligned}
\text{minimize } & J_h(u_h, q_h) = \frac{1}{2}\|u_h - u_{dh}\|^2_{L^2(\Omega_h)} + \frac{\alpha}{2}\|q_h\|^2_{L^2(\Omega_h)} \\
\text{subject to } & A_h u_h = q_h \\
& \eta_h \geq u_h \\
& \beta_h \geq q_h
\end{aligned}
\tag{3.26}
$$

where $u_h \in H_0^1(\Omega_h) \cap H^2(\Omega_h)$, and $A_h : H_0^1(\Omega_h) \cap H^2(\Omega_h) \to L^2(\Omega_h)$, and $q_{,h}\, u_{dh}, \eta_h$, and β_h are all in $L^2(\Omega_h)$. The primal NRAL method can also be utilized to solve this discretized problem.

The alternative to this finite dimensional methodology is referred to as a function space, or Optimize-Than-Discretize (OTD), approach. In this methodology the original problem is left intact, and the optimization method is formulated in the same space the original optimization problem, and discretization of the space Ω is performed only when required to numerically solve a set of equations. There are advantages and disadvantages to both approaches, and one discussion of is included by Gunzburger in [19].

In a function space primal NRAL method, the unconstrained minimization step finding where $\nabla_x \mathcal{L}_k(x, \lambda_g, \lambda_f) = 0$ would be the point at which discretization occurs. When comparing problems (2.3) to (3.1) we see that there is now just one equality constraint and two inequality constraints. The system of equations which is equivalent to $\nabla_x \mathcal{L}_k(x, \lambda_g, \lambda_f) = 0$ becomes finding the $\hat{u}$ and $\hat{q}$ which satisfies the following system of equations.

$$\nabla_u J(u, q) - \lambda_f^u, \Psi'(k(\eta - u) - A^\dagger \lambda_g - k A^\dagger (Au - q) = 0 \tag{3.27a}$$

$$\nabla_q J(u, q) - \lambda_f^q f \Psi'(k(\beta - q)) + q\lambda_g - k(Au - q) = 0 \tag{3.27b}$$

This unconstrained minimization is followed by the updates to λ_g, λ_f^u, and λ_f^q.

$$\hat{\lambda}_f^u = \lambda_f^u \Psi' \left(k(\eta - \hat{u}) \right) \tag{3.28a}$$

$$\hat{\lambda}_f^q = \lambda_f^q \Psi' \left(k(\beta - \hat{q}) \right) \tag{3.28b}$$

$$\hat{\lambda}_g = \lambda_g - k(A\hat{u} - \hat{q}) \tag{3.28c}$$

The following chapters discuss variations on primal dual methods associated with

NRAL methods for solving problems similar to (2.3). Chapter 4 introduces and analyses the PDAL method in function space which is used for solving problems with only the PDE constraint. Chapter 5 introduces and analyzes a mixed primal/primal-dual NRAL method which uses the PDAL method to solve the inner problem. Finally, Chapter 6 introduces and analyzes a full primal-dual NRAL method for solving problems similar to (2.3) but with control constraints only.

Chapter 4: Quadratic Convergence of a PDAL Method for Optimization with Elliptic Equality Constraints

4.1 Problem Definition

The general problem examined in this chapter involves a PDECO problem with no additional inequality constraints. Let u, q, A, and Ω be as defined in Section 2.1. Additional, define $\mathcal{J}(u,q) : \mathcal{W} \times L^2(\Omega) \to \mathbb{R}$ be a twice continuously Fréchet differentiable function, which is convex within Ω.

$$\begin{gathered} \text{minimize } \mathcal{J}(u,q) \\ \text{subject to } Au = q \text{ in } \Omega \end{gathered} \tag{4.1}$$

Let $u^* \in \mathcal{W}$ and $q^* \in L^2$ be the solution to problem (4.1), and define its Lagrangian, $L(u,q,\lambda) : \mathcal{W} \times L^2 \times L^2 \to \mathbb{R}$.

$$L(u,q,\lambda) = \mathcal{J}(u,q) - (\lambda, Au - q) \tag{4.2}$$

Due to the elliptic nature of A it is known that there must exist a $\lambda^* \in L^2$ such that the following first order optimality conditions are true.

$$\nabla L(u^*, q^*, \lambda^*) = \begin{pmatrix} \nabla_u \mathcal{J}(u^*, q^*) - A^\dagger \lambda^* \\ \nabla_q \mathcal{J}(u^*, q^*) + \lambda^* \end{pmatrix} = 0 \tag{4.3a}$$

$$Au^* - q^* = 0 \tag{4.3b}$$

The second order optimality conditions also hold for Problem (4.1), due to the strong convexity of $\mathcal{J}$.

4.2 The PDAL Method

The AL method begins with the addition of a penalty term to the Lagrangian, $L(u, q, \lambda)$. This results in the augmented Lagrangian, $\mathcal{L}_{AL,k}(u, q, \lambda) : \mathcal{W} \times L^2(\Omega) \times L^2(\Omega) \to \mathbb{R}$, with $k > 0$.

$$\begin{aligned} \mathcal{L}_{AL,k}(u, q, \lambda) &= L(u, q, \lambda) + \frac{k}{2}(Au - q, Au - q) \\ &= \mathcal{J}(u, q) - (\lambda, Au - q) + \frac{k}{2}(Au - q, Au - q) \end{aligned} \tag{4.4}$$

The gradient of $\mathcal{L}_{AL,k}(u, q, \lambda)$ can be computed as the following.

$$\nabla \mathcal{L}_{AL,k}(u, q, \lambda) = \begin{pmatrix} \nabla_u \mathcal{J}(u, q) - A^\dagger \lambda + kA^\dagger(Au - q) \\ \nabla_q \mathcal{J}(u, q) + \lambda - k(Au - q) \\ Au - q \end{pmatrix} \tag{4.5}$$

There are a number of important properties of $\mathcal{L}_{AL,k}$ at the solution, (u^*, q^*, λ^*).

The first of these can be trivially seen from its definition, and the second from its gradient.

$$\mathcal{L}_{AL,k}(u^*, q^*, \lambda^*) = L(u^*, q^*, \lambda^*) = \mathcal{J}(u^*, q^*) \tag{4.6}$$

$$\nabla \mathcal{L}_{AL,k}(u^*, q^*, \lambda^*) = \nabla L(u^*, q^*, \lambda^*) = \begin{pmatrix} \nabla_u \mathcal{J}(u^*, q^*) - A^\dagger \lambda^* \\ \nabla_q \mathcal{J}(u^*, q^*) + \lambda \\ Au - q \end{pmatrix} \tag{4.7}$$

We can therefore state that (u^*, q^*, λ^*) is a stationary point for both $L(u, q, \lambda)$ and $\mathcal{L}_{AL,k}$, and in fact is the solution to both the original problem and its augmented equivalent. One additional useful property of the augmented Lagrangian is its convexity, which is stated in the following lemma.

Lemma 4.2.1. *Let* (u^*, q^*, λ^*) *be a stationary point for Problem* (4.1)*. Then there exists a neighborhood* $B_1(u^*, q^*)$*,* $k_0 > 0$*, and* $\mu > 0$ *such that* $\mathcal{L}_{AL,k}(u, q, \lambda^*)$ *is strongly convex for all* $(u, q) \in B_1(u^*, q^*)$*,* $k > k_0$*, .*

Proof. Define $\xi = (u_\xi, q_\xi)$ where $u_\xi \in \mathcal{W}$, $q_\xi \in L^2(\Omega)$, and $\lambda_\xi \in L^2(\Omega)$. First compute $\nabla^2 \mathcal{L}_{AL,k}$ at the solution (u^*, q^*, λ^*).

$$\begin{aligned} \nabla^2 \mathcal{L}_{AL,k}(u^*, q^*, \lambda^*) &= \begin{pmatrix} \nabla^2_{uu} \mathcal{J}(u^*, q^*) + kA^\dagger A & \nabla^2_{uq} \mathcal{J}(u^*, q^*) - kA^\dagger \\ \nabla^2_{uq} \mathcal{J}(u^*, q^*) - kA & \nabla^2_{uu} \mathcal{J}(u^*, q^*) + kI \end{pmatrix} \\ &= \nabla^2 L(u^*, q^*, \lambda^*) + \begin{pmatrix} kA^\dagger A & -kA^\dagger \\ -kA & kI \end{pmatrix} \end{aligned} \tag{4.8}$$

Using strong convexity of $L(u, q)$ and recognizing that (4.8) can be written as

$$\nabla^2 \mathcal{L}_{AL,k}(u^*, q^*, \lambda^*) = \nabla L^2(u^*, q^*, \lambda^*) + k \begin{pmatrix} A & -I \end{pmatrix}^{\dagger} \begin{pmatrix} A & -I \end{pmatrix} \tag{4.9}$$

it can be directly seen that $\mathcal{L}_{AL,k}(u^*, q^*, \lambda^*)$ is strongly convex. $\square$

Like described in Section 3.2 the function space AL method is a SUMT method. Initial values for $u_{s=0}$, $q_{s=0}$, and $\lambda_{s=0}$ are selected. The first step of the SUMT iterations becomes the unconstrained minimization

$$(u_s, q_s) = \underset{(u,q) \in \mathcal{W} \times L^2(\Omega)}{\arg\min} \mathcal{L}_{AL,k}(u, q, \lambda_{s-1}) \tag{4.10}$$

with a fix λ_s. The Lagrange multiplier is then updated throughout Ω using

$$\lambda_s = \lambda_{s-1} - k\left(Au_s - q_s\right). \tag{4.11}$$

In the PDAL method this SUMT method of unconstrained minimization followed by the multiplier update is replaced with the solution of (u_s, q_s, λ_s) simultaneously at each iteration. By examination of (4.5) it can be seen that

$$\begin{aligned} \nabla_u \mathcal{L}_{AL,k}(u_s, q_s, \lambda_{s-1}) &= \nabla_u \mathcal{J}(u_s, q_s) - A^{\dagger}\left(\lambda_{s-1} - k(Au_s - q_s)\right) \\ &= \nabla_u \mathcal{J}(u_s, q_s) - A^{\dagger}\lambda_s \qquad (4.12) \\ &= \nabla_u L(u_s, q_s, \lambda_s) \end{aligned}$$

and

$$\begin{aligned}\nabla_q \mathcal{L}_{AL,k}(u_s, q_s, \lambda_{s-1}) &= \nabla_q \mathcal{J}(u_s, q_s) + \lambda_{s-1} - k(Au_s - q_s) \\ &= \nabla_q \mathcal{J}(u_s, q_s) + \lambda_s \\ &= \nabla_q L(u_s, q_s, \lambda_s).\end{aligned} \tag{4.13}$$

The PDAL method then becomes a method for solving (4.1) by solving the following system of equations.

$$\begin{aligned}\nabla_u L(u_s, q_s, \lambda_s) = \nabla_u \mathcal{J}(u_s, q_s) - A^\dagger \lambda_s = 0 \\ \nabla_q L(u_s, q_s, \lambda_s) = \nabla_q \mathcal{J}(u_s, q_s) + \lambda_s = 0 \\ \lambda_s - \lambda_{s-1} + k(Au_s - q_s) = 0\end{aligned} \tag{4.14}$$

This primal dual system (4.14) is solved using Newton's method. The Newton direction is solved for at each step by solving the system of equations derived by linearization of (4.14) about (u, q, λ). The linearization takes the form

$$M_{AL,k}(u_s, q_s, \lambda_s) \begin{pmatrix} \delta u \\ \delta q \\ \delta \lambda \end{pmatrix} = a_{AL}(u_s, q_s, \lambda_s), \tag{4.15}$$

where

$$M_{AL,k}(u_s, q_s, \lambda_s) = \begin{pmatrix} \nabla^2_{uu}\mathcal{J}(u_s, q_s) & \nabla^2_{uq}\mathcal{J}(u_s, q_s) & -A^\dagger \\ \nabla^2_{qu}\mathcal{J}(u_s, q_s) & \nabla^2_{qq}\mathcal{J}(u_s, q_s) & I_\lambda \\ A & -I_q & \frac{I_\lambda}{k} \end{pmatrix} \tag{4.16}$$

and

$$a_{AL}(u, q, \lambda) = \begin{pmatrix} -\nabla_u\mathcal{J}(u_s, q_s) + A^\dagger\lambda_s \\ -\nabla_q\mathcal{J}(u_s, q_s) - \lambda_s \\ -(Au_s - q_s) \end{pmatrix}. \tag{4.17}$$

Each iteration of the PDAL method becomes finding the Newton directions, $(\delta u, \delta q, \delta\lambda)$, from (4.15). This is followed by a simple update to the variables.

$$\begin{aligned} u_{s+1} &= u_s + \delta u \\ q_{s+1} &= q_s + \delta q \\ \lambda_{s+1} &= \lambda_s + \delta\lambda \end{aligned} \tag{4.18}$$

4.3 Local Convergence Analysis

The finite dimensional version of this PDAL method has been shown to have quadratic local convergence under appropriate assumptions [33]. The local convergence analysis shown here follows the outline seen in [33], but is presented here in the function space.

One key component in this analysis is the definition of the merit function $v(u, q, \lambda)$. This merit function both defines the distance between the current point in the solution and it will be used in the penalty parameter update strategy.

$$v(u, q, \lambda) = \max\{\|\nabla_u L(u, q, \lambda)\|, \|\nabla_q L(u, q, \lambda)\|, \|Au - q\|\} \tag{4.19}$$

A second component of this analysis is lemma 4.3.1. This lemma provides a bound on the norm of a Hilbert space operator's inverse, which will be used to bound $\|M_k(u, q, \lambda)^{-1}\|$ in the following analysis.

Lemma 4.3.1. *Define $\mathcal{A}$ and $\mathcal{B}$ to be Hilbert spaces. Let $F : \mathcal{A} \to \mathcal{B}$ be an invertible operator where $\|F^{-1}\| \leq N \ll \infty$. Define a small $\beta > 0$ and $G : \mathcal{A} \to \mathcal{B}$. If $\|F - G\| \leq \beta$ then*

$$\|G^{-1}\| \leq 2N \tag{4.20}$$

and

$$\|F^{-1} - G^{-1}\| \leq 2N^2\beta. \tag{4.21}$$

Proof. Invertibility of F and the bounds on $\|F^{-1}\|$ and $\|F - G\|$ allows G^{-1} to be bounded. First write G^{-1} as

$$\begin{aligned} G^{-1} &= (F - (F - G))^{-1} \\ &= \left(I - F^{-1}(F - G)\right)^{-1} F^{-1}. \end{aligned} \tag{4.22}$$

Then recall the Taylor series expansion of $(1-x)^{-1}$ and apply it to $(I-F^{-1}(F-G))^{-1}$, which leads to

$$\left(I - F^{-1}(F - G)\right)^{-1} = \left(I + \sum_{j=1}^{\infty} \left(F^{-1}(F - G)\right)^j\right). \tag{4.23}$$

By inserting (4.23) into (4.22), one can then bound $\|G^{-1}\|$ using the stated bounds on $\|F^{-1}\|$ and the Cauchy-Schwarz and triangle inequalities.

$$\begin{aligned}
\left\|\left(I+\sum_{j=1}^{\infty}\left(F^{-1}(F-G)\right)^{j}\right)F^{-1}\right\| &\leq \left\|\left(I+\sum_{j=1}^{\infty}\left(F^{-1}(F-G)\right)^{j}\right)\right\|\|F^{-1}\| \\
&\leq \left(1+\sum_{j=1}^{\infty}\left\|\left(F^{-1}(F-G)\right)^{j}\right\|\right)\|F^{-1}\| \\
&\leq N\left(1+\sum_{j=1}^{\infty}\left\|\left(F^{-1}(F-G)\right)^{j}\right\|\right) \\
&\leq N\left(1+\sum_{j=1}^{\infty}(N\beta)^{j}\right)
\end{aligned}$$

Finally, by selecting a small enough β we can assert that $N\beta < \frac{1}{2}$, leading to the initial claim of

$$\|G^{-1}\| \leq N\left(1+\sum_{i=1}^{\infty}\frac{1}{2^{j}}\right) = 2N$$

With this result in hand, we can easily prove the second claim. By noting that

$$\|F^{-1}-G^{-1}\| = \left\|F^{-1}(G-F)G^{-1}\right\|$$

and using the previous result we can see that

$$\|F^{-1}-G^{-1}\| \leq \|F^{-1}\|\|(F-G)\|\|G^{-1}\| \leq 2N^{2}\beta$$

$\square$

With Lemma 4.3.1 and the definition of $v(u,q,\lambda)$ the quadratic local convergence of the function space PDAL method can now be shown. In the following analysis the linearization of (4.5) results in the Newton system of equation for solving problem (4.1). Invertibility of the operator from this Newton system is known, and used in conjunction with Lemma 4.3.1 to bound $M_{AL,k}(u,q,\lambda)$. This bound, along with computed bounds on $a_{AL}(u,q,\lambda)$ are then used to bound the error after a Newton step.

Theorem 4.3.2. *Define* (u^*, q^*, λ^*) *to be the solution to* (4.1)*. Further define* $(\hat{u}, \hat{q}, \hat{\lambda})$ *to be the current solution after a single iteration using the Newton system* (4.15) *where* $k = v(u,q,\lambda)^{-1}$*. Then there exists a small parameter* $0 \leq \epsilon \ll 1$ *such that for any initial* $(u,q,\lambda) \in B_\epsilon(u^*, q^*, \lambda^*)$ *the bound on the error in* $(\hat{u}, \hat{q}, \hat{\lambda})$ *is*

$$\|(\hat{u}, \hat{q}, \hat{\lambda}) - (u^*, q^*, \lambda^*)\| \leq \rho \|(u,q,\lambda) - (u^*, q^*, \lambda^*)\|^2 \tag{4.24}$$

for some $\rho > 0$

Proof. First define the linearized system derived from the Lagrange system (4.5) for problem (4.1).

$$M_\infty(u,q,\lambda) \begin{pmatrix} \overline{\delta u} \\ \overline{\delta q} \\ \overline{\delta \lambda} \end{pmatrix} = a_{AL}(u,q,\lambda), \tag{4.25}$$

where

$$M_\infty(u,q,\lambda) = \begin{pmatrix} \nabla^2_{uu}\mathcal{J}(u,q) & \nabla^2_{uq}\mathcal{J}(u,q) & -A^\dagger \\ \nabla^2_{qu}\mathcal{J}(u,q) & \nabla^2_{qq}\mathcal{J}(u,q) & I_\lambda \\ A & -I_q & 0 \end{pmatrix}. \tag{4.26}$$

The strong convexity of $\mathcal{J}$ and definition of A can be used to show that the operator

$M_\infty(u,q,\lambda)$ is an invertible operator. First assume that $M_\infty(u,q,\lambda)$ is not invertible. Then there exists a $w=(w_u,w_q,w_\lambda)\in\mathcal{W}\times L^2\times L^2$, such that $M_\infty(u,q,\lambda)w=0$ for $w\neq 0$. See that $M_\infty(u,q,\lambda)w=0$ is equivalent to

$$\begin{pmatrix}\nabla^2_{uu}\mathcal{J}(u,q) & \nabla^2_{uq}\mathcal{J}(u,q)\\ \nabla^2_{qu}\mathcal{J}(u,q) & \nabla^2_{qq}\mathcal{J}(u,q)\end{pmatrix}\begin{pmatrix}w_u\\ w_q\end{pmatrix}+\begin{pmatrix}-A^\dagger\\ I_\lambda\end{pmatrix}w_\lambda=0 \tag{4.27a}$$

$$\begin{pmatrix}A & -I_q\end{pmatrix}\begin{pmatrix}w_u\\ w_q\end{pmatrix}=0 \tag{4.27b}$$

Multiplying (4.27a) by $(w_u \quad w_q)$ and using the fact that $(w_u,A^\dagger w_\lambda)=(Aw_u,w_\lambda)$ and (4.27b) leads to

$$\begin{pmatrix}w_u & w_q\end{pmatrix}\begin{pmatrix}-A^\dagger\\ I_\lambda\end{pmatrix}w_\lambda=w_\lambda\begin{pmatrix}A & -I_q\end{pmatrix}\begin{pmatrix}w_u\\ w_q\end{pmatrix}=0 \tag{4.28}$$

Then the second term on the left had side of the modified (4.27a) reduces down to

$$\begin{pmatrix}w_u & w_q\end{pmatrix}\begin{pmatrix}\nabla^2_{uu}\mathcal{J}(u,q) & \nabla^2_{uq}\mathcal{J}(u,q)\\ \nabla^2_{qu}\mathcal{J}(u,q) & \nabla^2_{qq}\mathcal{J}(u,q)\end{pmatrix}\begin{pmatrix}w_u\\ w_q\end{pmatrix}=0. \tag{4.29}$$

Stong convexity of $\mathcal{J}$ implies that (4.29) can only be true if $w_u=w_q=0$. Finally, with $w_u=w_q=0$, (4.27a) simplifies to $-A^\dagger w_\lambda=0$ and $w_\lambda=0$. The latter trivially indicates that $w_\lambda=0$, and therefore $M_\infty(u,q,\lambda)w=0$ if and only if $w=0$, and therefor $M_\infty(u,q,\lambda)$ is invertible.

Quadratic convergence of Newton's method for (u, q, λ) close to (u^*, q^*, λ^*) indicates that there must exist a $\rho_0 > 0$ such that

$$\|(\overline{u}, \overline{q}, \overline{\lambda}) - (u^*, q^*, \lambda^*)\| \leq \rho_0 \|(u, q, \lambda) - (u^*, q^*, \lambda^*)\|^2 \tag{4.30}$$

where $\overline{\xi} = \xi + \overline{\delta\xi}$ for $\xi = u, q, \lambda$.

In order to find a similar bound for $(\hat{u}, \hat{q}, \hat{\lambda})$ we begin with the following algebraic relations.

$$\begin{aligned}(\hat{u}, \hat{q}, \hat{\lambda}) - (u^*, q^*, \lambda^*) &= (u, q, \lambda) + (\delta u, \delta q, \delta\lambda) - (u^*, q^*, \lambda^*) \\ &= (u, q, \lambda) + (\delta u, \delta q, \delta\lambda) + (\overline{\delta u}, \overline{\delta q}, \overline{\delta\lambda}) - (\overline{\delta u}, \overline{\delta q}, \overline{\delta\lambda}) - (u^*, q^*, \lambda^*) \qquad (4.31) \\ &= (\overline{u}, \overline{q}, \overline{\lambda}) - (u^*, q^*, \lambda^*) + (\delta u, \delta q, \delta\lambda) - (\overline{\delta u}, \overline{\delta q}, \overline{\delta\lambda})\end{aligned}$$

Take the norm of both sides, recall the definition of $(\delta u, \delta q, \delta\lambda)$ and $(\overline{\delta u}, \overline{\delta q}, \overline{\delta\lambda})$, and apply the triangle inequality.

$$\begin{aligned}&\|(\hat{u}, \hat{q}, \hat{\lambda}) - (u^*, q^*, \lambda^*)\| = \|(\overline{u}, \overline{q}, \overline{\lambda}) - (u^*, q^*, \lambda^*) + (\delta u, \delta q, \delta\lambda) - (\overline{\delta u}, \overline{\delta q}, \overline{\delta\lambda})\| \\ &= \|(\overline{u}, \overline{q}, \overline{\lambda}) - (u^*, q^*, \lambda^*) + M_{AL,k}^{-1}(u, q, \lambda) a_{AL}(u, q, \lambda) - M_\infty^{-1}(u, q, \lambda) a_{AL}(u, q, \lambda)\| \\ &\leq \|(\overline{u}, \overline{q}, \overline{\lambda}) - (u^*, q^*, \lambda^*)\| + \|M_{AL,k}^{-1}(u, q, \lambda) a_{AL}(u, q, \lambda) - M_\infty^{-1}(u, q, \lambda) a_{AL}(u, q, \lambda)\| \\ &\leq \|(\overline{u}, \overline{q}, \overline{\lambda}) - (u^*, q^*, \lambda^*)\| + \|M_{AL,k}^{-1}(u, q, \lambda) - M_\infty^{-1}(u, q, \lambda)\| \|a_{AL}(u, q, \lambda)\|\end{aligned} \tag{4.32}$$

The using the bounds on $\|(\overline{u}, \overline{q}, \overline{\lambda}) - (u^*, q^*, \lambda^*)\|$ the above term can be written without reference to $(\overline{u}, \overline{q}, \overline{\lambda})$.

$$\begin{aligned} \|(\hat{u}, \hat{q}, \hat{\lambda}) - (u^*, q^*, \lambda^*)\| \leq & \rho_0 \|(u, q, \lambda) - (u^*, q^*, \lambda^*)\|^2 + \\ & \|M_{AL,k}^{-1}(u, q, \lambda) - M_\infty^{-1}(u, q, \lambda)\| \|a_{AL}(u, q, \lambda)\| \end{aligned} \tag{4.33}$$

$M_\infty(u, q, \lambda)$ is invertible, due to strong convexity of $\mathcal{J}$ and the definition of A. Therefore we can state that there exists an N, with $0 < N \ll \infty$, such that $\|M_\infty^{-1}(u, q, \lambda)\| \leq N$. By definition of $M_{AL,k}(u, q, \lambda)$ and $M_\infty(u, q, \lambda)$ we know that

$$\|M_{AL,k}(u, q, \lambda) - M_\infty(u, q, \lambda)\| = \frac{1}{k}. \tag{4.34}$$

Application of Lemma 4.3.1 then implies that

$$\|M_{AL,k}^{-1}(u, q, \lambda) - M_\infty^{-1}(u, q, \lambda)\| \leq \frac{2N^2}{k}. \tag{4.35}$$

Since $\mathcal{J}$ and the elements of A are twice continuously Fréchet differentiable and $\lambda \in L^2(\Omega)$ it is known that there must exist an $L_0 > 0$ such that $\|a_{AL}(u, q, \lambda)\| \leq L_0 \|(u, q, \lambda) - (u^*, q^*, \lambda^*)\|$. These two bounds are then used to further bound $\|(\hat{u}, \hat{q}, \hat{\lambda}) - (u^*, q^*, \lambda^*)\|$.

$$\|(\hat{u}, \hat{q}, \hat{\lambda}) - (u^*, q^*, \lambda^*)\| \leq \rho_0 \|(u, q, \lambda) - (u^*, q^*, \lambda^*)\|^2 + \frac{2N^2}{k} L_0 \|(u, q, \lambda) - (u^*, q^*, \lambda^*)\| \tag{4.36}$$

Recognize that $v(u, q, \lambda)$ is Lipschitz continuous, and that $v(u, q, \lambda) = 0$ if and only if $(u, q, \lambda) = (u^*, q^*, \lambda^*)$. Then there exists a $L_1 > 0$ such that $v(u, q, \lambda) \leq L_1 \|(u, q, \lambda) - (u^*, q^*, \lambda^*)\|$. Also recall that $k = v(u, q, \lambda)^{-1}$, and the second term in

(4.36) can be further bounded.

$$\begin{aligned}\frac{2N^2}{k} L_0 \|(u, q, \lambda) - (u^*, q^*, \lambda^*)\| &= 2N^2 L_0 v(u, q, \lambda) \|(u, q, \lambda) - (u^*, q^*, \lambda^*)\| \\ &\leq 2N^2 L_0 L_1 \|(u, q, \lambda) - (u^*, q^*, \lambda^*)\|^2\end{aligned} \tag{4.37}$$

Incorporating (4.37) in (4.36) results in the claim.

$$\begin{aligned}\|(\hat{u}, \hat{q}, \hat{\lambda}) - (u^*, q^*, \lambda^*)\| &\leq \rho_0 \|(u, q, \lambda) - (u^*, q^*, \lambda^*)\|^2 \\ &+ 2N^2 L_0 L_1 \|(u, q, \lambda) - (u^*, q^*, \lambda^*)\|^2 \\ &\leq \rho \|(u, q, \lambda) - (u^*, q^*, \lambda^*)\|^2\end{aligned}$$

where $\rho = \max\{\rho_0, 2N^2 L_0 L_1\}$. $\square$

Chapter 5: Linear Convergence of a NR-PDAL Method for State- and Control-Constrained Optimization with Elliptic Equality Constraints

The method analyzed in this chapter directly handles Problem (2.3) with all conditions specified in Section 2.1. This method is a mixed method which treats the inequality constraints in a standard primal NR methodology, but in each inner step of the NR method the PDE constraint is incorporated using a primal-dual AL method.

5.1 The NR-PDAL Method

Before defining the NR-PDAL method, additional details of Problem (2.3) must be defined, in additional to those shown in Chapter 2. Let $u^* \in \mathcal{W}$ and $q^* \in L^2$ be the solution to Problem (2.3). Due to the strong convexity of $\frac{1}{2}\|u - u_d\|_{L^2}^2 + \frac{\alpha}{2}\|q\|^2$ and the assumptions of problem (2.3), it is known that there exists a Lagrange multiplier tuple $(\lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*) \in L^2 \times \mathcal{C}^* \times \mathcal{C}^* \times L^2 \times L^2$ such that the optimality conditions (2.4) hold.

The derivation of the NR-PDAL method begins in much the same way as the classic NRAL method shown in section 3.3. Define the Lagrangian, $L(u, q, \lambda, \sigma_u, \sigma_l, \chi_u, \chi_l)$:

$\mathcal{W} \times L^2 \times L^2 \times \mathcal{C}^* \times \mathcal{C}^* \times L^2 \times L^2 \to \mathbb{R}$, be defined as

$$\begin{aligned} L(u, q, \lambda, \sigma_u, \sigma_l, \chi_u, \chi_l) =& \frac{1}{2}\|u - u_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|q\|^2 - (\lambda, Au - q) \\ & -(\sigma_u, \eta_u - u) - (\sigma_l, u - \eta_l) - (\chi_u, \beta_u - q) - (\chi_l, q - \beta_l) \end{aligned} \tag{5.1}$$

The modified Lagrangian from the NRAL method must now be defined. Unlike in section 3.3, the penalty and barrier parameters will be not be the same, resulting in two k values. The parameter k_p will denote the penalty parameter associated with the AL modification. The parameter k_b will be the barrier parameter associated with the NR modification. The modified Lagrangian from the NRAL method becomes

$$\begin{aligned} \mathcal{L}_k(u, q, \lambda, \sigma_u, \sigma_l, \chi_u, \chi_l) =& \frac{1}{2}\|u - u_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|q\|^2 - (\lambda, Au - q) \\ & + \frac{k_p}{2}(Au - q, Au - q) \\ & - \frac{1}{k_b}(\sigma_u, \Psi(k_b(\eta_u - u)) - \frac{1}{k_b}(\sigma_l, \Psi(k_b(u - \eta_l)) \\ & - \frac{1}{k_b}(\chi_u, \Psi(k_b(\beta_u - q)) - \frac{1}{k_b}(\chi_l, \Psi(k_b(q - \beta_l)) \end{aligned} \tag{5.2}$$

As described in section 3.3, the classic primal NRAL method would alternate between the unconstrained minimization step

$$(\hat{u}, \hat{q}) = \operatorname*{arg\,min}_{(u,q) \in \mathcal{W} \times L^2(\Omega)} \mathcal{L}_k(u, q, \lambda, \sigma_u, \sigma_l, \chi_u, \chi_l) \tag{5.3}$$

over fixed (λ, σ, χ), followed by the Lagrange multiplier updates

$$\hat{\lambda} = \lambda - k_p(A\hat{u} - \hat{q}) \tag{5.4a}$$

$$\hat{\sigma}_u = \sigma_u \Psi'(k_b(\eta_u - \hat{u})) \quad \hat{\sigma}_l = \sigma_l \Psi'(k_b(\hat{u} - \eta_l)) \tag{5.4b}$$

$$\hat{\chi}_u = \chi_u \Psi'(k_b(\beta_u - \hat{q})) \quad \hat{\chi}_l = \chi_l \Psi'(k_b(\hat{q} - \beta_l)) \tag{5.4c}$$

In the mixed primal/primal-dual NR-PDAL method the unconstrained minimization is replaced with a PDAL step. This PDAL step is formed very similar to the PDAL method shown in Chapter 4. First the gradient of $\mathcal{L}_k(u, q, \lambda, \sigma_u, \sigma_l, \chi_u, \chi_l)$ with respect to (u, q) is computed.

$$\begin{aligned}
\nabla_u \mathcal{L}_k(u, q, \lambda, \sigma_u, \sigma_l, \chi_u, \chi_l) &= (u - u_d) - A^\dagger \lambda + k_p A^\dagger (Au - q) \\
&\quad + \sigma_u \Psi'(k_b(\eta_u - u)) - \sigma_l \Psi'(k_b(u - \eta_l)) \\
&= (u - u_d) - A^\dagger(\lambda - k_p(Au - q)) + \sigma_u \Psi'(k_b(\eta_u - u)) \\
&\quad - \sigma_l \Psi'(k_b(u - \eta_l) \\
\nabla_q \mathcal{L}_k(u, q, \lambda, \sigma_u, \sigma_l, \chi_u, \chi_l) &= \alpha q + \lambda - k_p(Au - q) \\
&\quad + \chi_u \Psi'(k_b(\beta_u - q)) - \chi_l \Psi'(k_b(\beta_l - q))
\end{aligned} \tag{5.5}$$

By inserting $\hat{\lambda}$ and the updated $\hat{u}$ and $\hat{q}$ into $\nabla \mathcal{L}_k(u, q, \lambda, \sigma_u, \sigma_l, \chi_u, \chi_l)$ and setting the system of equations to 0 the following system of equations is found.

$$(\hat{u} - u_d) - A^{\dagger}\hat{\lambda} + \sigma_u \Psi'(k_b(\eta_u - \hat{u})) - \sigma_l \Psi'(k_b(\hat{u} - \eta_l)) = 0 \tag{5.6a}$$

$$\alpha\hat{q} + \hat{\lambda} + \chi_u \Psi'(k_b(\beta_u - \hat{q})) - \chi_l \Psi'(k_b(\hat{q} - \beta_l)) = 0 \tag{5.6b}$$

$$\hat{\lambda} - \lambda + k_p(A\hat{u} - \hat{q}) = 0 \tag{5.6c}$$

This system of equations is the same as the primal dual system of equations (4.14) seen in Chapter 4, with the following definition for $\mathcal{J}(u, q)$.

$$\begin{aligned} \mathcal{J}(u, q) = \frac{1}{2}\|u - u_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|q\|^2 - \sigma_u \Psi(k_b(\eta_u - u)) - \sigma_l \Psi(k_b(u - \eta_l)) \\ - \chi_u \Psi(k_b(\beta_u - q)) - \chi_l \Psi(k_b(q - \beta_l)) \end{aligned} \tag{5.7}$$

Since Ψ is concave and $\frac{1}{2}\|u - u_d\|^2_{L^2(\Omega)}$ is convex we know that $\mathcal{J}(u, q)$ is strongly convex. Therefore the assumptions from Theorem 4.3.2 all hold and the PDAL inner step of the NR-PDAL step should have local quadratic convergence.

The NR-PDAL method can now be defined as a sequential constrained minimization method, which first solves the PDAL system (5.6) under fixed Lagrange multipliers σ and χ. The Lagrange multipliers are then updated using (5.4b) and (5.4c).

5.2 Local Convergence Analysis

In this section the local convergence of the NR-PDAL method is analyzed, and shown to have linear local convergence when k is held fixed.

Theorem 5.2.1. *Define* $(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*)$ *to be the solution to Problem* (2.3).

Then there exists a $k_0 > 0$ *and* $\delta > 0$ *such that for all* $k_p, k_b > k_0$ *and* $0 < \epsilon < \min\{\sigma_u \in A_{u\eta}, \sigma_l \in A_{l\eta}, \chi_u \in A_{u\beta}, \chi_l \in A_{l\beta}\}$ *the following are true:*

(i) *There exists a solution* $(\hat{u}, \hat{q}, \hat{\lambda})$ *to system of equations* (5.6) *for a given* (σ, χ).

(ii) *For the solution* $(\hat{u}, \hat{q}, \hat{\lambda})$ *from* (i) *the following are bounds on* $\|(\hat{u}, \hat{q}, \hat{\lambda}) - (u^*, q^*, \lambda^*)\|$ *and* $\|(\hat{\sigma}_u, \hat{\sigma}_l, \hat{\chi}_u, \hat{\chi}_l) - (\sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*)\|$.

$$\max\{\|\hat{u} - u^*\|, \|\hat{q} - q^*\|, \|\hat{\lambda} - \lambda^*\|, \|\hat{\sigma}_u - \sigma_u^*\|, \|\hat{\sigma}_l - \sigma_l^*\|, \|\hat{\chi}_u - \chi_u^*\|, \|\hat{\chi}_l - \chi_l^*\|\}$$
$$\leq \frac{C}{k_b} \max\{\|\sigma_u - \sigma_u^*\|, \|\sigma_l - \sigma_l^*\|, \|\chi_u - \chi_u^*\|, \|\chi_l - \chi_l^*\|\} \tag{5.8}$$

Proof. Begin with the following definitions. Define

$$\tau = (\tau_{l\eta}, \tau_{u\eta}, \tau_{u\beta}, \tau_{l\beta}) \tag{5.9}$$

where $\tau_{i\eta} = k_b^{-1}(\sigma_i - \sigma_i^*)$ and $\tau_{i\beta} = k_b^{-1}(\chi_i - \chi_i^*)$, for $i = u, l$. Also define the sets

$S_\epsilon(0,\delta) = \{x \in \Omega \mid \tau_\epsilon \leq \delta\}$ for $\epsilon = u\eta, l\eta, u\beta, l\beta$ and $D_{\epsilon\delta}(\sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, k_0)$, where

$$D_{\epsilon,\delta}(\sigma^*, \chi^*, k_0) = \begin{cases} k_p \geq k_0 \\ k_b \geq k_0 \\ \sigma_u > \epsilon, |\sigma_u - \sigma_u^*| \leq k_b\delta \text{ for } x \in A_{u\eta} \\ \sigma_l > \epsilon, |\sigma_l - \sigma_l^*| \leq k_b\delta \text{ for } x \in A_{l\eta} \\ \sigma_u \leq k_b\delta \text{ for } x \in P_{u\eta} \\ \sigma_l \leq k_b\delta \text{ for } x \in P_{l\eta} \\ \chi_u > \epsilon, |\chi_u - \chi_u^*| \leq k_b\delta \text{ for } x \in A_{u\beta} \\ \chi_l > \epsilon, |\chi_l - \chi_l^*| \leq k_b\delta \text{ for } x \in A_{l\beta} \\ \chi_u \leq k_b\delta \text{ for } x \in P_{u\beta} \\ \chi_l \leq k_b\delta \text{ for } x \in P_{l\beta} \end{cases} \tag{5.10}$$

The Implicit Function theorem is used throughout this analysis in order to develop the bounds claimed by the Theorem 5.2.1. In order to use this an appropriate mapping functional must be defined. Begin by defining $\Theta_k'(u, q, \lambda, \hat{\sigma}_u, \hat{\sigma}_l, \hat{\chi}_u, \hat{\chi}_l, \tau)$.

$$\Theta_k'(\hat{u}, \hat{q}, \hat{\lambda}, \hat{\sigma}_u, \hat{\sigma}_l, \hat{\chi}_u, \hat{\chi}_l, \tau) = \begin{cases} \hat{u} - u_d - A^\dagger\hat{\lambda} + \hat{\sigma}_u - \hat{\sigma}_l \\ \alpha\hat{q} - \hat{\lambda} + \hat{\chi}_u - \hat{\chi}_l \\ \hat{\lambda} - \lambda + k_p(A\hat{u} - \hat{q}) \\ k_b^{-1}(k_b\tau_{u\eta} + \sigma_u^*)\Psi'(k_b(\eta_u - \hat{u})) - k_b^{-1}\hat{\sigma}_u \\ -k_b^{-1}(k_b\tau_{l\eta} + \sigma_l^*)\Psi'(k_b(\hat{u} - \eta_l)) - k_b^{-1}\hat{\sigma}_l \\ k_b^{-1}(k_b\tau_{u\beta} + \chi_u^*)\Psi'(k_b(\beta_u - \hat{q})) - k_b^{-1}\hat{\chi}_u \\ -k_b^{-1}(k_b\tau_{l\beta} + \chi_l^*)\Psi'(k_b(\hat{q} - \beta_l)) - k_b^{-1}\hat{\chi}_l \end{cases} \tag{5.11}$$

Within $P_{u\eta}$ it is known that $\sigma_u^* = 0$, and therefore within this region $\tau_{u\eta} = k_b^{-1}(\sigma_u -$

$\sigma_u^*) = k_b^{-1}\sigma_u$. This, along with the definition $\hat{\sigma}_u = \sigma_u \Psi'(k_b(\eta_u - \hat{u}))$ implies that

$$\begin{aligned} k_b^{-1}(k_b\tau_{u\eta} + \sigma_u^*)\Psi'(k_b(\eta_u - \hat{u})) - k_b^{-1}\hat{\sigma}_u &= k_b^{-1}(k_b k_b^{-1}\sigma_u)\Psi'(k_b(\eta_u - \hat{u})) \\ &\quad - k_b^{-1}\sigma_u\Psi'(k_b(\eta_u - \hat{u})) \\ &= k_b^{-1}\sigma_u\Psi'(k_b(\eta_u - \hat{u})) - k_b^{-1}\sigma_u\Psi'(k_b(\eta_u - \hat{u})) \\ &= 0 \end{aligned} \tag{5.12}$$

everywhere within $P_{u\eta}$. Similar analysis can be performed for σ_l, χ_u, and χ_l in their respective passive regions.

$$\begin{aligned} k_b^{-1}(k_b\tau_{l\eta} + \sigma_l^*)\Psi'(k_b(\hat{u} - \eta_l) - k_b^{-1}\hat{\sigma}_l = 0 \text{ in } P_{l\eta} \\ k_b^{-1}(k_b\tau_{u\beta} + \chi_u^*)\Psi'(k_b(\beta_u - \hat{q})) - k_b^{-1}\hat{\chi}_u = 0 \text{ in } P_{u\beta} \\ k_b^{-1}(k_b\tau_{l\beta} + \chi_l^*)\Psi'(k_b(\hat{q} - \beta_l)) - k_b^{-1}\hat{\chi}_l = 0 \text{ in } P_{l\beta} \end{aligned} \tag{5.13}$$

Due to this behavior the last two equations in $\Theta_k'(\hat{u}, \hat{q}, \hat{\lambda}, \hat{\sigma}_u, \hat{\sigma}_l, \hat{\chi}_u, \hat{\chi}_l, \tau)$ may be altered to only apply to the active regions, resulting in a new mapping function.

$$\Theta_k(\hat{u},\hat{q},\hat{\lambda},\hat{\sigma}_u,\hat{\sigma}_l,\hat{\chi}_u,\hat{\chi}_l,\tau) = \begin{cases} \hat{u} - u_d - A^\dagger\hat{\lambda} + \hat{\sigma}_u - \hat{\sigma}_l \\ \alpha\hat{q} - \hat{\lambda} + \hat{\chi}_u - \hat{\chi}_l \\ \hat{\lambda} - \lambda + k_p(A\hat{u} - \hat{q}) \\ k_b^{-1}(k_b\tau_{u\eta} + \sigma_u^*)\Psi'(k_b(\eta_u - \hat{u})) - k_b^{-1}\hat{\sigma}_u \text{ for } x \in A_{u\eta} \\ -k_b^{-1}(k_b\tau_{l\eta} + \sigma_l^*)\Psi'(k_b(\hat{u} - \eta_l)) - k_b^{-1}\hat{\sigma}_l \text{ for } x \in A_{l\eta} \\ k_b^{-1}(k_b\tau_{u\beta} + \chi_u^u*)\Psi'(k_b(\beta_u - \hat{q})) - k_b^{-1}\hat{\chi}_u \text{ for } x \in A_{u\beta} \\ -k_b^{-1}(k_b\tau_{l\beta} + \chi_l^*)\Psi'(k_b(\hat{q} - \beta_l)) - k_b^{-1}\hat{\chi}_l \text{ for } x \in A_{l\beta} \end{cases} \tag{5.14}$$

In order to use the implicit function theorem for $\Theta_k(\hat{u},\hat{q},\lambda,\hat{\sigma}_u,\hat{\sigma}_l,\hat{\chi}_u,\hat{\chi}_l,\tau)$ we must show that the function satisfies the conditions of the theorem. The first of these conditions requires

$$\Theta_k(u^*,q^*,\lambda^*,\sigma_u^*,\sigma_l^*,\chi_u^*,\chi_l^*,0) = 0 \tag{5.15}$$

which can be seen using the definition of τ, $\hat{\sigma}_u$, $\hat{\sigma}_l$, $\hat{\chi}_u$, $\hat{\chi}_l$, and the optimality conditions (2.4).

The second condition required by the implicit function theorem is invertibility of $\nabla\Theta_k(\hat{u},\hat{q},\hat{\lambda},\hat{\sigma}_u,\hat{\sigma}_l,\hat{\chi}_u,\hat{\chi}_l,\tau)$ at $(u^*,q^*,\lambda^*,\sigma_u^*,\sigma_l^*,\chi_u^*,\chi_l^*,0)$. First define the following operators.

$$\begin{aligned} \Psi_{u\eta} &= -(k_b\tau_{u\eta} + \sigma_u^*)\Psi''(k_b(\eta_u - \hat{u})) \\ \Psi_{l\eta} &= (k_b\tau_{l\eta} + \sigma_l^*)\Psi''(k_b(\hat{u} - \eta_l)) \\ \Psi_{u\beta} &= -(k_b\tau_{u\beta} + \chi_u^*)\Psi''(k_b(\beta_u - \hat{q})) \\ \Psi_{l\beta} &= (k_b\tau_{l\beta} + \chi_l^*)\Psi''(k_b(\hat{q} - \beta_l)) \end{aligned} \tag{5.16}$$

Then evaluate $\nabla\Theta$.

$$\nabla\Theta_k(\hat{u},\hat{q},\hat{\lambda},\hat{\sigma}_u,\hat{\sigma}_l,\hat{\chi}_u,\hat{\chi}_l,\tau) =$$

$$\begin{pmatrix} I_u & 0 & -A^\dagger & I_{\sigma_u} & -I_{\sigma_l} & 0 & 0 \\ 0 & \alpha I_q & -I_\lambda & 0 & 0 & I_{\chi_u} & -I_{\chi_l} \\ k_p A & -k_p I_q & I & 0 & 0 & 0 & 0 \\ \Psi_{u\eta} & 0 & 0 & -k_b^{-1} I_{\sigma_u} & 0 & 0 & 0 \\ \Psi_{l\eta} & 0 & 0 & 0 & -k_b^{-1} I_{\sigma_l} & 0 & 0 \\ 0 & \Psi_{u\beta} & 0 & 0 & 0 & -k_b^{-1} I_{\chi_u} & 0 \\ 0 & \Psi_{l\beta} & 0 & 0 & 0 & 0 & -k_b^{-1} I_{\chi_l} \end{pmatrix} \tag{5.17}$$

Divide the third line of $\nabla\Theta_k(\hat{u},\hat{q},\hat{\lambda},\hat{\sigma},\hat{\chi},\tau)$ by k_p and the last four lines by k_b and evaluate at $\tau = 0$.

$$\nabla\Theta_k(u^*,q^*,\lambda^*,\sigma_u^*,\sigma_l^*,\chi_u^*,\chi_l^*,0)$$

$$= \begin{pmatrix} I_u & 0 & -A^\dagger & I_{\sigma_u} & -I_{\sigma_l} & 0 & 0 \\ 0 & \alpha & -I_\lambda & 0 & 0 & I_{\chi_u} & -I_{\chi_l} \\ A & -I_q & k_p^{-1} I & 0 & 0 & 0 & 0 \\ -\sigma_u^* \Psi''(0) & 0 & 0 & -k_b^{-1} I_{\sigma_u} & 0 & 0 & 0 \\ \sigma_l^* \Psi''(0) & 0 & 0 & 0 & -k_b^{-1} I_{\sigma_l} & 0 & 0 \\ 0 & -\chi_u^* \Psi''(0) & 0 & 0 & 0 & -k_b^{-1} I_{\chi_u} & 0 \\ 0 & \chi_l^* \Psi''(0) & 0 & 0 & 0 & 0 & -k_b^{-1} I_{\chi_l} \end{pmatrix} \tag{5.18}$$

The operator $\nabla\Theta_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)$ may be directly shown to be invertible under appropriately specified A, but for the general case presented here Lemma 4.3.1 will be used to show invertibility. Recall that conditions of the Lemma requires an invertible operator that close enough to $\nabla\Theta_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)$. One potential operator can be found by evaluating $\nabla\Theta_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)$ as k_b approaches infinity.

$$\begin{aligned}\nabla\Theta_\infty(u^*, q^*, \lambda^*, \sigma^*, \chi^*, 0) &= \lim_{k\to\infty} \nabla\Theta_k(u^*, q^*, \lambda^*, \sigma^*, \chi^*, 0) \\ &= \begin{pmatrix} I_u & 0 & -A^\dagger & I_{\sigma_u} & -I_{\sigma_l} & 0 & 0 \\ 0 & \alpha & -I_\lambda & 0 & 0 & I_{\chi_u} & -I_{\chi_l} \\ A & -I_q & k_p^{-1} I & 0 & 0 & 0 & 0 \\ -\sigma_u^* \Psi''(0) & 0 & 0 & 0 & 0 & 0 & 0 \\ \sigma_l^* \Psi''(0) & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\chi_u^* \Psi''(0) & 0 & 0 & 0 & 0 & 0 \\ 0 & \chi_l^* \Psi''(0) & 0 & 0 & 0 & 0 & 0 \end{pmatrix}\end{aligned} \tag{5.19}$$

Define $w = (w_u, w_q, w_\lambda, w_{\sigma_u}, w_{\sigma_l}, w_{\chi_u}, w_{\chi_l})$, where $w_u \in \mathcal{W}$, $w_q \in L^2(\Omega)$, $w_\lambda \in L^2(\Omega)$,

$w_{\sigma_u}, w_{\sigma_l} \in \mathcal{C}^*$, $w_{\chi_u}, w_{\chi_l} \in L^2(\Omega)$ and evaluate $\nabla\Theta_\infty(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)w = 0$.

$$w_u - A^\dagger w_\lambda + w_{\sigma_u} - w_{\sigma_l} = 0 \tag{5.20a}$$

$$\alpha w_q - w_\lambda + w_{\chi_u} - w_{\chi_l} = 0 \tag{5.20b}$$

$$A w_u - w_q + \frac{1}{k_p} w_\lambda = 0 \tag{5.20c}$$

$$-\sigma_u^* \Psi''(0) w_u = 0 \quad \sigma_l^* \Psi''(0) w_u = 0 \tag{5.20d}$$

$$-\chi_u^* \Psi''(0) w_q = 0 \quad \chi_l^* \Psi''(0) w_q = 0 \tag{5.20e}$$

If $\nabla\Theta_\infty(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)$ was not invertible then there must exist a w such that $w_\xi = 0$ for at least one of $\xi = u, q, \lambda, \sigma_u, \sigma_l, \chi_u, \chi_l$. By definition of Ψ we have $\Psi''(0) < 0$, and by the strict complementarity assumption we know that $\sigma_u^* > 0$, $\sigma_l^* > 0$, $\chi_u^* > 0$, and $\chi_l^* > 0$. Therefore (5.20d) and (5.20e) imply that $w_u = 0$ and $w_q = 0$. Equation (5.20c) then implies that $w_\lambda = 0$. One is then left with (5.20a) and (5.20b) implying $w_{\sigma_u} - w_{\sigma_l} = 0$ and $w_{\chi_u} - w_{\chi_l} = 0$. Furthermore, as $\nabla\Theta_\infty$ operates only in the respective active regions, the w's associated with inequality constraints in (5.20b) and (5.20a) are active in separate regions. Therefore either $w_{\sigma_u} = 0$ or $w_{\sigma_l} = 0$ in any given region. Similarly, either $w_{\chi_u} = 0$ or $w_{\chi_l} = 0$ in any given region. $w_{\sigma_u} = w_{\sigma_l} = w_{\chi_u} = w_{\chi_l} = 0$. Therefore $\nabla\Theta_\infty(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)w = 0$ if an only if $w = 0$, and there must exist a $\rho_0 > 0$ such that

$$\|\nabla\Theta_\infty^{-1}(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)\| \leq \rho_0. \tag{5.21}$$

Lemma 4.3.1 requires a bound on the difference between the two operators under consideration. This bound can be found by computing

$$\nabla\Theta_\infty(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0) - \nabla\Theta_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0) =$$

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & k_b^{-1} I_{\sigma_u} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & k_b^{-1} I_{\sigma_l} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & k_b^{-1} I_{\chi_u} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & k_b^{-1} I_{\chi_l} \end{pmatrix} \tag{5.22}$$

and therefore

$$\|\nabla\Theta_\infty(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0) - \nabla\Theta_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)\| = \|k_b^{-1}\| \tag{5.23}$$

Then application of Lemma 4.3.1 implies that $\nabla\Theta_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)$ is invertible, and is bounded.

$$\|\nabla\Theta_k^{-1}(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)\| \leq 2\rho_0^2 \|k_b^{-1}\| \leq 2\rho_0^2. \tag{5.24}$$

At the solution it has now been shown that $\Theta_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0) = 0$ and that $\nabla\Theta_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)$ is invertible. This allows the second implicit function theorem to be used to complete the proof of *(i)*. First define $\xi(\tau, k_b)$, for $\xi = u, q, \lambda, \sigma_u, \sigma_l, \chi_u, \chi_l$, to be functions in $S(K, \delta) = \{(k, \tau) : k_0 \leq k \leq k_1, \|\tau\| \leq \delta\}$. By the second implicit function theorem there exists a $k_1 > k_0$ such that for any $k \in [k_0, k_1]$ there exists a $\delta > 0$ such that $\xi(0, k_b) = \xi^*$, for $\xi = u, q, \lambda, \sigma_u, \sigma_l, \chi_u, \chi_l$.

This completes the proof of claim *(i)*.

(ii): The claimed bound on the Lagrange multipliers within $P_{u\eta}$, $P_{l\eta}$, $P_{u\beta}$, and $P_{l\beta}$ are considered first. From the previous section we saw that there must exist a $\delta > 0$ such that for any $(k_b, \tau) \in S(K, \delta)$ there exists an $\epsilon_0 > 0$ such that

$$\max\{\|u(\tau, k_b) - u^*\|, \|q(\tau, k_b) - q^*\|, \|\lambda(\tau, k_b) - \lambda^*\|\} \leq \epsilon_0. \tag{5.25}$$

In the passive regions it is also known that there exist a $U_{u\eta} > 0$, $U_{l\eta} > 0$, $U_{u\beta} > 0$, and $U_{l\beta} > 0$ such that

$$\eta_u - \hat{u} > \frac{U_{u\eta}}{2} \qquad \hat{u} - \eta_l > \frac{U_{l\eta}}{2} \tag{5.26a}$$

$$\beta_u - \hat{q} > \frac{U_{u\beta}}{2} \qquad \hat{q} - \beta_u > \frac{U_{l\beta}}{2} \tag{5.26b}$$

Recall that in the passive regions $\sigma_u^* = 0$, $\sigma_l^* = 0$, $\chi_u^* = 0$, and $\chi^* = 0$, then $\hat{\sigma}_u$, $\hat{\sigma}_l$, $\hat{\chi}_u$, and $\hat{\chi}_l$ may be written as follows.

$$\hat{\sigma}_u = (\sigma_u - \sigma_u^*)\Psi'(k_b(\eta_u - \hat{u})) \qquad \hat{\sigma}_l = (\sigma_l - \sigma_l^*)\Psi'(k_b(\hat{u} - \eta_l)) \tag{5.27a}$$

$$\hat{\chi}_u = (\chi_u - \chi_u^*)\Psi'(k_b(\beta_u - \hat{q})) \qquad \hat{\chi}_l = (\chi_l - \chi_l^*)\Psi'(k_b(\hat{q} - \beta_l)) \tag{5.27b}$$

By the conditions required of $\Psi(t)$ there must exist a $a_{\sigma_u} > 0$, $a_{\sigma_l} > 0$, $a_{\chi_u} > 0$, and

$a_{\chi_l} > 0$ such that

$$\Psi'(k_b(\eta_u - \hat{u})) < a_{\sigma_u}(k_b(\eta_u - \hat{u}) + 1)^{-1} \tag{5.28a}$$

$$\Psi'(k_b(\hat{u} - \eta_l)) < a_{\sigma_l}(k_b(\hat{u} - \eta_l) + 1)^{-1} \tag{5.28b}$$

$$\Psi'(k(\beta_u - \hat{q})) < a_{\chi_u}(k_b(\beta_u - \hat{q}) + 1)^{-1} \tag{5.28c}$$

$$\Psi'(k(\hat{q} - \beta_l)) < a_{\chi_l}(k_b(\hat{q} - \beta_l) + 1)^{-1} \tag{5.28d}$$

Therefore

$$\begin{aligned} \hat{\sigma}_u = \hat{\sigma}_u - \sigma_u^* &\leq a_{\sigma_u}(\sigma_u - \sigma_u^*)(k_b(\eta_u - \hat{u}) + 1)^{-1} \\ &\leq (a_{\sigma_u}(\sigma_u - \sigma_u^*))(k_b(\eta_u - \hat{u}))^{-1} \\ &\leq a_{\sigma_u}(\sigma_u - \sigma_u^*)2(U_{u\eta}k_b)^{-1} \end{aligned} \tag{5.29}$$

and similarly

$$\hat{\sigma}_l = \hat{\sigma}_l - \sigma_l^* \leq a_{\sigma_l}(\sigma_l - \sigma_l^*)2(U_{l\eta}k_b)^{-1} \tag{5.30a}$$

$$\hat{\chi}_u = \hat{\chi}_u - \chi_u^* \leq a_{\chi_u}(\chi_u - \chi_u^*)2(U_{u\beta}k_b)^{-1} \tag{5.30b}$$

$$\hat{\chi}_l = \hat{\chi}_l - \chi_l^* \leq a_{\chi_l}(\chi_l - \chi_l^*)2(U_{l\beta}k_b)^{-1} \tag{5.30c}$$

which confirms the bounds

$$\max\{\|\hat{\sigma}_u - \sigma_u^*\|, \hat{\sigma}_l - \sigma_l^*\|, \|\hat{\chi}_u - \chi_u^*\|, \|\hat{\chi}_l - \chi_l^*\|\}$$
$$\leq \frac{C_0}{k_b}\|\max\{\|\sigma_u - \sigma_u^*\|, \sigma_l - \sigma_l^*\|, \|\chi_u - \chi_u^*\|, \|\chi_l - \chi_l^*\|\} \tag{5.31}$$

where $C_0 = \max\left\{a_{\sigma_u}\frac{U_{u\eta}}{2}, a_{\sigma_l}\frac{U_{l\eta}}{2}, a_{\chi_u}\frac{U_{u\beta}}{2}, a_{\chi_l}\frac{U_{l\beta}}{2}\right\}$.

The mapping Θ_k will again be used in order to prove the claimed bounds for $(\hat{u}, \hat{q}, \hat{\lambda})$ everywhere in Ω and $(\hat{\sigma}_u, \hat{\sigma}_l, \hat{\chi}_u, \hat{\chi}_l)$ in their respective active regions. For this usage the derivative of Θ_k with respect to τ must be evaluated and set to 0. Set

$$\nabla_\tau \Theta_k(\hat{u}, \hat{q}, \hat{\lambda}, \hat{\sigma}_u, \hat{\sigma}_l, \hat{\chi}_u, \hat{\chi}_l, \tau) = \left[\frac{d\Theta_k(\cdot)}{d\tau_{u\eta}}, \frac{d\Theta_k(\cdot)}{d\tau_{l\eta}}, \frac{d\Theta_k(\cdot)}{d\tau_{u\beta}}, \frac{d\Theta_k(\cdot)}{d\tau_{l\beta}}\right] = [0, 0, 0, 0] \tag{5.32}$$

where

$$\frac{d\Theta_k(\cdot)}{d\tau_{u\eta}} = \begin{pmatrix} \hat{u}_{\tau_{u\eta}} - A^\dagger \hat{\lambda}_{\tau_{u\eta}} + \hat{\sigma}_{u,\tau_{u\eta}} - \hat{\sigma}_{l,\tau_{u\eta}} \\ \alpha \hat{q}_{\tau_{u\eta}} + \hat{\sigma}_{\tau_{u\eta}} + \hat{\chi}_{u,\tau_{u\eta}} - \hat{\chi}_{l,\tau_{u\eta}} \\ \hat{\lambda}_{\tau_{u\eta}} + k_p(A\hat{u}_{\tau_{u\eta}} - \hat{q}_{\tau_{u\eta}}) \\ \Psi'(k_b(\eta_u - \hat{u})) - (k_b\tau_{u\eta} + \sigma_u^*)\Psi''(k_b(\eta_u - \hat{u}))\hat{u}_{\tau_{u\eta}} - k_b^{-1}\hat{\sigma}_{u,\tau_{u\eta}} \\ \sigma_l^* \Psi''(k_b(\hat{u} - \eta_l))\hat{u}_{\tau_{u\eta}} - k_b^{-1}\hat{\sigma}_{l,\tau_{u\eta}} \\ -\chi_u^* \Psi''(k_b(\beta_u - \hat{q}))\hat{q}_{\tau_{u\eta}} - k_b^{-1}\hat{\chi}_{u,\tau_{u\eta}} \\ \chi_l^* \Psi''(k_b(\hat{q} - \beta_l))\hat{q}_{\tau_{u\eta}} - k_b^{-1}\hat{\chi}_{l,\tau_{u\eta}} \end{pmatrix} \tag{5.33}$$

$$\frac{d\Theta_k(\cdot)}{d\tau_{l\eta}} = \begin{pmatrix} \hat{u}_{\tau_{l\eta}} - A^{\dagger}\hat{\lambda}_{\tau_{l\eta}} + \hat{\sigma}_{u,\tau_{l\eta}} - \hat{\sigma}_{l,\tau_{l\eta}} \\ \alpha\hat{q}_{\tau_{l\eta}} + \hat{\sigma}_{\tau_{l\eta}} + \hat{\chi}_{u,\tau_{l\eta}} - \hat{\chi}_{l,\tau_{l\eta}} \\ \hat{\lambda}_{\tau_{l\eta}} + k_p(A\hat{u}_{\tau_{l\eta}} - \hat{q}_{\tau_{l\eta}}) \\ -\sigma_u^{*}\Psi''(k_b(\eta_u - \hat{u}))\hat{u}_{\tau_{l\eta}} - k_b^{-1}\hat{\sigma}_{u,\tau_{l\eta}} \\ \Psi'(k_b(\hat{u} - \eta_l)) - (k_b\tau_{l\eta} + \sigma_l^{*})\Psi''(k_b(\hat{u} - \eta_l))\hat{u}_{\tau_{l\eta}} - k_b^{-1}\hat{\sigma}_{l,\tau_{l\eta}} \\ -\chi_u^{*}\Psi''(k_b(\beta_u - \hat{q}))\hat{q}_{\tau_{l\eta}} - k_b^{-1}\hat{\chi}_{u,\tau_{l\eta}} \\ \chi_l^{*}\Psi''(k_b(\hat{q} - \beta_l))\hat{q}_{\tau_{l\eta}} - k_b^{-1}\hat{\chi}_{l,\tau_{l\eta}} \end{pmatrix} \tag{5.34}$$

$$\frac{d\Theta_k(\cdot)}{d\tau_{u\beta}} = \begin{pmatrix} \hat{u}_{\tau_{u\beta}} - A^{\dagger}\hat{\lambda}_{\tau_{u\beta}} + \hat{\sigma}_{u,\tau_{u\beta}} - \hat{\sigma}_{l,\tau_{u\beta}} \\ \alpha\hat{q}_{\tau_{u\beta}} + \hat{\sigma}_{\tau_{u\beta}} + \hat{\chi}_{u,\tau_{u\beta}} - \hat{\chi}_{l,\tau_{u\beta}} \\ \hat{\lambda}_{\tau_{u\beta}} + k_p(A\hat{u}_{\tau_{u\beta}} - \hat{q}_{\tau_{u\beta}}) \\ -\sigma_u^{*}\Psi''(k_b(\eta_u - \hat{u}))\hat{u}_{\tau_{u\beta}} - k_b^{-1}\hat{\sigma}_{u,\tau_{u\beta}} \\ \sigma_l^{*}\Psi''(k_b(\hat{u} - \eta_l))\hat{)}u_{\tau_{u\beta}} - k_b^{-1}\hat{\sigma}_{l,\tau_{u\beta}} \\ \Psi'(k_b(\beta_u - \hat{q})) - (k_b\tau_{u\beta} + \chi_u^{*})\Psi''(k_b(\beta_u - \hat{q}))\hat{q}_{\tau_{u\beta}} - k_b^{-1}\hat{\chi}_{u,\tau_{u\beta}} \\ \chi_l^{*}\Psi''(k_b(\hat{q} - \beta_l))\hat{q}_{\tau_{u\eta}} - k_b^{-1}\hat{\chi}_{l,\tau_{u\eta}} \end{pmatrix} \tag{5.35}$$

$$\frac{d\Theta_k(\cdot)}{d\tau_{l\beta}} = \begin{pmatrix} \hat{u}_{\tau_{l\beta}} - A^{\dagger}\hat{\lambda}_{\tau_{l\beta}} + \hat{\sigma}_{u,\tau_{l\beta}} - \hat{\sigma}_{l,\tau_{l\beta}} \\ \alpha\hat{q}_{\tau_{l\beta}} + \hat{\sigma}_{\tau_{l\beta}} + \hat{\chi}_{u,\tau_{l\beta}} - \hat{\chi}_{l,\tau_{l\beta}} \\ \hat{\lambda}_{\tau_{l\beta}} + k_p(A\hat{u}_{\tau_{l\beta}} - \hat{q}_{\tau_{l\beta}}) \\ -\sigma_u^{*}\Psi''(k_b(\eta_u - \hat{u}))\hat{u}_{\tau_{l\beta}} - k_b^{-1}\hat{\sigma}_{u,\tau_{l\beta}} \\ \sigma_l^{*}\Psi''(k_b(\hat{u} - \eta_l))\hat{u}_{\tau_{l\beta}} - k_b^{-1}\hat{\sigma}_{l,\tau_{l\beta}} \\ -\chi_u^{*}\Psi''(k_b(\beta_u - \hat{q}))\hat{q}_{\tau_{l\eta}} - k_b^{-1}\hat{\chi}_{u,\tau_{l\eta}} \\ \Psi'(k_b(\hat{q} - \beta_l)) - (k_b\tau_{l\beta} + \chi_l^{*})\Psi''(k_b(\hat{q} - \beta_l))\hat{q}_{\tau_{l\beta}} - k_b^{-1}\hat{\chi}_{l,\tau_{l\beta}} \end{pmatrix} \tag{5.36}$$

Recognize that (5.32) can be represented as a linear operator on $(\xi_{\tau_{u\eta}}, \xi_{\tau_{l\eta}}, \xi_{\tau_{u\beta}}, \xi_{\tau_{l\beta}})$ for $\xi = u, q, \lambda, \sigma_u, \sigma_l, \chi_u, \chi_l$. Rewrite (5.32) as the linear operator, moving the $\Psi'(\cdot)$

terms to the right hand side since they are not multiplied by the dependent variables. The variables $\hat{\sigma}_u$, $\hat{\sigma}_l$, $\hat{\chi}_u$, and $\hat{\chi}_l$ are decomposed into their active and passive regions, with the values corresponding to the active region are retained on the left hand side and the portion corresponding to the passive region are moved to the right hand side.

$$T_k(\hat{u}, \hat{q}, \hat{\lambda}, \hat{\sigma}_u, \hat{\sigma}_l, \hat{\chi}_u, \hat{\chi}_l, \tau) \begin{pmatrix} \hat{u}_{\tau_{u\eta}} & \hat{u}_{\tau_{l\eta}} & \hat{u}_{\tau_{u\beta}} & \hat{u}_{\tau_{l\beta}} \\ \hat{q}_{\tau_{u\eta}} & \hat{q}_{\tau_{l\eta}} & \hat{q}_{\tau_{u\beta}} & \hat{q}_{\tau_{l\beta}} \\ \hat{\lambda}_{\tau_{u\eta}} & \hat{\lambda}_{\tau_{l\eta}} & \hat{\lambda}_{\tau_{u\beta}} & \hat{\lambda}_{\tau_{l\beta}} \\ \hat{\sigma}_{u,\tau_{u\eta}} & \hat{\sigma}_{u,\tau_{l\eta}} & \hat{\sigma}_{u,\tau_{u\beta}} & \hat{\sigma}_{u,\tau_{l\eta}} \\ \hat{\sigma}_{l,\tau_{u\eta}} & \hat{\sigma}_{l,\tau_{l\eta}} & \hat{\sigma}_{l,\tau_{u\beta}} & \hat{\sigma}_{l,\tau_{l\eta}} \\ \hat{\chi}_{u,\tau_{u\eta}} & \hat{\chi}_{u,\tau_{l\eta}} & \hat{\chi}_{u,\tau_{u\beta}} & \hat{\chi}_{u,\tau_{l\eta}} \\ \hat{\chi}_{l,\tau_{u\eta}} & \hat{\chi}_{l,\tau_{l\eta}} & \hat{\chi}_{l,\tau_{u\beta}} & \hat{\chi}_{l,\tau_{l\eta}} \end{pmatrix} = t_k(\hat{u}, \hat{q}, \hat{\lambda}, \hat{\sigma}_u, \hat{\sigma}_l, \hat{\chi}_u, \hat{\chi}_l) \tag{5.37}$$

where

$$T_k(\cdot) = \tag{5.38a}$$

$$\begin{pmatrix} I_u & 0 & -A^\dagger & I_{\sigma_u} & -I_{\sigma_l} & 0 & 0 \\ 0 & \alpha I_q & I_\lambda & 0 & 0 & I_{\chi_u} & -I_{\chi_l} \\ k_p A & -k_p I_q & I_\lambda & 0 & 0 & 0 & 0 \\ -(k_b\tau_{u\eta} - \sigma_u^*)\Psi'(k_b(\eta_u - \hat{u})) & 0 & 0 & -k_b^{-1} I_{\sigma_u} & 0 & 0 & 0 \\ (k_b\tau_{l\eta} - \sigma_l^*)\Psi'(k_b(\hat{u} - \eta_l)) & 0 & 0 & 0 & -k_b^{-1} I_{\sigma_l} & 0 & 0 \\ 0 & -(k_b\tau_{u\beta} - \chi_u^*)\Psi''(k_b(\beta_u - \hat{q})) & 0 & 0 & 0 & -k_b^{-1} I_{\chi_u} & 0 \\ 0 & (k_b\tau_{l\beta} - \chi_l^*)\Psi''(k_b(\hat{q} - \beta_l)) & 0 & 0 & 0 & 0 & -k_b^{-1} I_{\chi_l} \end{pmatrix}$$

$$t_k(\cdot) = \begin{pmatrix} -\hat{\sigma}_{u\tau_{u\eta}} & \hat{\sigma}_{u\tau_{l\eta}} & -\hat{\sigma}_{u\tau_{u\beta}} & \hat{\sigma}_{u\tau_{l\beta}} \\ -\hat{\sigma}_{l\tau_{u\eta}} & \hat{\sigma}_{l\tau_{l\eta}} & -\hat{\sigma}_{l\tau_{u\beta}} & \hat{\sigma}_{l\tau_{l\beta}} \\ -\hat{\chi}_{u\tau_{u\eta}} & \hat{\chi}_{u\tau_{l\eta}} & -\hat{\chi}_{u\tau_{u\beta}} & \hat{\chi}_{u\tau_{l\beta}} \\ -\hat{\chi}_{l\tau_{u\eta}} & \hat{\chi}_{l\tau_{l\eta}} & -\hat{\chi}_{l\tau_{u\beta}} & \hat{\chi}_{l\tau_{l\beta}} \\ 0 & 0 & 0 & 0 \\ -\Psi'(k_b(\eta_u - \hat{u})) & 0 & 0 & 0 \\ 0 & -\Psi'(k_b(\hat{u} - \eta_l)) & 0 & 0 \\ 0 & 0 & -\Psi'(k_b(\beta_u - \hat{q})) & 0 \\ 0 & 0 & 0 & -\Psi'(k_b(\hat{q} - \beta_l)) \end{pmatrix} \tag{5.38b}$$

Within regions $P_{u\eta}$, $P_{l\eta}$, $P_{u\beta}$, and $P_{l\beta}$ recall that

$$\hat{\sigma}_u = k_b\tau_{u\eta}\Psi'(k_b(\eta_u - \hat{u})) \tag{5.39a}$$

$$\hat{\sigma}_l = k_b\tau_{l\eta}\Psi'(k_b(\hat{u} - \eta_l)) \tag{5.39b}$$

$$\hat{\chi}_u = k_b\tau_{u\beta}\Psi'(k_b(\beta_u - \hat{q})) \tag{5.39c}$$

$$\hat{\chi}_l = k_b\tau_{l\beta}\Psi'(k_b(\hat{q} - \beta_l)). \tag{5.39d}$$

Compute the derivatives of $\hat{\sigma}_u$, $\hat{\sigma}_l$, $\hat{\chi}_u$, and $\hat{\chi}_l$ with respect to τ.

$$\hat{\sigma}_{u,\tau_{u\eta}} = k_b\left(\Psi'(k_b(\eta_u - \hat{u})) - \tau_{u\eta}\Psi''(k_b(\eta_u - \hat{u}))k_b u_{\tau_{u\eta}}\right) \tag{5.40a}$$

$$\hat{\sigma}_{u,\tau_X} = -\tau_{u\eta}\Psi''(k_b(\eta_u - \hat{u}))k_b u_{\tau_X}, X = l\eta, u\beta, l\beta \tag{5.40b}$$

$$\hat{\sigma}_{l,\tau_{l\eta}} = k_b\left(\Psi'(k_b(\hat{u} - \eta_l)) + \tau_{l\eta}\Psi''(k_b(\hat{u} - \eta_l))k_b u_{\tau_{l\eta}}\right) \tag{5.40c}$$

$$\hat{\sigma}_{l,\tau_X} = \tau_{l\eta}\Psi''(k_b(\hat{u} - \eta_l))k_b u_{\tau_X}, X = u\eta, u\beta, l\beta \tag{5.40d}$$

$$\hat{\chi}_{u,\tau_{u\beta}} = k_b\left(\Psi'(k_b(\beta_u - \hat{q})) - \tau_{u\beta}\Psi''(k_b(\beta_u - \hat{q}))k_b q_{\tau_{u\beta}}\right) \tag{5.40e}$$

$$\hat{\chi}_{u,\tau_X} = -\tau_{u\beta}\Psi''(k_b(\beta_u - \hat{q}))k_b q_{\tau_X}, X = u\eta, l\eta, l\beta \tag{5.40f}$$

$$\hat{\chi}_{l,\tau_{l\beta}} = k_b\left(\Psi'(k_b(\hat{q} - \eta_l)) + \tau_{l\eta}\Psi''(k_b(\hat{q} - \eta_l))k_b q_{\tau_{l\eta}}\right) \tag{5.40g}$$

$$\hat{\chi}_{l,\tau_X} = \tau_{l\beta}\Psi''(k_b(\hat{q} - \beta_l))k_b q_{\tau_X}, X = u\eta, l\eta, u\beta \tag{5.40h}$$

Recall that the goal of this step is to use the implicit function theorem by investigating $\nabla_\tau \Theta_k$ at $\tau = 0$. At $\tau_\eta = 0$ and $\tau_\beta = 0$ the following is known about the solution variables.

$$\hat{u}(0,k) = u^* \qquad \hat{q}(0,k) = q^* \qquad \hat{\lambda}(0,k) = \lambda^*$$

$$\begin{aligned}
\hat{\sigma}_u(0,k) &= \sigma_u^* > 0 \text{ in } A_{u\eta} \qquad & \hat{\sigma}_u(0,k) &= 0 \text{ in } P_{u\eta} \\
\hat{\sigma}_l(0,k) &= \sigma_l^* > 0 \text{ in } A_{l\eta} \qquad & \hat{\sigma}_l(0,k) &= 0 \text{ in } P_{u\eta} \\
\hat{\chi}_u(0,k) &= \chi_u^* > 0 \text{ in } A_{u\beta} \qquad & \hat{\chi}_u(0,k) &= 0 \text{ in } P_{u\beta} \\
\hat{\chi}_l(0,k) &= \chi_l^* > 0 \text{ in } A_{l\beta} \qquad & \hat{\chi}_l(0,k) &= 0 \text{ in } P_{l\beta}
\end{aligned} \tag{5.41}$$

The system $T_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)(\cdots) = t_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)$ may now be evaluated.

$$T_k(u^*,q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0) =$$

$$\begin{pmatrix} I_u & 0 & -A^\dagger & I_{\sigma_u} & -I_{\sigma_l} & 0 & 0 \\ 0 & \alpha I_q & I_\lambda & 0 & 0 & I_{\chi_u} & -I_{\chi_l} \\ k_p A & -k_p I_q & I_\lambda & 0 & 0 & 0 & 0 \\ -\sigma_u^* \Psi'(0) & 0 & 0 & -k_b^{-1} I_{\sigma_u} & 0 & 0 & 0 \\ \sigma_l^* \Psi'(0) & 0 & 0 & 0 & -k_b^{-1} I_{\sigma_l} & 0 & 0 \\ 0 & -\chi_u^* \Psi'(0) & 0 & 0 & 0 & -k_b^{-1} I_{\chi_u} & 0 \\ 0 & \chi_l^* \Psi'(0) & 0 & 0 & 0 & 0 & -k_b^{-1} I_{\chi_l} \end{pmatrix} \tag{5.42}$$

$$t_k(u^*,q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0) =$$

$$\begin{pmatrix} -k_b \Psi'(k_b(\eta_u - \hat{u})) & 0 & 0 & 0 \\ 0 & k_b \Psi'(k_b(\hat{u} - \eta_l)) & 0 & 0 \\ 0 & 0 & -k_b \Psi'(k_b(\beta_u - \hat{q})) & 0 \\ 0 & 0 & 0 & k_b \Psi'(k_b(\hat{q} - \beta_l)) \\ 0 & 0 & 0 & 0 \\ -\Psi'(k_b(\eta_u - \hat{u})) & 0 & 0 & 0 \\ 0 & -\Psi'(k_b(\hat{u} - \eta_l)) & 0 & 0 \\ 0 & 0 & -\Psi'(k_b(\beta_u - \hat{q})) & 0 \\ 0 & 0 & 0 & -\Psi'(k_b(\hat{q} - \beta_l)) \end{pmatrix} \tag{5.43}$$

Recognize that $T_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0) = \nabla\Theta_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)$, and therefore it is known that there must exist a ρ_0 such that $\|T_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)^{-1}\| \leq 2\rho_0^2$. The norm of the left hand side, $t_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)$, may also be bounded by utilizing the known upper bounds on $\Psi'(t)$, $\eta_u - \hat{u}$, $\hat{u} - \eta_l$, $\beta_u - \hat{q}$, and $\hat{q} - \beta_l$. In particular, by applying (3.6a) and (5.26) one receives the following bound.

$$\begin{aligned}\Psi'(k_b(\eta_u - \hat{u})) &\leq \frac{a}{k_b(\eta_u - \hat{u}) + 1} \\ &\leq \frac{a}{k_b(\eta_u - \hat{u})} \\ &\leq 2a(k_b U_{\hat{u}\eta})^{-1}\end{aligned} \tag{5.44}$$

A similar analysis may be performed for the remaining terms in $t_k(\cdot)$, which results in the following bound.

$$\begin{aligned}&\|t_k(u^*, q^*, \lambda^*, \sigma_u^*, \sigma_l^*, \chi_u^*, \chi_l^*, 0)\| \\ &\qquad \leq \max\{\|2ak_b(U_{u\eta}k_b)^{-1}\|, \|2ak_b(U_{l\eta}k_b)^{-1}\|, \|2ak_b(U_{u\beta}k_b)^{-1}\|, \|2ak_b(U_{l\beta}k_b)^{-1}\|, \\ &\qquad\qquad \|2a(U_{u\eta}k_b)^{-1}\|, \|2a(U_{l\eta}k_b)^{-1}\|, \|2a(U_{u\beta}k_b)^{-1}\|, \|2a(U_{l\beta}k_b)^{-1}\|\} \\ &\qquad \leq 2a \max\{\|(U_{u\eta})^{-1}\|, \|(U_{l\eta})^{-1}\|, \|(U_{u\beta})^{-1}\|, \|(U_{l\beta})^{-1}\|\}.\end{aligned} \tag{5.45}$$

For some small $\delta > 0$, the smoothness of the map $\Theta_k(\hat{u}, \hat{q}, \hat{\lambda}, \hat{\sigma}_u, \hat{\sigma}_l, \hat{\chi}_u, \hat{\chi}_l)$ implies that for $(k_b, \tau_{u\eta}, \tau_{l\eta}, \tau_{u\beta}, \tau_{l\beta}) \in S(k, \delta)$,

$$\left\| \begin{matrix} \hat{u}_{\tau_{u\eta}} & \hat{u}_{\tau_{l\eta}} & \hat{u}_{\tau_{u\beta}} & \hat{u}_{\tau_{l\beta}} \\ \hat{q}_{\tau_{u\eta}} & \hat{q}_{\tau_{l\eta}} & \hat{q}_{\tau_{u\beta}} & \hat{q}_{\tau_{l\beta}} \\ \hat{\lambda}_{\tau_{u\eta}} & \hat{\lambda}_{\tau_{l\eta}} & \hat{\lambda}_{\tau_{u\beta}} & \hat{\lambda}_{\tau_{l\beta}} \\ \hat{\sigma}_{u,\tau_{u\eta}} & \hat{\sigma}_{u,\tau_{l\eta}} & \hat{\sigma}_{u,\tau_{u\beta}} & \hat{\sigma}_{u,\tau_{l\beta}} \\ \hat{\sigma}_{l,\tau_{u\eta}} & \hat{\sigma}_{l,\tau_{l\eta}} & \hat{\sigma}_{l,\tau_{u\beta}} & \hat{\sigma}_{l,\tau_{l\beta}} \\ \hat{\chi}_{u,\tau_{u\eta}} & \hat{\chi}_{u,\tau_{l\eta}} & \hat{\chi}_{u,\tau_{u\beta}} & \hat{\chi}_{u,\tau_{l\beta}} \\ \hat{\chi}_{l,\tau_{u\eta}} & \hat{\chi}_{l,\tau_{l\eta}} & \hat{\chi}_{l,\tau_{u\beta}} & \hat{\chi}_{l,\tau_{l\beta}} \end{matrix} \right\| \leq \|T_k^{-1}(\cdot)\| \|t_k(\cdot)\| \leq 2\rho_0^2 C_3 \tag{5.46}$$

where $C_3 = 2a \max\{\|(U_{u\eta})^{-1}\|, \|(U_{l\eta})^{-1}\|, \|(U_{u\beta})^{-1}\|, \|(U_{l\beta})^{-1}\|\}$.

The norm of the derivatives with respect to τ is now bounded. To recover the terms required for the claim we perform an integration step.

$$\begin{aligned} \int_0^\tau \begin{pmatrix} \hat{u}_{\tau_{u\eta}} & \hat{u}_{\tau_{l\eta}} & \hat{u}_{\tau_{u\beta}} & \hat{u}_{\tau_{l\beta}} \\ \hat{q}_{\tau_{u\eta}} & \hat{q}_{\tau_{l\eta}} & \hat{q}_{\tau_{u\beta}} & \hat{q}_{\tau_{l\beta}} \\ \hat{\lambda}_{\tau_{u\eta}} & \hat{\lambda}_{\tau_{l\eta}} & \hat{\lambda}_{\tau_{u\beta}} & \hat{\lambda}_{\tau_{l\beta}} \\ \hat{\sigma}_{u,\tau_{u\eta}} & \hat{\sigma}_{u,\tau_{l\eta}} & \hat{\sigma}_{u,\tau_{u\beta}} & \hat{\sigma}_{u,\tau_{l\beta}} \\ \hat{\sigma}_{l,\tau_{u\eta}} & \hat{\sigma}_{l,\tau_{l\eta}} & \hat{\sigma}_{l,\tau_{u\beta}} & \hat{\sigma}_{l,\tau_{l\beta}} \\ \hat{\chi}_{u,\tau_{u\eta}} & \hat{\chi}_{u,\tau_{l\eta}} & \hat{\chi}_{u,\tau_{u\beta}} & \hat{\chi}_{u,\tau_{l\beta}} \\ \hat{\chi}_{l,\tau_{u\eta}} & \hat{\chi}_{l,\tau_{l\eta}} & \hat{\chi}_{l,\tau_{u\beta}} & \hat{\chi}_{l,\tau_{l\beta}} \end{pmatrix} d \begin{pmatrix} u \\ q \\ \lambda \\ \sigma_u \\ \sigma_l \\ \chi_u \\ \chi_l \end{pmatrix} &= \begin{pmatrix} \hat{u}(\tau,k) - \hat{u}(0,k) \\ \hat{q}(\tau,k) - \hat{q}(0,k) \\ \hat{\lambda}(\tau,k) - \lambda(0,k) \\ \hat{\sigma}_u(\tau,k) - \sigma_u(0,k) \\ \hat{\sigma}_l(\tau,k) - \sigma_l(0,k) \\ \hat{\chi}_u(\tau,k) - \chi_u(0,k) \\ \hat{\chi}_l(\tau,k) - \chi_l(0,k) \end{pmatrix} \\ &= \begin{pmatrix} \hat{u}(\tau,k) - u^* \\ \hat{q}(\tau,k) - q^* \\ \hat{\lambda}(\tau,k) - \lambda^* \\ \hat{\sigma}_u(\tau,k) - \sigma_u^* \\ \hat{\sigma}_l(\tau,k) - \sigma_l^* \\ \hat{\chi}_u(\tau,k) - \chi_u^* \\ \hat{\chi}_l(\tau,k) - \chi_l^* \end{pmatrix} \end{aligned} \tag{5.47}$$

It can therefore be seen that

$$\left\| \begin{matrix} \hat{u}(\tau,k)-u^* \\ \hat{q}(\tau,k)-q^* \\ \hat{\lambda}(\tau,k)-\lambda^* \\ \hat{\sigma}_u(\tau,k)-\sigma_u^* \\ \hat{\sigma}_l(\tau,k)-\sigma_l^* \\ \hat{\chi}_u(\tau,k)-\chi_u^* \\ \hat{\chi}_l(\tau,k)-\chi_l^* \end{matrix} \right\| = \left\| \int_0^\tau T_k^{-1}(\cdot,\xi)t_k(\cdot)d\xi \right\|$$

$$\le \int_0^\tau \|T_k^{-1}(\cdot,\xi)\|\|t_k(\cdot)\|d\xi$$

$$\le \int_0^\tau \|\rho_0 C_3\|d\xi$$

$$\le \rho_0 C_3 \|\tau\| \tag{5.48}$$

Recalling the definition of τ in (5.9) we see that

$$\|\tau\| = \max\{\|k_b^{-1}(\sigma_u-\sigma_u^*)\|, \|k_b^{-1}(\sigma_l-\sigma_l^*)\|, \|k_b^{-1}(\chi_u-\chi_u^*)\|, \|k_b^{-1}(\chi_l-\chi_l^*)\|\}$$

$$= k_b^{-1}\max\{\|(\sigma_u-\sigma_u^*)\|, \|(\sigma_l-\sigma_l^*)\|, \|(\chi_u-\chi_u^*)\|, \|(\chi_l-\chi_l^*)\|\} \tag{5.49}$$

Noting that τ is simply a function of σ and χ it can be seen that

$$\max\{\|\hat{u}-u^*\|, \|\hat{q}-q^*\|, \|\hat{\lambda}-\lambda^*\|, \|\hat{\sigma}_u-\sigma_u^*\|, \|\hat{\sigma}_l-\sigma_l^*\|, \|\hat{\chi}_u-\chi_u^*\|, \|\hat{\chi}_l-\chi_l^*\|\}$$

$$\le \frac{\rho_0 C_3}{k_b}\max\{\|\sigma_u-\sigma_u^*\|, \|\sigma_l-\sigma_l^*\|, \|\chi_u-\chi_u^*\|, \|\chi_l-\chi_l^*\|\} \tag{5.50}$$

Recognize that the term on the left hand side of this inequality is only over the Lagrange multipliers associated with the constraints in their respective active domains. Inclusion of (5.31) therefore implies that

$$\max\{\|\hat{u}-u^*\|,\|\hat{q}-q^*\|,\|\hat{\lambda}-\lambda^*\|,\|\hat{\sigma}_u-\sigma_u^*\|,\|\hat{\sigma}_l-\sigma_l^*\|,\|\hat{\chi}_u-\chi_u^*\|,\|\hat{\chi}_l-\chi_l^*\|\}$$
$$\leq \frac{C}{k_b}\max\{\|\sigma_u-\sigma_u^*\|,\|\sigma_l-\sigma_l^*\|,\|\chi_u-\chi_u^*\|,\|\chi_l-\chi_l^*\|\} \tag{5.51}$$

where $C = \max\{C_0, \rho_0 C_3\}$. This completes the claim.

□

Chapter 6: Super-linear Convergence of a PDNRAL Method for Control-Constrained Optimization with Elliptic Equality Constraints

The subject of this chapter is a full primal dual NRAL method, this time for an optimization problem with elliptic PDE constrained that has constraints on the just control.

$$
\begin{aligned}
&\text{minimize } J(u,q) = \frac{1}{2}\|u - u_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|q\|^2_{L^2(\Omega)} \\
&\text{subject to } Au = q \text{ in } \Omega \qquad (6.1) \\
&\qquad\qquad \beta(q) \geq 0 \text{ a.e. in } \Omega
\end{aligned}
$$

where $u \in \mathcal{W}$, and $A : \mathcal{W} \to L^2(\Omega)$ is a uniformly elliptic, self-adjoint operator, and q, u_d, and β are all in $L^2(\Omega)$. Furthermore β is required to be concave and strictly monotonic, and $\alpha > 0$.

Problem (6.1), assumed to satisfy strict complementarity. Furthermore, the strong convexity of $\mathcal{J}(u,q)$ allow one to assume that the second order optimality conditions are satisfied.

6.1 Optimality Conditions

Begin by defining the Lagrangian for problem (6.1) in the usual way, with $\lambda \in \mathcal{W}$ and let $\chi \in L^2(\Omega)$.

$$L(u, q, \lambda, \chi) = \frac{1}{2}\|u - u_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|q\|^2_{L^2(\Omega)} - (\lambda, Au - q) - (\chi, \beta(q)) \tag{6.2}$$

The first order optimality conditions for this problem are known [23]. Let (u^*, q^*) be the solution to Problem (6.1), then there must exist a Lagrange multipliers $\lambda^* \in \mathcal{W}$ and $\chi^* \in L^2(\Omega)$ such that the following conditions hold.

$$\nabla_u L(u^*, q^*, \lambda^*, \chi^*) = (u^* - u_d) - A^\dagger \lambda^* = 0 \tag{6.3a}$$

$$\nabla_q L(u^*, q^*, \lambda^*, \chi^*) = \alpha q^* + \lambda^* - \chi^* \nabla_q \beta(q^*) = 0 \tag{6.3b}$$

$$\nabla_\lambda L(u^*, q^*, \lambda^*, \chi^*) = Au^* - q^* = 0 \tag{6.3c}$$

$$\chi^* \geq 0 \qquad \beta(q^*) \geq 0 \qquad (\chi^*, \beta(q^*)) = 0 \tag{6.3d}$$

6.2 The PDNRAL Method

The derivation of the PDNRAL method begins much in the same way as the NR-PDAL method from Chapter 5. The Lagrangian is first augmented and modified in the normal NRAL way.

$$\begin{aligned} \mathcal{L}_k(u, q, \lambda, \chi) = \frac{1}{2}\|u - u_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|q\|^2_{L^2(\Omega)} - (\lambda, Au - q) \\ + \frac{k}{2}(Au - q, Au - q) - \frac{1}{k}(\chi, \varPsi(k\beta(q))) \end{aligned} \tag{6.4}$$

Compute the gradient of $\mathcal{L}_k$.

$$\begin{aligned}\nabla_u \mathcal{L}_k(u, q, \lambda, \chi) &= (u - u_d) - A^\dagger \lambda + k A^\dagger (Au - q) \\ &= (u - u_d) - A^\dagger (\lambda - k(Au - q))\end{aligned} \tag{6.5}$$

$$\nabla_q \mathcal{L}_k(u, q, \lambda, \chi) = \alpha q + \lambda - k(Au - q) - \chi \Psi(k\beta(q)) \nabla_q \beta(q)$$

Construct the variables $\hat{\lambda}$ and $\hat{\chi}$ using the NRAL Lagrange multiplier update inspired formula.

$$\hat{\lambda} = \lambda - k(A\hat{u} - \hat{q}) \tag{6.6a}$$

$$\hat{\chi} = \chi \Psi'(k\beta(\hat{q})) \tag{6.6b}$$

In the NR-PDAL method the $\hat{\lambda}$ variable, along with the updated $\hat{u}$ and $\hat{q}$, was inserted into (6.5) to construct the inner system to be solved at each PDAL step, which was followed by the NR multiplier update. The PDNRAL method is a full primal dual method which solves for all variables at once, doing away with the inner optimization step. Therefore both $\hat{\lambda}$ and $\hat{\chi}$ are inserted into (6.5), which leads to the following system of equations which must be solved.

$$\begin{aligned}\nabla_u L(\hat{u}, \hat{q}, \hat{\lambda}, \hat{\chi}) &= (\hat{u} - u_d) - A^\dagger \hat{\lambda} = 0 \\ \nabla_q L(\hat{u}, \hat{q}, \hat{\lambda}, \hat{\chi}) &= \alpha \hat{q} + \hat{\lambda} - \hat{\chi} \nabla_q \beta(\hat{q}) = 0 \\ \hat{\lambda} - \lambda + k(A\hat{u} - \hat{q}) &= 0 \\ \hat{\chi} - \chi \Psi'(k\beta(\hat{q})) &= 0\end{aligned} \tag{6.7}$$

The PDNRAL method then becomes solving (6.7) using Newton's method.

6.3 Local Convergence Analysis

The finite dimensional primal-dual NRAL method was first introduced as the Exterior Point Method (EPM) in [18], where it was shown to have 1.5-q-superlinear convergence under appropriate conditions. The analysis that follows is done in function space over this elliptically constrained optimization problem with control constraints, and confirms that the method retains superlinear convergence.

The first step in this analysis is the definition of the merit function $v(u, q, \lambda, \chi) \in \mathcal{W} \times L^2 \times \mathcal{W} \times L^2$.

$$\begin{aligned} v(u, q, \lambda, \chi) = \max\{&\|\nabla_u L(u, q, \lambda, \chi)\|, \|\nabla_q L(u, q, \lambda, \chi)\|, \|Au - q\|, \\ &- \min(\beta(q)), \|\chi\beta(q)\|, - \min(\chi)\} \end{aligned} \tag{6.8}$$

This function serves as both a measure of error in the current solution as well as an input to the update strategy for the barrier/penalty parameter k. After each successful Newton step a new k will be the be selected.

$$k = \frac{1}{\sqrt{v(u, q, \lambda, \chi)}} \tag{6.9}$$

The system of equations that is solved at each Newton step can be computed in the usual way, by linearizing (6.7) about the solution u^*, q^*, λ^*, and χ^*. The Newton system is

$$M_k(u,q,\lambda,\chi)\begin{pmatrix}\delta u\\ \delta q\\ \delta\lambda\\ \delta\chi\end{pmatrix} = a_k(u,q,\lambda,\chi) \tag{6.10}$$

where

$$M_k(u,q,\lambda,\chi) = \begin{pmatrix} I_u & 0 & -A^{\dagger} & 0 \\ 0 & \alpha I_q - \chi\nabla^2_{qq}\beta(q) & I_\lambda & -\nabla_q\beta(q) \\ kA & -ku & -I_\lambda & 0 \\ 0 & k\chi\Psi''(k\beta(q))\nabla_q\beta(q) & 0 & I_\chi \end{pmatrix} \tag{6.11}$$

and

$$a_k(u,q,\lambda,\chi) = \begin{pmatrix} -(u-u_d)+A^{\dagger}\lambda \\ -\alpha q - \lambda + \chi\nabla_q\beta(q) \\ -k(Au-q) \\ \chi(\Psi'(k\beta(q))-1) \end{pmatrix} \tag{6.12}$$

The convergence analysis requires the particular bounds on $v(u,q,\lambda,\chi)$, which are proven in the following lemma.

Lemma 6.3.1. *Define $z=(u,q,\lambda,\chi)$ and z^* to be the solution to Problem* (6.1). *Define $B_\epsilon(z^*)=\{z:\|z-z^*\|\le\epsilon\}$. Then there exists a small enough $\epsilon>0$ such that for all $z\in B_\epsilon(z^*)$ there exists a L_1 and L_2 such that $L_2>L_1>0$ and*

$$L_1\|z-z^*\| \le v(z) \le L_2\|z-z^*\| \tag{6.13}$$

Proof. By definition of $v(z)$ and its implication that $v(z^*) = 0$ it is evident that there must exist an $L_2 > 0$ such that $v(z) \leq L_2 \|z - z^*\|$.

The lower bound $L_1 \|z - z^*\|$ is computed first for χ in Ω_P. Within Ω_P it must be that there exists a $\tau_1 > 0$ such that $\beta(q) \geq \tau_1$. By definition of $v(z)$ we have the $\|\chi \beta(q)\| \leq v(z)$, and therefore

$$v(z) \geq ||\chi \beta(q)\| \geq \|\chi \tau_1\| = \tau_1 \|\chi\| \tag{6.14}$$

In order to bound the remainder of the variables in $\|z - z^*\|$ the optimality conditions (6.3) will be linearized about z^*, with χ only being considered within Ω_A. After incorporation of the known optimality conditions the resulting system of equations is

$$M_\infty(z) \begin{pmatrix} u - u^* \\ q - q^* \\ \lambda - \lambda^* \\ \chi - \chi^* \end{pmatrix} = \begin{pmatrix} -(u - u_d) + A^\dagger \lambda \\ -\alpha q - \lambda + \chi \nabla_q \beta(q) \\ -Au + q \\ -\beta(q) \end{pmatrix} \tag{6.15}$$

where

$$M_\infty(z) = \begin{pmatrix} I_u & 0 & -A^\dagger & 0 \\ 0 & \alpha I_q - \chi \nabla^2_{qq} \beta(q) & I_\lambda & -\nabla_q \beta(q) \\ A & -I_u & 0 & 0 \\ 0 & -\nabla_q \beta(q) & 0 & 0 \end{pmatrix}. \tag{6.16}$$

To prove that $M_\infty(z)$ is invertible one can use a contradiction by assuming it is not invertible. Then there must exist a non-zero vector $w = (w_u, w_q, w_\lambda, w_\chi)$ such that

$M_\infty(z)w = 0$. Write $M_\infty(z)w = 0$ as the following system of equations:

$$\begin{pmatrix} I_u & 0 \\ 0 & \alpha I_q - \chi \nabla^2_{qq}\beta(q) \end{pmatrix} \begin{pmatrix} w_u \\ w_q \end{pmatrix} + \begin{pmatrix} -A^\dagger & 0 \\ I_\lambda & -\nabla_q \beta(q) \end{pmatrix} \begin{pmatrix} w_\lambda \\ w_\chi \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{6.17a}$$

$$\begin{pmatrix} A & -I_u \\ 0 & -\nabla_q \beta(q) \end{pmatrix} \begin{pmatrix} w_u \\ w_q \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{6.17b}$$

Multiplying (6.17a) by (w_u, w_q) gives

$$\begin{pmatrix} w_u & w_q \end{pmatrix} \begin{pmatrix} I_u & 0 \\ 0 & \alpha I_q - \chi \nabla^2_{qq}\beta(q) \end{pmatrix} \begin{pmatrix} w_u \\ w_q \end{pmatrix} + \begin{pmatrix} w_u & w_q \end{pmatrix} \begin{pmatrix} -A^\dagger & 0 \\ I_\lambda & -\nabla_q \beta(q) \end{pmatrix} \begin{pmatrix} w_\lambda \\ w_\chi \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{6.18}$$

The second term on the left hand side of (6.18) can be rearranged to show that

$$\begin{pmatrix} w_u & w_q \end{pmatrix} \begin{pmatrix} -A^\dagger & 0 \\ I_\lambda & -\nabla_q \beta(q) \end{pmatrix} \begin{pmatrix} w_\lambda \\ w_\chi \end{pmatrix} = \begin{pmatrix} w_\lambda & w_\chi \end{pmatrix} \begin{pmatrix} A & -I_u \\ 0 & -\nabla_q \beta(q) \end{pmatrix} \begin{pmatrix} w_u \\ w_q \end{pmatrix} \tag{6.19}$$

But (6.17b) is already known, and therefore the terms on both sides of (6.19) are equal to zero. All that remains of (6.18) then is

$$\begin{pmatrix} w_u & w_q \end{pmatrix} \begin{pmatrix} I_u & 0 \\ 0 & \alpha I_q - \chi \nabla^2_{qq}\beta(q) \end{pmatrix} \begin{pmatrix} w_u \\ w_q \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{6.20}$$

Since $M_\infty(z)$ is constructed in Ω_A it is known that $\chi > 0$. Additionally it is known that $\nabla^2_{qq}\beta(q) < 0$. Therefore $\alpha I_q - \chi \nabla^2_{qq}\beta(q) > 0$, and (6.20) implies that $w_u = w_q = 0$.

With w_u and w_q equal to zero one is left with he second term in (6.17a), which is equivalent to

$$-A^{\dagger}w_{\lambda} = 0 \tag{6.21a}$$

$$w_{\lambda} - \nabla_q \beta(q) w_{\chi} = 0 \tag{6.21b}$$

By the self-adjoint requirement on A we know that $A^{\dagger}$ is also uniformly elliptic. This fact, along with $w_{\lambda_{\partial\Omega}} = 0$ allows for the Weak Maximum Principle to be used to state that $w_{\lambda} = 0$. With $w_{\lambda} = 0$ and recalling strict monotonicity of $\beta(q)$, (6.21b) requires $w_{\chi} = 0$. Therefore $M_{\infty}(z)w = 0$ only if $w = 0$, and $M_{\infty}(z)$ must be invertible. Then there must exist a $\rho_0 > 0$ such that $\|M_{\infty}(z)^{-1}\| < \rho_0$. This implies that $\|z - z^*\|$ is bounded, and this bound will be used to form the lower bound on $v(z)$.

$$\|z - z^*\| \leq \rho_0 \left\| \begin{matrix} -(u - u_d) + A^{\dagger}\lambda \\ -\alpha q - \lambda + \chi \nabla_q \beta(q) \\ -Au + q \\ -\beta(q) \end{matrix} \right\|_{\infty}$$

$$= \rho_0 \max\{\|u - u_d - A^{\dagger}\lambda\|_{\Omega_A}, \|\alpha q + \lambda - \chi \nabla_q \beta(q)\|_{\Omega_A}, \|Au - q\|_{\Omega_A}, \|\beta(q)\|_{\Omega_A}\} \tag{6.22}$$

Using definition of $v(z)$ and $\|\cdot\|_{\Omega_A} \leq \|\cdot\|_{\Omega}$ it can be seen than

$$\begin{aligned}
\max\{\|u - u_d - A^{\dagger}\lambda\|_{\Omega_A}, &\|\alpha q + \lambda - \chi \nabla_q \beta(q)\|_{\Omega_A}, \|Au - q\|_{\Omega_A}\} \\
&\leq \max\{\|u - u_d - A^{\dagger}\lambda\|_{\Omega}, \|\alpha q + \lambda - \chi \nabla_q \beta(q)\|_{\Omega}, \|Au - q\|_{\Omega}\}. \\
&\leq v(z)
\end{aligned} \tag{6.23}$$

Within Ω_A there must exist a $\tau_2 > 0$ such that $|\beta(q)| \leq \tau_2$, and therefore

$$\|\beta(q)\| \leq \tau_2 \tag{6.24}$$

Finally then, $v(z)$ can be bounded below by

$$L_1 \|z - z^*\| \leq v(z) \tag{6.25}$$

where

$$L_1^{-1} = \max\{\|u - u_d - A^{\dagger}\lambda\|_{\Omega}, \|\alpha q + \lambda - \chi \nabla_q \beta(q)\|_{\Omega}, \|Au - q\|_{\Omega}, \tau_2\} \tag{6.26}$$

□

The upper and lower bounds on $v(z)$ now defined the convergence analysis of the PDNRAL method for control constrained problems may proceed.

Theorem 6.3.2. *Define $z^* = (u^*, q^*, \lambda^*, \chi^*)$ to be the solution to Problem* (6.1)*, and define $B_\epsilon(z^*) = \{z : \|z - z^*\| \leq \epsilon\}$. Let $\hat{z} = (\hat{u}, \hat{q}, \hat{\lambda}, \hat{\chi})$ be the solution to the single step after the solution to the system of equations* (6.10)*, where $k = v(z)^{-0.5}$. Then* *there exists a small positive $\epsilon \ll 1$ such that for any $z \in B_\epsilon(z^*)$ the error on $\hat{z}$ is*

$$\|\hat{z} - z^*\| \leq \rho \|z - z^*\|^{\frac{3}{2}} \tag{6.27}$$

for some $\rho > 0$.

Proof. Define $\partial z = (\partial u, \partial q, \partial \lambda, \partial \chi)$ to be the step taken at each PDNRAL step, i.e. the solution to (6.10). To analyze this problem the system of equations will be modified by splitting the χ equations into both the active and passive regions. This modified system of equations results in a new $M_k(z)$ and $a_k(z)$.

$$\widehat{M}_k(z) = \begin{pmatrix} I_u & 0 & -A^\dagger & 0 & 0 \\ 0 & \alpha I_q & -I_\lambda \chi \nabla^2_{qq}\beta(q) & -\nabla_q\beta(q) I_{\chi,\Omega_A} & -\nabla_q\beta(q) I_{\chi,\Omega_P} \\ kA & -kI_q & -I_\lambda & 0 & 0 \\ 0 & k\chi_{\Omega_A}\Psi''(k\beta(q))\nabla_q\beta(q) & 0 & I_{\chi,\Omega_A} & 0 \\ 0 & k\chi_{\Omega_P}\Psi''(k\beta(q))\nabla_q\beta(q) & 0 & 0 & I_{\chi,\Omega_P} \end{pmatrix} \tag{6.28}$$

$$\hat{a}_k(z) = \begin{pmatrix} -(u - u_d) + A^\dagger \lambda \\ -\alpha q - \lambda + \chi \nabla_q \beta(q) \\ -k(Au - q) \\ \chi_{\Omega_A}(\Psi'(k\beta(q)) - 1) \\ \chi_{\Omega_P}(\Psi'(k\beta(q)) - 1) \end{pmatrix} \tag{6.29}$$

Using $\hat{\chi}_{\Omega_P} = \chi_{\Omega_P} + \partial \chi_{\Omega_P}$ the equation for χ_{Ω_P} can be rewritten as

$$\hat{\chi}_{\Omega_P} = \chi_{\Omega_P}\Psi'(k\beta(q)) - k\chi_{\Omega_P}\Psi''(k\beta(q))\nabla_q\beta(q)\partial q. \tag{6.30}$$

Using requirements (3.6a) and (3.6b) there must exist an $a > 0$ such that $\Psi'(k\beta(q)) \leq a(k\beta(q)+1)^{-1}$, and a $b > 0$ such that $-\Psi''(k\beta(q)) \leq b(k\beta(q)+1)^{-2}$. Additionally it is known that within Ω_P there exists a ξ_1 and ξ_2 such that $\beta(q) \geq \xi_1$.

$$
\begin{aligned}
\hat{\chi}_{\Omega_P} &\leq \chi_{\Omega_P}\left(a(k\beta(q)+1)^{-1} + kb(k(\beta(q)+1)^{-2})\nabla_q\beta(q)\partial q\right) \\
&\leq \chi_{\Omega_P}\left(a(k\beta(q))^{-1} + kb(k(\beta(q))^{-2})\nabla_q\beta(q)\partial q\right) \\
&\leq \chi_{\Omega_P}k^{-1}\left(a\xi_1^{-1} + b\xi_1^{-2}\nabla_q\beta(q)\partial q\right)
\end{aligned}
\tag{6.31}
$$

Continuity of $\beta(q)$ and boundedness of the space Ω_P imply there exists a $\xi_2 > 0$ and $\xi_3 > 0$ and such that $\|\nabla_q\beta(q)\| \leq \xi_2$ and $\|\partial q\| \leq \xi_3$. Then the norm of $\hat{\chi}_{\Omega_P}$ can be further bounded.

$$
\begin{aligned}
\|\hat{\chi}_{\Omega_P}\| &\leq \left\|\chi_{\Omega_P}k^{-1}\left(a\xi_1^{-1} + b\xi_1^{-2}\nabla_q\beta(q)\partial q\right)\right\| \\
&\leq k^{-1}\|\chi_{\Omega_P}\|\left\|a\xi_1^{-1} + b\xi_1^{-2}\nabla_q\beta(q)\partial q\right\| \\
&\leq k^{-1}\|\chi_{\Omega_P}\|\left\|a\xi_1^{-1} + b\xi_1^{-2}\xi_2\xi_3\right\|
\end{aligned}
\tag{6.32}
$$

By definition it is known that $\|\chi - \chi^*\| \leq \|z - z^*\|$. There exists an $L_1 > 0$ such that $L_2\|\chi - \chi^*\| \geq v(z)$. But by the k update strategy $k = v(z)^{-\frac{1}{2}}$, and therefore

$$
k^{-1} \leq (L_2\|z - z^*\|)^{\frac{1}{2}}. \tag{6.33}
$$

Finally, within Ω_P $\chi^* = 0$, so $\|\chi\| \leq \|z - z^*\|$. This results in the claimed bound on χ within Ω_P.

$$
\|\hat{\chi}_{\Omega_P}\| \leq (L_2)^{\frac{1}{2}}\left\|a\xi_1^{-1} + b\xi_1^{-2}\xi_2\xi_3\right\|\|z - z^*\|^{\frac{3}{2}} = C_1\|z - z^*\|^{\frac{3}{2}} \tag{6.34}
$$

The remaining functionals (u, q, λ, and χ_{Ω_A}) will be treated via the primal dual system $\widehat{M}_k(z)\partial z = \hat{a}_k(z)$ with the χ_{Ω_P} equation eliminated. The λ and χ_{Ω_A} equations are also modified by dividing them by k and $k\chi_{\Omega_A}\Psi''(k\beta(q))$, respectively, resulting in the reduced system of equations $M_k(z)\widehat{\partial z} = a_k$, where

$$M_k(z) = \begin{pmatrix} I_u & 0 & -A^\dagger & 0 \\ 0 & \alpha I_q - \chi\nabla^2_{qq}\beta(q) & I_\lambda & -\nabla_q\beta(q)I_{\chi,\Omega_q} \\ A & -I_q & -k^{-1}I_\lambda & 0 \\ 0 & I_q & 0 & (k\chi_{\Omega_A}\Psi''(k\beta(q)))^{-1} \end{pmatrix} \tag{6.35}$$

and

$$a_k = \begin{pmatrix} -(u-u_d) + A^\dagger\lambda \\ -\alpha q - \lambda + \chi\nabla_q\beta(q) \\ -Au + q \\ (k\Psi''(k\beta(q)))^{-1}(\Psi'(k\beta(q)) - 1) \end{pmatrix} \tag{6.36}$$

The bounds on $\widehat{\partial z}$ will be formed by comparison with a single step, $\overline{\partial z}$, found via Newton's method applied to the subset of (6.3) where that subset consists of just Ω_A. Define $\overline{z} = z + \overline{\partial z}$.

$$\begin{aligned} \|\hat{z} - z^*\| &= \|(z + \widehat{\partial z}) + (\overline{\partial z} - \overline{\partial z}) - z^*\| \\ &= \|\overline{z} - z^* + \widehat{\partial z} - \overline{\partial z}\| \\ &\le \|\overline{z} - z^*\| + \|\widehat{\partial z} - \overline{\partial z}\| \end{aligned} \tag{6.37}$$

This Newton step, $\overline{\partial z}$, is computed as the solution to $M_\infty(z)\overline{\partial z} = a_\infty(z)$, where

$$M_\infty(z) = \begin{pmatrix} I_u & 0 & -A^\dagger & 0 \\ 0 & \alpha I_q - \chi\nabla^2_{qq}\beta(q) & I_\lambda & -\nabla_q\beta(q)I_{\chi,\Omega_q} \\ A & -I_q & 0 & 0 \\ 0 & I_q & 0 & 0 \end{pmatrix} \tag{6.38}$$

and

$$a_\infty = \begin{pmatrix} -(u-u_d) + A^\dagger\lambda \\ -\alpha q - \lambda + \chi\nabla_q\beta(q) \\ -Au + q \\ -\beta(q) \end{pmatrix}. \tag{6.39}$$

Invertibility of the operator $M_\infty(z)$ has already been established, and there must exist a $\rho_0 > 0$ such that $\|M_\infty(z)^{-1}\| < \rho_0$. Invertibility of $M_k(z)$ is established using Lemma 4.3.1. Recognize that

$$\begin{aligned} \|M_\infty - M_k\| &= \left\| \begin{matrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & k^{-1}I_\lambda & 0 \\ 0 & 0 & 0 & -(k\chi_{\Omega_A}\Psi''(k\beta(q)))^{-1} \end{matrix} \right\| \\ &\le \max\{\|k^{-1}\|, \|(k\chi_{\Omega_A}\Psi''(k\beta(q)))^{-1}\|\} \end{aligned} \tag{6.40}$$

By the definition of $\Psi''(t)$ condition (3.5d) there must exist a $\xi_4 > 0$ such that

$\Psi''(t) \geq \xi_4^{-1}$, and therefore

$$\|\Psi''(k\beta(q))^{-1}\| \leq \|\xi_4\|. \tag{6.41}$$

Additionally within Ω_A there must exist a $\xi_5 > 0$ such that $\chi_A \geq \xi_5$.

Therefore the bounds on $\|M_\infty - M_k\|$ may be written as

$$\begin{aligned}\|M_\infty - M_k\| &\leq \max\{\|k^{-1}\|, \|(k\chi_{\Omega_A}\Psi''(k\beta(q)))^{-1}\|\} \\ &\leq \max\{\|(L_2\|z - z^*\|)^{\frac{1}{2}}\|, \|(L_2\|z - z^*\|)^{\frac{1}{2}}\|\|\xi_5\|\|\xi_4\|\} \\ &\leq \max\{L_2^{\frac{1}{2}}, L_2^{\frac{1}{2}}\xi_5\xi_4\}\|z - z^*\|^{\frac{1}{2}} \\ &= C_2\|z - z^*\|^{\frac{1}{2}}\end{aligned} \tag{6.42}$$

The invertibility of $M_\infty(z)$ and bounds on $\|M_\infty(z) - M_k(z)\|$ allow use of Lemma 4.3.1 to state that $M_k(z)$ is invertible and the following bounds hold.

$$\|M_k^{-1}(z)\| \leq 2\rho_0 \tag{6.43}$$

With invertibility of $M_\infty(z)$ and $M_k(z)$ (6.37) may be rewritten as

$$\begin{aligned}
\|\hat{z}-z^*\| &\leq \|\overline{z}-z^*\| + \|M_\infty^{-1}(z)a_\infty(z) - M_k^{-1}(z)a_k(z)\| \\
&=\leq \|\overline{z}-z^*\| + \|M_\infty^{-1}(z)a_\infty(z) - M_k^{-1}(z)a_k(z) - M_k^{-1}(z)a_\infty(z) + M_k^{-1}(z)a_\infty(z)\| \\
&\leq \|\hat{z}-z^*\| + \|M_\infty^{-1}(z)\|\|M_k^{-1}(z)\|\|M_\infty(z)-M_k(z)\|\|a_\infty(z)\| \\
&\quad + \|M_k^{-1}(z)\|\|a_\infty(z)-a_k(z)\| \\
&\leq \|\hat{z}-z^*\| + 2\rho_0^2 C_2\|z-z^*\|^{\frac{1}{2}}\|a_\infty(z)\| + 2\rho_0\|a_\infty(z)-a_k(z)\|
\end{aligned} \tag{6.44}$$

The definitions of $v(z)$, $a_\infty(z)$, and Lemma 6.3.1 imply that

$$\|a_\infty(z)\| \leq v(z) \leq L_2\|z-z^*\|. \tag{6.45}$$

The remaining bound that must be established on

$$\begin{aligned}
\|a_\infty(z)-a_k(z)\| &= \left\| \begin{matrix} 0 \\ 0 \\ 0 \\ -\beta(q) - (k\Psi''(k\beta(q)))^{-1}(\Psi'(k\beta(q))-1) \end{matrix} \right\| \\
&= \|-\beta(q) - (k\Psi''(k\beta(q)))^{-1}(\Psi'(k\beta(q))-1)\|
\end{aligned} \tag{6.46}$$

The Lagrange interpolatory equation will be used twice in order to construct a form in which allows this term to be bounded. Let t_1, t_2, t_3 and t_4 be in $\mathbb{R}$, then there must exist a θ_1 and $\theta_2 \in (0,1)$ such that

$$\Psi''(\theta_1 t_1 + (1-\theta_1)t_2) = \frac{\Psi'(t_1) - \Psi'(t_2)}{t_1 - t_2} \tag{6.47}$$

and

$$\Psi'''(\theta_2 t_3 + (1-\theta_2)t_4) = \frac{\Psi''(t_3) - \Psi''(t_4)}{t_3 - t_4} \tag{6.48}$$

Recognize that with in Ω_A we have $\beta(q^*) = 0$, and that $\Psi'(0) = 1$. Let $t_1 = k\beta(q)$ and $t_2 = k\beta(q^*)$. Then (6.47) becomes

$$\Psi'(k\beta(q)) - 1 = \Psi''(\theta_1 k\beta(q))k\beta(q) \tag{6.49}$$

Equation (6.49) may then be inserted into (6.46).

$$\begin{aligned} \|a_\infty(z) - a_k(z)\| &= \left\| -\beta(q) - \frac{(\Psi''(\theta_1 k\beta(q))k\beta(q))}{k\Psi''(k\beta(q))} \right\| \\ &= \left\| -\beta(q) \frac{\Psi''(k\beta(q)) - \Psi''(\theta_1 k\beta(q))}{\Psi''(k\beta(q))} \right\| \end{aligned} \tag{6.50}$$

Next define $t_3 = \theta_1 k\beta(q)$ and $t_4 = k\beta(q)$. Then (6.48) becomes

$$\Psi''(\theta_1 k\beta(q)) - \Psi''(k\beta(q)) = \Psi'''(t_5)(\theta_1 - 1)k\beta(q) \tag{6.51}$$

where $t_5 = (\theta_2\theta_1 + (1-\theta_2))k\beta(q)$. Inserting (6.51) results in

$$\begin{aligned}
\|a_\infty(z) - a_k(z)\| &= \left\| \beta(q) \frac{\Psi'''(t_5)(\theta_1 - 1)k\beta(q)}{\Psi''(k\beta(q))} \right\| \\
&\le |\theta_1 - 1| \|k^{-1}k\beta(q)\| \|\Psi'''(t_5)\| \|k\beta(q)\| \|\Psi''(k\beta(q))^{-1}\| \\
&\le |\theta_1 - 1| \|k^{-1}\| \|k\beta(q)\|^2 \|\Psi'''(t_5)\| \|\Psi''(k\beta(q))^{-1}\|
\end{aligned} \tag{6.52}$$

Using the known bounds on $v(z)$, $k^{-1} = v(z)^{-\frac{1}{2}}$, it is known that

$$\begin{aligned}
\|k\beta(q)\| &\le \left((L_1\|z - z^*\|)^{-\frac{1}{2}}\right)(v(z)) \\
&\le \left((L_1\|z - z^*\|)^{-\frac{1}{2}}\right)(L_2\|z - z^*\|) \\
&\le L_1^{-\frac{1}{2}} L_2 \|z - z^*\|^{\frac{1}{2}}.
\end{aligned} \tag{6.53}$$

Then using (3.7), (6.41), and (6.33)

$$\begin{aligned}
\|a_\infty(z) - a_k(z)\| &\le |\theta_1 - 1| (L_2\|z - z^*\|)^{\frac{1}{2}} (L_1^{-1} L_2^2 \|z - z^*\|) c \|\xi_4\| \\
&\le C_4 \|z - z^*\|^{\frac{3}{2}}.
\end{aligned} \tag{6.54}$$

Finally, using (6.53) and (6.44) the bound on $\|\hat{z} - z^*\|$ is established.

$$\begin{aligned}
\|\hat{z} - z^*\| &\le \|\overline{z} - z^*\| + 2\rho_0^2 C_2 L_2 \|z - z^*\|^{\frac{3}{2}} + 2\rho_0 C_4 \|z - z^*\|^{\frac{3}{2}} \\
&\le \|\overline{z} - z^*\| + C_5 \|z - z^*\|^{\frac{3}{2}}
\end{aligned} \tag{6.55}$$

where $C_5 = 2\rho_0^2 C_2 L_2 + 2\rho_0 C_4$. Since $\overline{z}$ is the results of a single step of Newton's Method it is expected that the region $B_\epsilon(z^*)$ is small enough such that the method must have quadratic convergence, and therefore there must exist a $C_6 > 0$ such that $\|\overline{z} - z^*\| \leq C_6\|z - z^*\|^2$. Define $C = \max\{C_6, C_5\}$ and recognized that $\|z - z^*\|^2 \leq \|z - z^*\|^{\frac{3}{2}}$, then (6.55) becomes

$$\|\hat{z} - z^*\| \leq C\|z - z^*\|^{\frac{3}{2}} \tag{6.56}$$

which completes the claim.

$\square$

Chapter 7: Numerical Investigations of Analyzed Methods

Thus far in this document the PDAL, NR-PDAL, and PDNRAL methods have been used exclusively in their infinite dimensional form. In the remainder of this document, the implementations of the three methods will be described. The implementations are used for sample problems relevant to the method, and the predicted convergence rates from Chapters 4, 5, and 6 are confirmed.

7.1 Implementations Background Matter

The infinite dimensional form of these methods can only be used for actually solving these constrained problems for very limited cases. In order to implement a more general solver some portion of the method must be modified such that the infinite dimensional systems of equations are replaced with discretized versions. Multiple discretization methods, such as the finite difference, finite volume, and finite element methods are available and can be used for this purpose. In this work the finite element method was selected as the discretization method.

All following implementations use the `libMesh` [25] C++ library to aid in constructing the Finite Element solvers. The `libMesh` library is a collection of data management and numerical routines designed to ease the process of creating finite element implementations for solving PDEs. This includes many of the required features of any similar library, including definitions of many element types and quadrature methods, and the ability to create, store, query, and manipulate meshes.

7.2 PDAL Implementation and Example

In order to numerically verify quadratic convergence a sample problem was constructed and solved using the PDAL method. The following problem (7.1) is a parameter estimation problem with an elliptic PDE constraint.

$$\begin{aligned} &\text{minimize } \frac{1}{4}\left(\|u-u_d\|^2_{L^2(\Omega)} + \alpha\|q\|^2_{L^2(\Omega)}\right)^2 \\ &\text{subject to } -\nabla^2 u = q \text{ in } \Omega \\ &\qquad u = 0 \text{ on } \partial\Omega \end{aligned} \tag{7.1}$$

By denoting

$$\mathcal{J}(u,q) = \frac{1}{4}\left(\|u-u_d\|^2_{L^2(\Omega)} + \alpha\|q\|^2_{L^2(\Omega)}\right)^2 \tag{7.2}$$

and $A = -\nabla^2$ we see that this is the same form as Problem (4.1).

The first order optimality conditions (4.14) for this problem will be derived, along with the Newton system (4.15). In this problem statement, $u \in \mathcal{W}$ is the state, u_d is the desired value of u, $q \in L^2(\Omega)$ is a coefficient of the PDE and is the control which is to be found. The domain Ω is the space on which the PDE is to be evaluated. $\partial\Omega$ is the boundary of Ω.

The Lagrangian for this problem is

$$L(u,q,\lambda) = \frac{1}{4}\left(\|u-u_d\|^2 + \alpha\|q\|^2\right)^2 - \left(\lambda, \nabla^2 u + q\right)$$

where $\lambda \in H_0^1(\Omega)$ and λ_∂ are the Lagrange multipliers associated with the PDE and boundary constraints, though because $u = 0$ is enforced on the boundary the final term is not required and can be dropped. The first order optimality conditions for this problem

$$\nabla_u L(u, q, \lambda)(h) = ((u - u_d)^3 + \alpha q^2(u - u_d), h) - (\lambda, \nabla^2 h) = 0 \tag{7.3a}$$

$$\nabla_q L(u, q, \lambda)(h) = (\alpha q(u - u_d)^2 + \alpha^2 q^3, h) - (\lambda, h) = 0 \tag{7.3b}$$

$$\nabla_\lambda L(u, q, \lambda)(h) = (\nabla^2 u, h) + (q, h) = 0 \tag{7.3c}$$

Since (7.3) must be true for all $h \in \mathcal{W}$ we can choose $h \in \mathcal{W}_0$. Application of the Fundamental Lemma of the Calculus of Variations to (7.3b) and (7.3c) immediately leads to the following two equations.

$$\alpha q(u - u_d)^2 + \alpha^2 q^3 - \lambda = 0$$

$$\nabla^2 u + q = 0$$

Equation (7.3a) cannot be directly dealt with in a similar way due to the Laplacian of h. But Green's second identity can be used to transfer the Laplacian onto λ, resulting in

$$((u - u_d)^3 + \alpha q^2(u - u_d), h) - (\nabla^2 \lambda, h) = 0 \tag{7.5}$$

which does allow use of the Fundamental Lemma of the Calculus of Variations, leading to the adjoint equation

$$(u - u_d)^3 + \alpha q^2(u - u_d) - \nabla^2 \lambda = 0$$

as the optimality condition in Ω derived from (7.3a). Finally, the complete set of first order optimality conditions is then

$$(u - u_d)^3 + \alpha q^2 (u - u_d) - \nabla^2 \lambda = 0 \text{ in } \Omega$$

$$\alpha q (u - u_d)^2 + \alpha^2 q^3 - \lambda = 0 \text{ in } \Omega$$

$$\nabla^2 u + q = 0 = 0 \text{ in } \Omega$$

The augmented Lagrangian for (7.1) is

$$\mathcal{L}_k(u, q, \lambda) = \frac{1}{4}\left(\|u - u_d\|_{L^2}^2 + \frac{\alpha}{2}\|q\|_{L^2}^2\right)^2 - \left(\lambda, \nabla^2 u + q\right)_\Omega + \frac{k}{2}\|\nabla^2 u + q\|^2 \tag{7.7}$$

The first order optimality conditions resulting from (7.7), when using the dummy variable $\hat{\lambda}$ is

$$(\hat{u} - u_d)^3 + \alpha \hat{q}^2 (\hat{u} - u_d) - \nabla^2 \hat{\lambda} = 0 \text{ in } \Omega \tag{7.8a}$$

$$\alpha \hat{q} (\hat{u} - u_d)^2 + \alpha^2 \hat{q}^3 - \hat{\lambda} = 0 \text{ in } \Omega \tag{7.8b}$$

$$\hat{\lambda} - \lambda + k\left(\nabla^2 \hat{u} + \hat{q}\right) = 0 \text{ in } \Omega. \tag{7.8c}$$

In order to derive the Newton system equivalent to (4.15), equations (7.8) are linearized about the solution, which leads to the following system of equations. Note that the hats $\hat{()}$ are removed for clarity, as the Newton system always refers to the current u, q, and λ.

$$(u + \delta u - u_d)^3 + \alpha(q + \delta q)^2(u + \delta u - u_d) - \nabla^2(\lambda + \delta\lambda) = 0 \tag{7.9a}$$

$$\alpha q(u + \delta u - u_d)^2 + \alpha^2(q + \delta q)^3 - (\lambda + \delta\lambda) = 0 \tag{7.9b}$$

$$\delta\lambda + k\left(\nabla^2(u + \delta u) + (q + \delta q)\right) = 0. \tag{7.9c}$$

By dropping the second order terms and reallocating terms to their appropriate side we get the final Newton system that is solved in each PDAL step.

$$3(u - u_d)^2 + \alpha q^2)\delta u + 2\alpha q(u - u_d)\delta q - \nabla^2\delta\lambda = -(u - u_d)^3 - \alpha q^2(u - u_d) + \nabla^2\lambda \tag{7.10a}$$

$$2\alpha q(u - u_d)\delta u + \alpha(u - u_d)^2 + 3\alpha^2 q^2)\delta q - \delta\lambda = -\alpha q(u - u_d)^2 - \alpha^2 q^3 - \lambda \tag{7.10b}$$

$$\nabla^2\delta u + \delta q + \frac{1}{k}\delta\lambda = -\nabla^2 u - q \tag{7.10c}$$

The general method for solving (7.1) with the PDAL method is an iterative method, and is shown in Algorithm 1. This algorithm, like any Newton based method, iterates by solving (7.10) and updating the variables with the resulting solution. This method, still in its function space description, is of limited direct use due to the nature of (7.1).This system of equstions is a non-linear system of PDEs, for which there is generally no analytical solution. This system of equations must therefore be solved numerically, using some choice of discretization methods.

Multiple discretization schemes may be selected to solve (7.10), and the Finite Element Method was chosen here. The first step required to solve (7.10) using a standard Galerkin Finite Element scheme is first representing the equation in its weak form. Let $\varphi \in \mathcal{W}_0$, and multiply all equations (7.10) through by φ and integrate over

Algorithm 1 Function Space PDAL Algorithm

Choose initial values for u, q, and λ.
Pick $k > 0$.
repeat
Solve (7.10) for δu, δq, and $\delta\lambda$ given current values of u, q, and λ
Update the variables

$$\begin{aligned} u &= u + \delta u \\ q &= q + \delta q \\ \lambda &= \lambda + \delta\lambda \end{aligned} \tag{7.11}$$

Compute the error:

$$\mathcal{E} = \|(u - u_d) - \nabla^2\lambda - \lambda q\| + \|\alpha q - \lambda u\| \tag{7.12}$$

until $\mathcal{E} < tol$

Ω..

$$((3(u-u_d)^2 + \alpha q^2)\delta u, \varphi) + (2\alpha q(u-u_d)\delta q, \varphi) - (\nabla^2\delta\lambda, \varphi)$$

$$= -((u-u_d)^3, \varphi) - \alpha(q^2(u-u_d), \varphi) + (\nabla^2\lambda, \varphi) \tag{7.13a}$$

$$(2\alpha q(u-u_d)\delta u, \varphi) + (\alpha(u-u_d)^2 + 3\alpha^2 q^2)\delta q, \varphi) - (\delta\lambda, \varphi)$$

$$= -(\alpha q(u-u_d)^2, \varphi) - (\alpha^2 q^3, \varphi) - (\lambda, \varphi) \tag{7.13b}$$

$$(\nabla^2\delta u, \varphi) + (\delta q, \varphi) + \frac{1}{k}(\delta\lambda, \varphi) = -(\nabla^2 u, \varphi) - (q, \varphi) \tag{7.13c}$$

Apply Green's identities to reduce all differentiation to first order and we arrive at the following system of equations.

$$((3(u-u_d)^2+\alpha q^2)\delta u,\varphi)+(2\alpha q(u-u_d)\delta q,\varphi)+(\nabla\delta\lambda,\nabla\varphi)$$

$$=-((u-u_d)^3,\varphi)-\alpha(q^2(u-u_d),\varphi)-(\nabla\lambda,\nabla\varphi) \tag{7.14a}$$

$$(2\alpha q(u-u_d)\delta u,\varphi)+(\alpha(u-u_d)^2+3\alpha^2q^2)\delta q,\varphi)-(\delta\lambda,\varphi)$$

$$=-(\alpha q(u-u_d)^2,\varphi)-(\alpha^2q^3,\varphi)-(\lambda,\varphi) \tag{7.14b}$$

$$-(\nabla\delta u,\nabla\varphi)+(\delta q,\varphi)+\frac{1}{k}(\delta\lambda,\varphi)=(\nabla u,\nabla\varphi)-(q,\varphi) \tag{7.14c}$$

The system of equations (7.14) solves equations (7.10) in the weak sense if (7.14) is true for all $\varphi\in\mathcal{W}_0$.

The second step required for solving (7.10) using the Finite Element Method is to discretize the domain. Let the domain Ω_h be defined to be a triangularization of the full domain Ω. Similarly, $u_h,\delta u_h,\lambda_h,\delta\lambda_h,q_h,$ and δq_h are defined to be the discretized versions of u, δu, λ, $\delta\lambda$, q, and δq, respectively. The Lagrange interpolation functions were chosen to represent the test function φ from (7.14). Therefore we set $\varphi(x)=\sum_{j=1}^n\varphi_j(x)$ for all $x\in\Omega_h$, where n is the number of elements in Ω_h.

The standard continuous Galerkin method [35] was followed by defining the discretized representations of u, δu, q, δq, λ, and $\delta\lambda$.

$$\xi(x)\approx\xi_h(x)=\sum_{j=1}^n\xi_j\varphi_j(x)\quad\text{ for }\xi=u,\delta u,q,\delta q,\lambda,\delta\lambda \tag{7.15}$$

Finally, equations (7.14) were discretized by inserting these approximations and the interpolatory test functions. To simplify the resulting equation the homogeneous

Dirichlet boundary conditions on u and λ were imposed, which then lead to the following linear system of equations.

$$\begin{pmatrix} ((3(u_i-u_{d,i})^2+\alpha q_i^2)\varphi_i,\varphi_j) & (2\alpha q_i(u_i-u_{d,i})\varphi_i,\varphi_j) & (\nabla\varphi_i,\nabla\varphi_j) \\ (2\alpha q_i(u_i-u_{d,i})\varphi_i,\varphi_j) & ((\alpha(u_i-u_{d,i})^2+3\alpha^2 q_i^2)\varphi_i,\varphi_j) & -(\varphi_i,\varphi_j) \\ -(\nabla\varphi_i,\nabla\varphi_j) & (\varphi_i,\varphi_j) & \frac{1}{k}(\varphi_i,\varphi_j) \end{pmatrix} \begin{pmatrix} \delta u_i \\ \delta q_i \\ \delta\lambda_i \end{pmatrix} = \begin{pmatrix} -((u_i-u_{d,i})^3,\varphi_i)-\alpha(q_i^2(u_i-u_{d,i}),\varphi_i)-(\nabla\lambda_i,\nabla\varphi_i) \\ -(\alpha q_i(u_i-u_{d,i})^2,\varphi_i)-(\alpha^2 q_i^3,\varphi_i)-(\lambda_i,\varphi_i) \\ (\nabla u_i,\nabla\varphi_i)-(q_i,\varphi_i) \end{pmatrix} \tag{7.16}$$

For ease of implementation (7.16) will be redefined as

$$\begin{pmatrix} K_{uu} & K_{uq} & K_{u\lambda} \\ K_{qu} & K_{qq} & K_{q\lambda} \\ K_{\lambda u} & K_{\lambda q} & K_{\lambda\lambda} \end{pmatrix} \begin{pmatrix} \delta u_i \\ \delta q_i \\ \delta\lambda_i \end{pmatrix} = \begin{pmatrix} b_u \\ b_q \\ b_\lambda \end{pmatrix} \tag{7.17}$$

where

$$K_{uu} = ((3(u_i - u_{d,i})^2 + \alpha q_i^2)\varphi_i, \varphi_j) \tag{7.18a}$$

$$K_{uq} = (2\alpha q_i(u_i - u_{d,i})\varphi_i, \varphi_j) \tag{7.18b}$$

$$K_{u\lambda} = (\nabla\varphi_i, \nabla\varphi_j) \tag{7.18c}$$

$$K_{qu} = (2\alpha q_i(u_i - u_{d,i})\varphi_i, \varphi_j) \tag{7.18d}$$

$$K_{qq} = ((\alpha(u_i - u_{d,i})^2 + 3\alpha^2 q_i^2)\varphi_i, \varphi_j) \tag{7.18e}$$

$$K_{q\lambda} = -(\varphi_i, \varphi_j) \tag{7.18f}$$

$$K_{\lambda u} = -(\nabla\varphi_i, \nabla\varphi_j) \tag{7.18g}$$

$$K_{\lambda q} = (\varphi_i, \varphi_j) \tag{7.18h}$$

$$K_{\lambda\lambda} = \frac{1}{k}(\varphi_i, \varphi_j) \tag{7.18i}$$

and

$$b_u = -((u_i - u_{d,i})^3, \varphi_i) - \alpha(q_i^2(u_i - u_{d,i}), \varphi_i) - (\nabla\lambda_i, \nabla\varphi_i) \tag{7.19a}$$

$$b_q = -(\alpha q_i(u_i - u_{d,i})^2, \varphi_i) - (\alpha^2 q_i^3, \varphi_i) - (\lambda_i, \varphi_i) \tag{7.19b}$$

$$b_\lambda = (\nabla u_i, \nabla\varphi_i) - (q_i, \varphi_i) \tag{7.19c}$$

The Finite Element library `libMesh` [25] was used to implement the discretized system of equations (7.17) using second order elements. The resulting implementation is documented in Algorithm 2. The MUMPS direct solver [1] was used through its interface within PETSc [3] to solve (7.14) at each step. The variables u, q, and λ were initialized to zero throughout Ω, and homogeneous Dirichlet boundary conditions on the Newton directions δu and $\delta\lambda$ were imposed on the solution at each PDAL step.

Problem (7.1) was solved using the PDAL method in the two dimensional space $\Omega = [-1, 1]$. The desired state u_d was defined as

$$u_d(x, y) = e^{-x}(\cos(\pi x))(x - 1)^3(x + 1)^3.$$

The regularization parameter α was set to 10^{-6}.

The resulting implementation of the PDAL method was run with multiple mesh densities, with edge lengths ranging from $\frac{1}{16}$ to $\frac{1}{512}$. The convergence parameter

$$e_k = \max\{\|u_k - u_{k-1}\|_{L^2(\Omega)}, \|q_k - q_{k-1}\|_{L^2(\Omega)}\}$$

was monitored during each run to confirm quadratic local convergence and to check for mesh independence of the PDAL method. The iterations ended when $e_k \leq 10^{-12}$.

The resulting state, control, and Lagrange multipliers are seen in Figure 7.1.

The results in Figure 7.2 do demonstrate the desired quadratic convergence starting between iterations 18 and 22, depending on the mesh case. In addition, the behavior of the method under different mesh densities remained nearly constant, requiring only one additional iteration per mesh as as the meshes became more refined.

7.3 NR-PDAL Implementation and Example

A second parameter estimation problem with elliptic constraints was constructed in order to verify the predicted linear convergence of the NR-PDAL method. But in this case state and control constraints were added. For this problem the linear operator,

Algorithm 2 PDAL Implementation

Construct vectors u, q, λ, δu, δq, and $\delta\lambda$ and initialize them to 0
Initialize $k = k_0$
Compute the initial error $\mathcal{E}$
while $\mathcal{E} < tol$ **do**
  for each element n **do**
    Compute the elemental matrices
    for each quadrature point p **do**
      Get values of $\mathbf{JxW}$, φ, and $\nabla\varphi$ at point p
      Compute the values of u, q, λ, and $\nabla\lambda$ at point p
      $K^n_{uu} = \sum_{i=0}^{n_u}\sum_{j=0}^{n_u} \mathbf{JxW}((3(u-u_d(p))^2 + \alpha q^2)\varphi[i], \varphi[j])$
      $K^n_{uq} = \sum_{i=0}^{n_u}\sum_{j=0}^{n_q} \mathbf{JxW}(2\alpha q(u-u_d(p))\varphi[i], \varphi[j])$
      $K^n_{u\lambda} = \sum_{i=0}^{n_u}\sum_{j=0}^{n_\lambda} \mathbf{JxW}(\nabla\varphi[i], \nabla\varphi[j])$
      $b^n_u = \sum_{i=0}^{n_u} \mathbf{JxW}(-((u-u_d(p))^3, \varphi[i]) - \alpha(q^2(u-u_d(p)), \varphi[i]) - (\nabla\lambda, \nabla\varphi[i]))$
      $K^n_{qu} = \sum_{i=0}^{n_q}\sum_{j=0}^{n_u} \mathbf{JxW}(2\alpha q(u-u_d(p))\varphi[i], \varphi[j])$
      $K^n_{qq} = \sum_{i=0}^{n_q}\sum_{j=0}^{n_q} \mathbf{JxW}((\alpha(u-u_d(p0=))^2 + 3\alpha^2 q^2)\varphi[i], \varphi[j])$
      $K^n_{q\lambda} = \sum_{i=0}^{n_q}\sum_{j=0}^{n_\lambda} \mathbf{JxW}(-\varphi[i], \varphi[j])$
      $b^n_q = \sum_{i=0}^{n_q} \mathbf{JxW}(-(\alpha q(u-u_d(p))^2, \varphi[i]) - (\alpha^2 q^3, \varphi[i]) - (\lambda, \varphi[i]))$
      $K^n_{\lambda u} = \sum_{i=0}^{n_\lambda}\sum_{j=0}^{n_u} \mathbf{JxW}(-\nabla\varphi[i], \nabla\varphi[j]))$
      $K^n_{\lambda q} = \sum_{i=0}^{n_\lambda}\sum_{j=0}^{n_q} \mathbf{JxW}(\varphi[i], \varphi[j])$
      $K^n_{\lambda\lambda} = \sum_{i=0}^{n_\lambda}\sum_{j=0}^{n_\lambda} \mathbf{JxW}(\frac{1}{k}\varphi[i], \varphi[j])$
      $b^n_\lambda = \sum_{i=0}^{n_\lambda} \mathbf{JxW}((\nabla u, \nabla\varphi[i]) - (q, \varphi[i]))$
    end for
    Add elemental K^n matrix and b^n to the global system (7.17)
  end for
  Zero out the off-diagonal elements in each row corresponding to the homogeneous boundary conditions on δu and $\delta\lambda$.
  Solve (7.17) for $(\delta u_i, \delta q_i, \delta\lambda_i)^T$ using the MUMPS direct solver
  Update the variables

$$\begin{aligned} u_i &= u_i + \delta u_i \\ q_i &= q_i + \delta q_i \\ \lambda_i &= \lambda_i + \delta\lambda_i \end{aligned} \tag{7.20}$$

  Compute the error $\mathcal{E}$ and merit function $v(u, q, \lambda)$.
  Update $k = v^{-1}(u, q, \lambda)$
end while

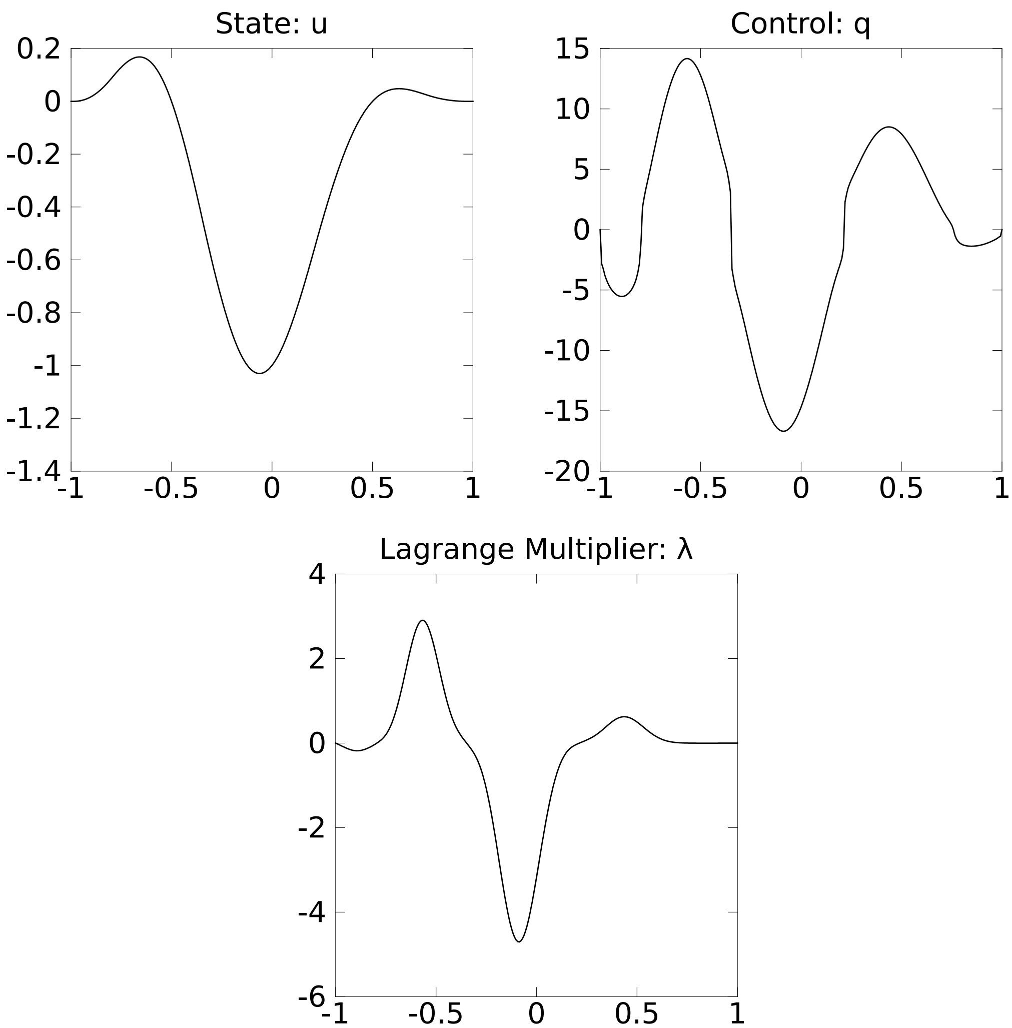


Figure 7.1: State, Control, and Lagrange Multiplier for the PDAL Example

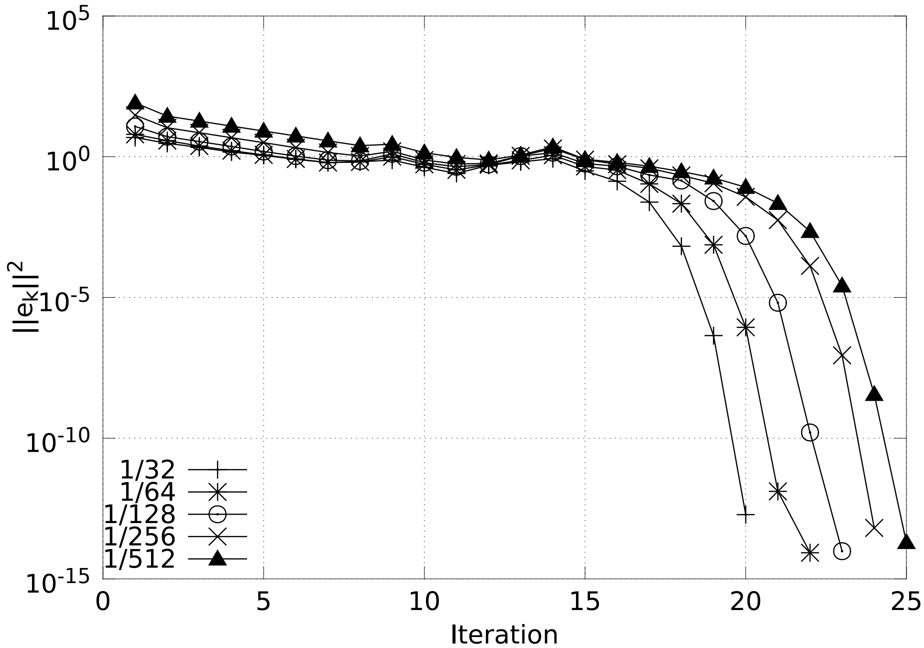


Figure 7.2: Convergence for the PDAL example

A, is set to be $-\nabla^2$, and the domain Ω is the real line $[-1, 1]$. A single lower bound

$$\eta_l = (x - 8))/10 \tag{7.21}$$

and a single upper bound

$$\beta_u = 12 \tag{7.22}$$

are used in this example. The resulting problem can then be generally stated as

$$\begin{aligned} &\text{minimize } J(u, q) = \frac{1}{2}\|u - u_d\|^2 + \frac{\alpha}{2}\|q\|^2 \\ &\text{subject to } -\nabla^2 u = q \text{ in } \Omega \\ &u \geq \eta_l \text{ a.e. in } \Omega \\ &\beta_u \geq q \text{ a.e. in } \Omega \end{aligned} \tag{7.23}$$

where $u, u_d \in \mathcal{W}$ and $q, \eta_l, \beta_u \in L^2$. The desired state is set to be

$$u_d = e^{-x} cos(\pi x)(x-1)^3(x+1)^3 \tag{7.24}$$

Finally, the regularization parameter α is set to 1e-7.

The Lagrangian for this problem is

$$L(u, q, \lambda, \sigma, \kappa) = \frac{1}{2}\|u - u_d\|^2 + \frac{\alpha}{2}\|q\|^2 - (\lambda, -\nabla^2 u - q) - (\sigma_l, u - \eta_t) - (\chi_u, \beta_u - q) \tag{7.25}$$

where $\lambda \in L^2$, $\sigma_l \in C^*$, and $\chi_u \in L^2$. The Lagrangian will be modified using the method described in Chapter 5. Let Ψ be as defined in in Section 3.1. k_p and k_b are defined to be positive barrier parameters for the PDE constraint and inequality constraints, respectively. The resulting modified Lagrangian becomes

$$\begin{aligned} \mathcal{L}_k(u, q, \lambda, \sigma_l, \chi_u) = \frac{1}{2}\|u - u_d\|^2 + \frac{\alpha}{2}\|q\|^2 - (\lambda, -\nabla^2 u - q) + \frac{k_p}{2}(\nabla^2 u - q, \nabla^2 u - q) \\ - \frac{1}{k_b}(\sigma_l, \Psi(k_b(u - \eta_t)) - \frac{1}{k_b}(\chi_u, \Psi(k_b(\beta_u - q)) \end{aligned} \tag{7.26}$$

Following the construction of the NR-PDAL method described in Chapter 5, the inner step is the solution to the constrained elliptic constrained problem, which is followed by the Lagrange multiplier updates. The constrained problem for this system at iteration s, as defined by the primal-dual system (5.6), becomes

$$
\begin{aligned}
(u_s - u_d) - \nabla^2 \lambda_s + \sigma_{u,s-1} \Psi'(k_p(\eta_u - u_s) &= 0 \\
\alpha q_s + \lambda_s + \chi_{u,s-1} \Psi'(k_p(\beta_u - q_s) &= 0 \\
\lambda_s - \lambda_{s-1} + k_b(\nabla^2 u_s - q_s) &= 0
\end{aligned}
\tag{7.27}
$$

and the Lagrange multiplier updates, (5.4b) and (5.4c), are the following.

$$\sigma_{u,s} = \sigma_{u,s-1} \Psi'(k_b(\eta_u - u_s)) \tag{7.28a}$$

$$\chi_{l,s} = \chi_{l,s-1} \Psi'(k_b(\beta_l - q_s)) \tag{7.28b}$$

For this problem, the Newton system to be solved at each PDAL step is found via linearization of to (7.29) about u_s, q_s, and, λ_s.

$$
\begin{aligned}
\delta u - \sigma_l k_b \Psi''(k_b(u - \eta_l))\delta u + \nabla^2 \delta\lambda &= -(u - u_d) + \sigma_l \Psi'(k_b(u - \eta)) - \nabla^2 \lambda \\
\alpha \delta q + \chi_u k_b \Psi''(k_b(\beta_u - q))\delta q + \delta\lambda &= -\alpha q + \chi_u \Psi'(k_b(\beta_u - q)) - \lambda \\
k_p \nabla^2 \delta u + k_p \delta q + \delta\lambda &= k_p(\nabla^2 u + q)
\end{aligned}
\tag{7.29}
$$

The NR-PDAL method, which can be described as a sequentially constraint minimization technique, is composed of the inner PDAL step, which solves for (7.27) using the linearization (7.29). The functional space algorithm is shown here.

As in Chapter 4 this Newton system is still only defined in its infinite dimensional form, and must be discretized. The Finite Element method is again chosen to solve this system of equations. Therefore the system (7.29) must be first written in its weak

Algorithm 3 Function Space NR-PDAL Algorithm

Choose initial values for u, q, λ, σ_u, and χ_l.
Pick $k_p > 0$ and $k_b > 0$.
repeat
  repeat
    Solve (7.27) for δu, δq, and $\delta\lambda$ given current values of u, q, λ, σ_u, and χ_l.
    Update the variables

$$\begin{aligned} u &= u + \delta u \\ q &= q + \delta q \\ \lambda &= \lambda + \delta\lambda \end{aligned} \tag{7.30}$$

    Compute the error in the inner step: abc

$$\mathcal{E} = \|(u - u_d) - \nabla^2\lambda + \sigma_u \Psi'(k_p(\eta_u - u))\| + \|\alpha q - \lambda + \chi_u \Psi'(k_p(\beta_l - q))\| \tag{7.31}$$

  until $\mathcal{E} < tol$
  Update Lagrange Multipliers on the inequality constraints

$$\begin{aligned} \sigma_u &= \sigma_u \Psi'(k_p(\eta_u - u)) \\ \chi_l &= \chi_l \Psi'(k_p(\beta_l - q)) \end{aligned} \tag{7.32}$$

  Compute the total error, $\mathcal{E}_t$
  Update the k_b and k_p parameters.
until $\mathcal{E}_t < tol$

form. Let $\varphi \in \mathcal{W}_0$ and multiply (7.29) through by φ, then reduce all differentiation to first order.

$$\begin{gathered}(\delta u - \sigma_{u,s} k_b \Psi''(k_b(u_s - \eta_l))\delta u, \varphi) - (\nabla \delta\lambda, \nabla\varphi) = -(u_s - u_d, \varphi) + (\sigma_{u,s}\Psi'(k_b(u_s - \eta_l)), \varphi) + (\nabla\lambda_s, \varphi)\\ \alpha(\delta q + \chi_{l,s} k_b \Psi''(k_b(\beta_l - q_s))\delta q, \varphi) + (\delta\lambda, \varphi) = -\alpha(q_s, \varphi) + (\chi_{l,s}\Psi'(k_b(\beta_s - q_s)), \varphi) - (\lambda_s, \varphi)\\ -k_p(\nabla\delta u, \nabla\varphi) + k_p(\delta q, \varphi) + (\delta\lambda, \varphi) = k_p(-(\nabla u_s, \nabla\varphi) + (q_s, \varphi))\end{gathered} \tag{7.33}$$

The domain Ω_h is defined to be a triangularization of the full domain Ω. The Lagrange interpolation functions are chosen to represent the test function φ, and the standard continuous Galerkin method [35] was followed in by defining the discretized approximations. Let

$$\xi(x) \approx \xi_h(x) = \sum_{j=1}^{n} \xi_j \varphi_j(x) \text{ for all } x \in \Omega \tag{7.34}$$

for $\xi = u_s, \delta u, q_s, \delta q, \lambda_s, \delta\lambda, \sigma_{u,s},$ and $\chi_{l,s}$. These discretized variables are then inserted into (7.33), resulting the following system of equations, which was implemented using the FE software library `libMesh` [25]. Note that the iteration count, s, is dropped for clarity from here through the remainder of this section.

$$\begin{gathered}\begin{pmatrix} (\varphi_i - \sigma_{u,i} k_b \Psi''(k_b(u_i - \eta_l)\varphi_i, \varphi_j) & 0 & -(\nabla\varphi_i, \nabla\varphi_j)\\ 0 & \alpha(\varphi_i + \chi_{l,i} k_b \Psi''(k_b(\beta_l - q_i))\varphi_i, \varphi_j) & (\varphi_i, \varphi_j)\\ -k_p(\nabla\varphi_i, \nabla\varphi_j) & k_p(\varphi_i, \varphi_j) & (\varphi_i, \varphi_j)\end{pmatrix} \begin{pmatrix}\delta u_h\\ \delta q_h\\ \delta\lambda_h\end{pmatrix} =\\ \begin{pmatrix} -(u_i - u_d, \varphi_i) + (\sigma_{u,i}\Psi'(k_b(u_i - \eta_u)), \varphi_i) + (\nabla\lambda_i, \varphi_i)\\ -\alpha(q_i, \varphi_i) + (\chi_{l,i}\Psi'(k_b(\beta_l - q_i)), \varphi) - (\lambda_i, \varphi_i)\\ k_p(-(\nabla u_i, \nabla\varphi_i) + (q_i, \varphi_i))\end{pmatrix}\end{gathered} \tag{7.35}$$

The results from each solution are used to update the current values of u, q, and λ.

Redefine (7.35) as the following in order to ease the description of the implementation of the NR-PDAL method for this example problem.

$$\begin{pmatrix} K_{uu} & 0 & K_{u\lambda} \\ 0 & K_{qq} & K_{q\lambda} \\ K_{\lambda u} & K_{\lambda q} & K_{\lambda\lambda} \end{pmatrix} \begin{pmatrix} \delta u_i \\ \delta q_i \\ \delta \lambda_i \end{pmatrix} = \begin{pmatrix} b_u \\ b_q \\ b_\lambda \end{pmatrix} \tag{7.36}$$

where

$$K_{uu} = ((1 - \sigma_{u,i} k_b \Psi''(k_b(u_i - \eta_l)))\varphi_i, \varphi_j) \tag{7.37a}$$

$$K_{u\lambda} = -(\nabla\varphi_i, \nabla\varphi_j) \tag{7.37b}$$

$$K_{qq} = \alpha((1 + \chi_{l,i} k_b \Psi''(k_b(\beta_l - q_i)))\varphi_i, \varphi_j) \tag{7.37c}$$

$$K_{q\lambda} = (\varphi_i, \varphi_j) \tag{7.37d}$$

$$K_{\lambda u} = -k_p(\nabla\varphi_i, \nabla\varphi_j) \tag{7.37e}$$

$$K_{\lambda q} = k_p(\varphi_i, \varphi_j) \tag{7.37f}$$

$$K_{\lambda\lambda} = (\varphi_i, \varphi_j) \tag{7.37g}$$

and

$$b_u = -(u_i - u_d, \varphi_i) + (\sigma_{u,i}\Psi'(k_b(u_i - \eta_u)), \varphi_i) + (\nabla\lambda_i, \varphi_i) \tag{7.38a}$$

$$b_q = -\alpha(q_i, \varphi_i) + (\chi_{l,i}\Psi'(k_b(\beta_l - q_i)), \varphi) - (\lambda_i, \varphi_i) \tag{7.38b}$$

$$b_\lambda = k_p(-(\nabla u_i, \nabla\varphi_i) + (q_i, \varphi_i)) \tag{7.38c}$$

After each inner PDAL step completes, the discretized Lagrange multipliers associated with the inequalities are updated in the standard NR way.

$$\sigma_{u,i} = \sigma_{u,i}\Psi'(k_p(u_i - \eta_u)) \tag{7.41a}$$

$$\chi_{l,i} = \chi_{l,i}\Psi'(k_p(\beta_l - q_i)) \tag{7.41b}$$

It can be seen from the convergence analysis that the linear convergence should hold when problems have either a state constraint, a control constraint, or independent constraints on both. Therefore this example problem was modified in three ways. In each version of the problem the step size was monitored by evaluating

$$e_j = \max\left\{\|u_j - u_{j-1}\|_{L^2}, \|q_j - q_{j-1}\|_{L^2}\right\} \tag{7.42}$$

at each NR-PDAL iteration.

The space $[-1, 1]$ was discretized with multiple mesh densities, with element lengths ranging from $^1/_{128}$ to $^1/_{512}$. Multiple values of k were also used to confirm that the convergence constant depends on k. These same configurations were used for the case with both the state and control constraint, the state constraint only, and the control constraint only. The initial values for u, q, and λ were all set to zero. The initial values of the inequality constraint Lagrange multipliers were set to 1e-4.

Algorithm 4 NR-PDAL Implementation

Construct vectors u, q, λ, σ_u, β_l, δu, δq, and $\delta\lambda$
Initialize $k_p = k_0$ and $k_b = k_0$.
Compute the initial error $\mathcal{E}$
while $\mathcal{E}_t < tol$ **do**
  while $\mathcal{E} < tol$ **do**
    for each element n **do**
      Compute the elemental matrices and associated parameters (notably $\mathbf{JxW}$, which is the Jacobian transformation multiplied by the weighting function of the element).
      for each quadrature point p **do**
        Get values of $\mathbf{JxW}$, φ, and $\nabla\varphi$ at point p
        Compute the values of u, q, λ, $\nabla\lambda$, σ_u, and χ_l at point p
        $K^n_{uu} = \sum_{i=0}^{n_u}\sum_{j=0}^{n_u}\mathbf{JxW}((1-\sigma_u[i]k_b\Psi''(k_b(u[i]-\eta_l(u[i]))))\varphi[i]\varphi[j])$
        $K^n_{u\lambda} = \sum_{i=0}^{n_u}\sum_{j=0}^{n_\lambda}\mathbf{JxW}(-\nabla\varphi[i]\cdot\nabla\varphi[j])$
        $b^n_u = \sum_{i=0}^{n_u}\mathbf{JxW}(-(u-u(x,y)\varphi[i]) + \nabla\lambda\nabla[i] + \lambda u\varphi[i])$
        $K^n_{qu} = \sum_{i=0}^{n_q}\sum_{j=0}^{n_u}\mathbf{JxW}(\lambda\varphi[i]\varphi[j])$
        $K^n_{qq} = \sum_{i=0}^{n_q}\sum_{j=0}^{n_q}\mathbf{JxW}(\alpha\varphi[i]\varphi[j])$
        $K^n_{q\lambda} = \sum_{i=0}^{n_q}\sum_{j=0}^{n_\lambda}\mathbf{JxW}(-k\nabla\varphi[i]\nabla\varphi[j] + (kq\varphi[i]\varphi[j])$
        $b^n_q = \sum_{i=0}^{n_q}\mathbf{JxW}(-\alpha(u-u_d(x,y))\varphi[i] + \nabla\lambda\cdot\nabla\varphi[i] + \lambda u\varphi[i])$
        $K^n_{\lambda u} = \sum_{i=0}^{n_\lambda}\sum_{j=0}^{n_u}\mathbf{JxW}(k\nabla\varphi[i]\nabla\varphi[j] + (kq\varphi[i]\varphi[j]))$
        $K^n_{\lambda q} = \sum_{i=0}^{n_\lambda}\sum_{j=0}^{n_q}\mathbf{JxW}(u\varphi[i]\varphi[j])$
        $K^n_{\lambda\lambda} = \sum_{i=0}^{n_\lambda}\sum_{j=0}^{n_\lambda}\mathbf{JxW}(\varphi[i]\varphi[j])$
        $b^n_\lambda = \sum_{i=0}^{n_\lambda}\mathbf{JxW}(-\nabla u\nabla\varphi[i] - qu\varphi[i] + f(x,y)\varphi[i])$
      end for
      Add elemental K^n matrix and b^n to the global system (7.17)
    end for
    Account for boundary conditions on δu and $\delta\lambda$.
    Solve (7.17) for $(\delta u_i, \delta q_i, \delta\lambda_i)^T$ using the MUMPS direct solver
    Update the variables

$$\begin{aligned} u_i &= u_i + \delta u_i \\ q_i &= q_i + \delta q_i \\ \lambda_i &= \lambda_i + \delta\lambda_i \end{aligned} \tag{7.39}$$

    Compute the error $\mathcal{E}$
  end while
  Update the Lagrange multipliers associated with inequality constraints

$$\begin{aligned} \sigma_{u,i} &= \sigma_{u,i}\Psi'(k_p(u_i-\eta_u)) \\ \chi_{l,i} &= \chi_{l,i}\Psi'(k_p(\beta_l-q_i)) \end{aligned} \tag{7.40}$$

  Compute the error $\mathcal{E}_t$
end while

Table 7.1: State and Control Constraints

	1/128			1/256			1/512		
$k = k_b = k_p$	Inner	Outer	C	Inner	Outer	C	Inner	Outer	C
100	96	42	0.628	598	461	0.977	4666	4397	0.998
1000	44	21	0.350	198	111	0.863	835	651	0.981
10000	71	19	0.403	140	51	0.678	230	135	0.905

The resulting state, control, and Lagrange multipliers for the case with state and control constraints are seen in Figure 7.3. The characteristic spike in the highly non-regular state inequality Lagrange multiplier, σ, is quite evident. Evidence of oscillations in the solution can be seen in the control, q, which can result from the continuous Galerkin method with solutions with the steep gradients seen in the σ and q.

Tables 7.1, 7.2, and 7.3 provide the iteration counts and convergence constants for the three cases. The convergence rates are comparable for either of the case which included state constraints, and the convergence rate is slow, approaching values near one as the mesh density increases. In the case with only the control constraint, on the other hand, demonstrated improved convergence for all values of k and mesh density, and actually experienced improved convergence rates as the mesh density increased.

Despite the slow convergence rates experienced in these cases, it should be noticed that all cases which converged the results do indicate the predicted linear convergence. The author believes that this indicates the function space NR-PDAL method to show promise as a method for solving state constrained optimization problems. The rapid linear convergence experienced and improved performance on refined meshes in the control constrained problem show that the NR-PDAL method should perform well for these types of problems.

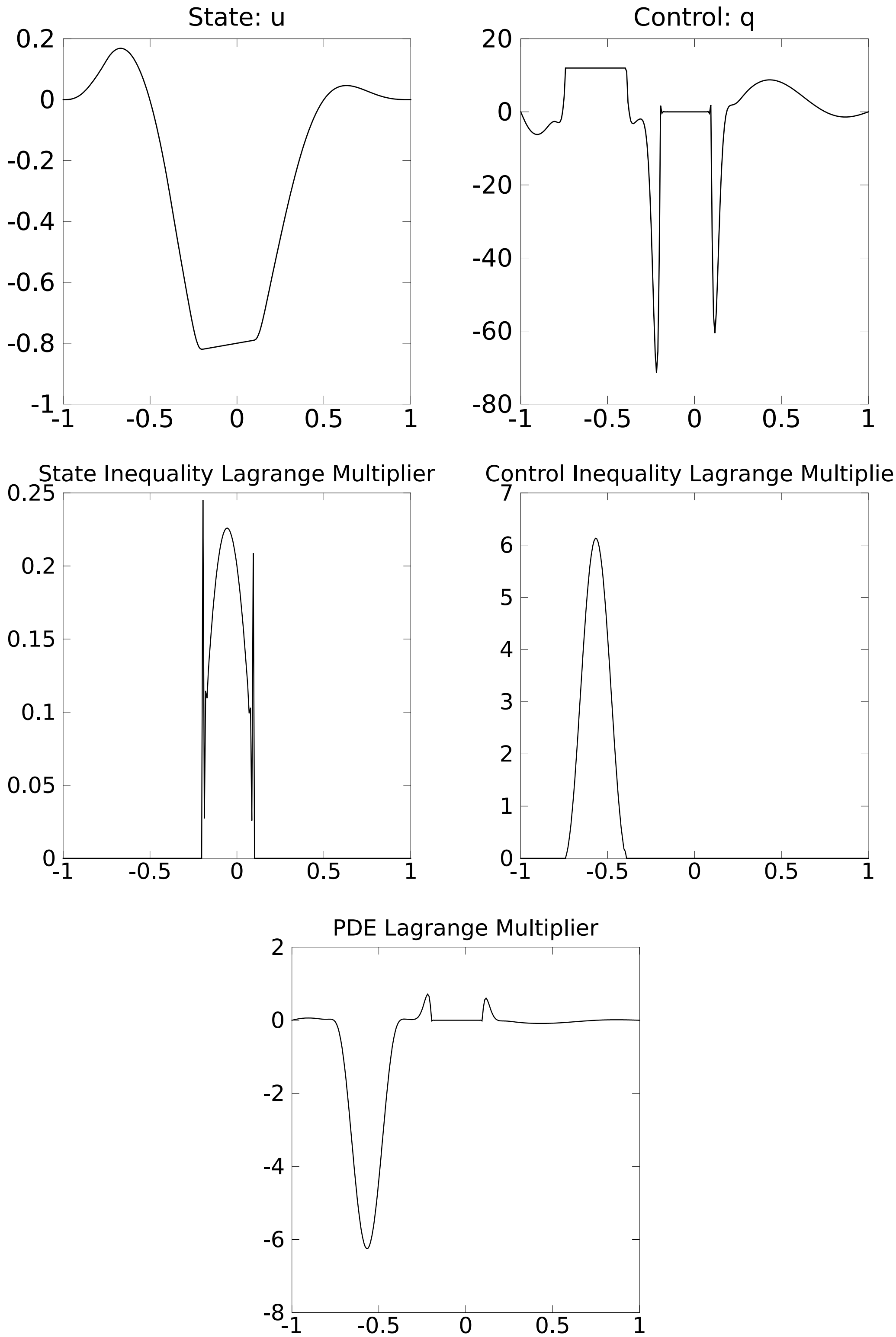


Figure 7.3: State, Control, and Lagrange Multipliers for the NR-PDAL Example

Table 7.2: State Constraint Only

	1/128			1/256			1/512		
$k = k_b = k_p$	Inner	Outer	C	Inner	Outer	C	Inner	Outer	C
100	78	42	0.628	577	461	0.969	4592	4346	0.998
1000	56	21	0.349	180	111	0.863	781	620	0.980
10000	47	19	0.402	123	51	0.678	222	143	0.910

Table 7.3: Control Constraint Only

	1/128			1/256			1/512		
$k = k_b = k_p$	Inner	Outer	C	Inner	Outer	C	Inner	Outer	C
100	44	9	0.054	64	19	0.515	44	9	0.054
1000	39	8	0.064	53	14	0.514	39	8	0.064
10000	38	7	0.144	48	10	0.511	38	6	0.143

7.4 PDNRAL Implementation and Example

The third elliptically constrained parameter estimation problem, only this time with just control constraints, was constructed in order to verify the predicted super-linear convergence of the PD-NRAL method. As in the other problem, the linear operator A is set to $-\nabla^2$, and the domain Ω is the real line $[-1, 1]$.

The desired state is set as

$$u_d = e^{-x} cos(\pi x)(x-1)^3(x+1)^3 \tag{7.43}$$

and a single upper bound

$$\beta(q) = 10 - q \tag{7.44}$$

is placed on the control.

The resulting problem is then stated as

$$\begin{aligned} \text{minimize } J(u,q) &= \frac{1}{2}\|u-u_d\|^2 + \frac{\alpha}{2}\|q\|^2 \\ \text{subject to } &-\nabla^2 u = q \text{ in } \Omega \\ &\beta(q) \geq 0 \text{ a.e. in } \Omega \end{aligned} \tag{7.45}$$

where $u, u_d \in \mathcal{W}$,and $q, \beta(q) \in L^2$. Finally, the regularization parameter α is set to 1e-7.

The Lagrangian for this problem is

$$L(u,q,\lambda,\kappa) = \frac{1}{2}\|u-u_d\|^2 + \frac{\alpha}{2}\|q\|^2 - (\lambda, \nabla^2 u + q) - (\chi_u, \beta(q)) \tag{7.46}$$

where $\lambda, \chi \in L^2$. The Lagrangian will again be modified by following the steps in Chapter 6. Let Ψ be define as in Section 3.1. A single positive barrier parameter, k, is used on the PDE constraint and inequality constraint. These steps define the following modified Lagrangian.

$$\begin{aligned} \mathcal{L}_k(u,q,\lambda,\beta_u) = \frac{1}{2}\|u-u_d\|^2 + \frac{\alpha}{2}\|q\|^2 - (\lambda, \nabla^2 u + q) + \frac{k}{2}(\nabla^2 u + q, \nabla^2 u + q) \\ - \frac{1}{k}(\chi, \Psi(k(\beta(q)))) \end{aligned} \tag{7.47}$$

Unlike the NR-PDAL method, this method is a full primal-dual method, and as such the inner system solution followed by a Lagrange multiplier update step is replaced by the solution of a single set of equations. This primal dual system is defined by (6.7), which for this specific problem becomes

$$(\hat{u} - u_d) - \nabla^2 \hat{\lambda} = 0 \tag{7.48a}$$

$$\alpha \hat{q} - \hat{\lambda} - \hat{\chi} \nabla \beta(\hat{q}) = 0 \tag{7.48b}$$

$$\hat{\lambda} - \lambda + k(\nabla^2 \hat{u} + \hat{q}) = 0 \tag{7.48c}$$

$$\hat{\chi} - \chi \Psi'(k(\beta(\hat{q}))) = 0 \tag{7.48d}$$

In order to solve for (7.48) using standard Newton iterations it must be linearized. The linearization of (7.48), is show below, with the hats $\hat{()}$ removed as all variables (u, q, λ, and χ) are considered to be at the same update level in the Newton system.

$$M_k(u, q, \lambda, \chi) \begin{pmatrix} \delta u \\ \delta q \\ \delta \lambda \\ \delta \chi \end{pmatrix} = a_k(u, q, \lambda, \chi) \tag{7.49}$$

$$M_k(u, q, \lambda, \chi) = \begin{pmatrix} I_u & 0 & -\nabla^2 & 0 \\ 0 & \alpha I_q & -I_\lambda & I_\chi \\ k\nabla^2 & kI_u & I_\lambda & 0 \\ 0 & -k\chi\Psi''(k(\beta(q))) & 0 & I_\chi \end{pmatrix} \tag{7.50}$$

and

$$a_k(u,q,\lambda,\chi) = \begin{pmatrix} -(u-u_d)+\nabla^2\lambda \\ -\alpha q+\lambda-\chi \\ -k(\nabla^2 u+q) \\ \chi(\Psi'(k(\beta(q))-1) \end{pmatrix} \tag{7.51}$$

where $M_k(u,q,\lambda,\chi)$ and $a_k(u,q,\lambda,\chi)$.

In order to solve the infinite dimensional (7.49) for this example problem, it must be first discretized. Again the Finite Element method is selected as the discretization method used to numerically solve this system of equations. Begin by defining $\varphi \in \mathcal{W}_0$ and rewriting (7.49) in its weak form with appropriate reduction of differentiation to first order.

$$(\delta u,\varphi)+(\nabla\delta\lambda,\nabla\varphi) = -(u-u_d,\varphi)-(\nabla\lambda,\nabla\varphi) \tag{7.52a}$$

$$\alpha(\delta q,\varphi)-(\delta\lambda,\varphi)+(\delta\chi,\varphi) = -\alpha(q,\varphi)+(\lambda-\chi,\varphi) \tag{7.52b}$$

$$-k(\nabla u,\nabla\varphi)+k(u\delta q,\varphi)+(\delta\lambda,\varphi) = -k(\nabla u,\nabla\varphi)-(q,\varphi) \tag{7.52c}$$

$$-k(\chi\Psi''(k(\beta(q))),\varphi)+(\delta\chi,\varphi) = (\chi(\Psi'(k(\beta_(q))-1)),\varphi) \tag{7.52d}$$

The domain Ω_h is defined to be a triangularization of the full domain Ω. The Lagrange interpolation functions are chose to represent the test function φ, and the standard continuous Galerkin [35] is again followed by defining the discretized approximations. Let

$$\xi(x) \approx \xi_h(x) = \sum_{j=1}^{n} \xi_j\varphi_j(x) \text{ for all } x \in \Omega \tag{7.53}$$

for $\xi = u, \delta u, q, \delta q, \lambda, \delta\lambda, \chi$, and $\delta\chi$. These variables are inserted into (7.52), resulting in the following system of equations, which was implemented using the FE software library `libMesh` [25].

$$\begin{pmatrix} (\varphi_i, \varphi_j) & 0 & (\nabla\varphi_i, \nabla\varphi_j) & 0 \\ 0 & \alpha(\varphi_i, \varphi_j) & -(\varphi_i, \varphi_j) & (\varphi_i, \varphi_j) \\ -(\nabla\varphi_i, \nabla\varphi_j) & (\varphi_i, \varphi_j) & k^{-1}(\varphi_i, \varphi_j) & 0 \\ 0 & -k(\chi_i \Psi''(k(\beta(q_i)))\varphi_i, \varphi_j) & 0 & (\varphi_i, \varphi_j) \end{pmatrix} \begin{pmatrix} \partial u_i \\ \partial q_i \\ \partial \lambda_i \\ \partial \chi_i \end{pmatrix}$$

$$= \begin{pmatrix} -(u_i - u_d, \varphi_i) - (\nabla\lambda_i, \nabla\varphi_i) \\ -\alpha(q_i, \varphi_i) + (\lambda_i - \chi_i, \varphi_i) \\ -(\nabla u_i, \nabla\varphi_i) - (q_i, \varphi_j) \\ (\chi_i \Psi'(k(\beta(q_i))) - 1, \varphi_i) \end{pmatrix} \tag{7.54}$$

Like in the previous section, this system of equations will be recast into the following simplified system of equations to allow for a better algorithmic description of the PDNRAL method for this example problem.

$$\begin{pmatrix} K_{uu} & 0 & K_{u\lambda} & 0 \\ 0 & K_{qq} & K_{q\lambda} & K_{q\chi} \\ K_{\lambda u} & K_{\lambda q} & K_{\lambda\lambda} & 0 \\ 0 & K_{\chi\lambda} & 0 & K_{\chi\chi} \end{pmatrix} \begin{pmatrix} \delta u_i \\ \delta q_i \\ \delta\lambda_i \\ \delta\chi_i \end{pmatrix} = \begin{pmatrix} b_u \\ b_q \\ b_\lambda \\ b_\chi \end{pmatrix} \tag{7.55}$$

where

$$K_{uu} = K_{\chi\chi} = K_{\lambda q} = -K_{q\lambda} = K_{q\chi} = (\varphi_i, \varphi_j) \tag{7.56a}$$

$$K_{qq} = \alpha(\varphi_i, \varphi_j) \tag{7.56b}$$

$$K_{\lambda\lambda} = k^{-1}(\varphi_i, \varphi_j) \tag{7.56c}$$

$$-K_{u\lambda} = K_{\lambda u} = (\nabla\varphi_i, \nabla\varphi_j) \tag{7.56d}$$

$$K_{\chi\lambda} = -(\chi_i \Psi''(k(\beta(q_i)))\varphi_i, \varphi_j) \tag{7.56e}$$

and

$$b_u = -(u_i - u_d, \varphi_i) - (\nabla\lambda_i, \varphi_i) \tag{7.57a}$$

$$b_q = -\alpha(q_i, \varphi_i) + (\lambda_i - \chi_i, \varphi_i) \tag{7.57b}$$

$$-(\nabla u_i, \nabla\varphi_i) - (q_i, \varphi_j) \tag{7.57c}$$

$$(\chi_i \Psi'(k(\beta(q_i))) - 1, \varphi_i) \tag{7.57d}$$

As with the previous problem, the space $[-1, 1]$ was discretized with multiple mesh densities (with element lengths ranging from 1/128 to 1/2048). The initial value for u, q, and λ was set to 0. The inequality constraint Lagrange multiplier, χ, was set to 1.0. The resulting state, control, and Lagrange multipliers for the case with state and control constraints are seen in Figure 7.4. The convergence rates for the different discretizations is shown in Figure 7.5, which demonstrates the predicted non-linear convergence rate. Also demonstrated in this graph is nearly mesh independent convergence rates, which shows that the PDNRAL method can be a good choice for

Algorithm 5 PDNRAL Implementation

Construct vectors u, q, λ, χ, δu, δq, $\delta\lambda$, and $\delta\chi$
Initialize $k = k_0$.
Compute the initial error $\mathcal{E}$
while $\mathcal{E} < tol$ **do**
  for each element n **do**
    Compute the elemental matrices and associated parameters (notably **JxW**, which is the Jacobian transformation multiplied by the weighting function of the element).
    for each quadrature point p **do**
      Get values of **JxW**, φ, and $\nabla\varphi$ at point p
      Compute the values of u, q, λ, $\nabla\lambda$, σ_u, and χ_l at point p
      $K^n_{uu} = \sum_{i=0}^{n_u}\sum_{j=0}^{n_u} \mathbf{JxW}(\varphi[i]\varphi[j])$
      $K^n_{u\lambda} = \sum_{i=0}^{n_u}\sum_{j=0}^{n_\lambda} \mathbf{JxW}(-\nabla\varphi[i]\cdot\nabla\varphi[j])$
      $b^n_u = \sum_{i=0}^{n_u} \mathbf{JxW}(-(u-u(x,y)\varphi[i]) + \nabla\lambda\nabla[i] + \lambda u\varphi[i])$
      $K^n_{qq} = \sum_{i=0}^{n_q}\sum_{j=0}^{n_q} \mathbf{JxW}(\alpha\varphi[i]\varphi[j])$
      $K^n_{q\lambda} = \sum_{i=0}^{n_q}\sum_{j=0}^{n_\lambda} \mathbf{JxW}(\varphi[i]\varphi[j])$
      $K^n_{q\chi} = \sum_{i=0}^{n_q}\sum_{j=0}^{n_\chi} \mathbf{JxW}(\varphi[i]\varphi[j])$
      $b^n_q = \sum_{i=0}^{n_q} \mathbf{JxW}(-\alpha q[i]\varphi[i] - (\lambda[i]+\chi[i])\varphi[i])$
      $K^n_{\lambda u} = \sum_{i=0}^{n_\lambda}\sum_{j=0}^{n_u} \mathbf{JxW}(\nabla\varphi[i]\nabla\varphi[j])$
      $K^n_{\lambda q} = \sum_{i=0}^{n_\lambda}\sum_{j=0}^{n_q} \mathbf{JxW}(-\varphi[i]\varphi[j])$
      $K^n_{\lambda\lambda} = \sum_{i=0}^{n_\lambda}\sum_{j=0}^{n_\lambda} \mathbf{JxW}(\varphi[i]\varphi[j]/k)$
      $b^n_\lambda = \sum_{i=0}^{n_\lambda} \mathbf{JxW}(-\nabla u[i]\nabla\varphi[i] + q[i]\varphi[i])$
      $K^n_{\chi q} = \sum_{i=0}^{n_\chi}\sum_{j=0}^{n_q} \mathbf{JxW}(k\chi[i]\Psi'(k(\beta(q[i])\varphi[i]\varphi[j])$
      $K^n_{\chi\chi} = \sum_{i=0}^{n_\chi}\sum_{j=0}^{n_\chi} \mathbf{JxW}(\varphi[i]\varphi[j])$
      $b^n_\chi = \sum_{i=0}^{n_\chi} \mathbf{JxW}((\chi[i]\Psi'(k\beta(q[i])) - 1)\varphi[i]))$
    end for
    Add elemental K^n matrix and b^n to the global system (7.17)
  end for
  Zero out the off-diagonal elements in each row corresponding to the homogeneous boundary conditions on δu and $\delta\lambda$.
  Solve (7.17) for $(\delta u_i, \delta q_i, \delta\lambda_i, \delta\chi_i)^T$ using the MUMPS direct solver
  Update the variables

$$\begin{aligned} u_i &= u_i + \delta u_i \\ q_i &= q_i + \delta q_i \\ \lambda_i &= \lambda_i + \delta\lambda_i \\ \chi_i &= \chi_i + \delta\chi_i \end{aligned} \tag{7.58}$$

  Compute the error $\mathcal{E}$
end while

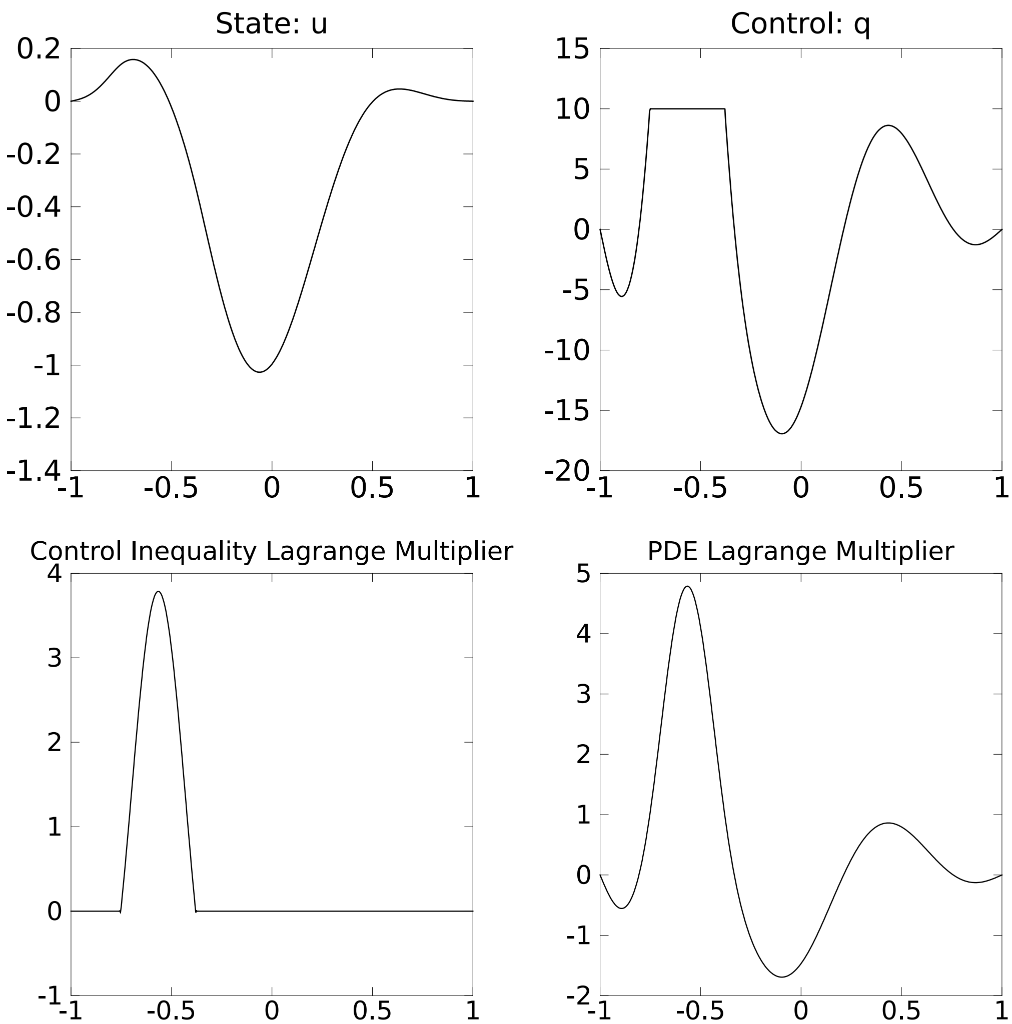


Figure 7.4: State, Control, and Lagrange Multipliers for the PDNRAL Example

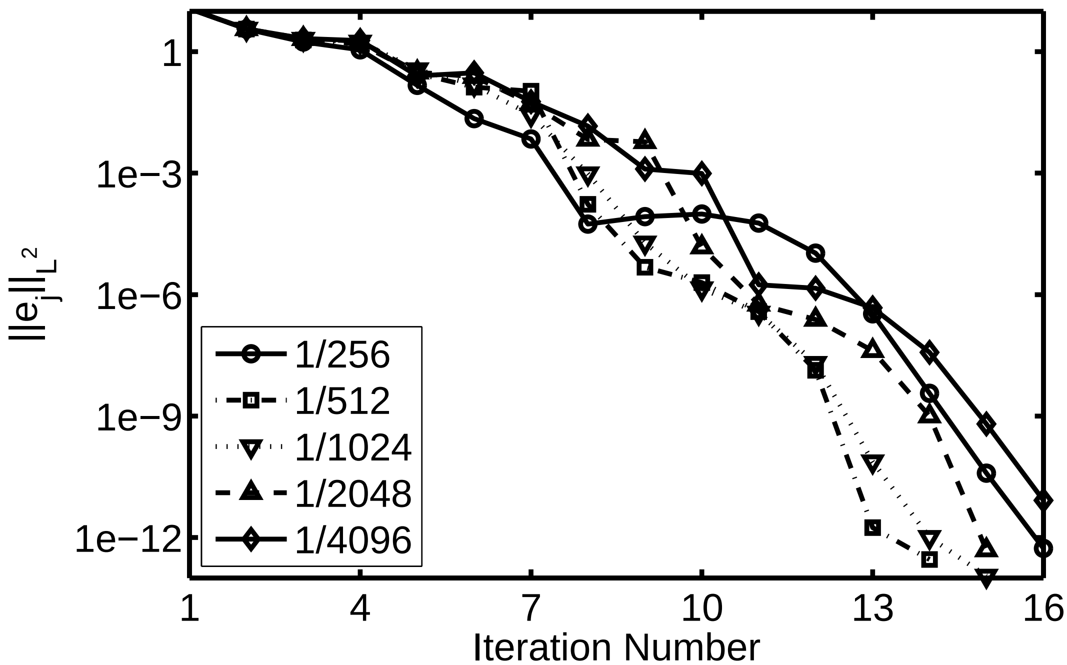


Figure 7.5: Convergence Plots for PDNRAL Example Problem

solving problems of this type.

Chapter 8: Conclusion

Function space optimization methods based on the Nonlinear Rescaling method have been examined here. A new variant of these methods, the NR-PDAL, was proposed and analyzed. This method was proven to have linear convergence rates for elliptically constrained problems with state and control constraints. An example problem was constructed which confirmed that the NR-PDAL method can experience the predicted linear convergence.

Two other methods were considered. The first of these is the PDAL method, which is a key component of the NR-PDAL method, was analyzed for elliptically constrained optimization problems. This method was proven to have quadratic convergence rates for problems of this type. In addition, the discretized problem was demonstrated to retain the quadratic convergence. Additionally, the PDAL method showed mesh independent convergence rates. These items all imply that the function space PDAL is an excellent method to use for problems of this type.

The last method examined was the function space PDNRAL method for elliptically constrained problems with control constraints. It was proven that for these problems the method is capable of superlinear convergence. An addition, a test case was constructed which demonstrated that the discretized implementation of the PDNRAL does retain superlinear convergence, and has little mesh dependence in the convergence rate.

It should be noted that while the NR-PDAL implementation for problems including state constraints did exhibit linear convergence rates, those rates were slow in the more refined mesh cases. In addition, the algorithm did not converge with lower

k values for the more refined mesh cases. This is not unexpected behavior, as the convergence analysis for the NR-PDAL method requires k to be large enough. For the refined mesh cases, k needed to be larger in order to attain convergence. There was a limit to how high the k could go in the implementations. The author believes that these issues are a function of the method used to discretize the function space algorithm. The standard continuous Galerkin method used for the finite element discretization may not be appropriate for the highly non-regular Lagrangian associated with state constraint. This method was chosen for its simplicity, and in the end was sufficient to demonstrate the linear convergence rate of the model. But future work could be performed to modify the discretized implementation of the NR-PDAL to improve the stability and convergence rate that result from the state constraint.

The excellent performance of the NR-PDAL and PDNRAL methods for problems with only control constraints indicates that the method may be promising for solving regularized state constrained problems [2, 40, 28] as well. The regularization is often performed by replacing the pure state constraint, such as $\eta_u \geq u$, with the following mixed control-state constraint,

$$\eta_u \geq u + \varepsilon q \tag{8.1}$$

for some small regularization parameter $\varepsilon > 0$. The inclusion of the regularization term, εq, has a rather profound effect, in that it converts the Lagrange multiplier from the simple measure ($\sigma_u \in \mathcal{C}^*$) to a function in L^2. The author expects that using the NR-PDAL method on regularized state constraints should lead to similar performance as control constrained problems.

In the end, methods derived from the NR principle have been proven and demonstrated to work both in theory and in practice for elliptically constrained problems with state and/or control constraints.

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Biography

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