



Journal of Applied and Computational Mechanics



Research Paper

A General Purpose Variational Formulation for Boundary Value Problems of Orders Greater than Two

Xuefeng Li¹✉

¹Department of Mathematics and Computer Science, Loyola University, New Orleans, LA 70118, U.S.A., Email: Li@Loyno.edu

Received April 24 2021; Revised July 02 2021; Accepted for publication July 03 2021.

Corresponding author: Xuefeng Li (Li@Loyno.edu)

© 2021 Published by Shahid Chamran University of Ahvaz

Abstract. We develop a new general purpose variational formulation, particularly suitable for solving boundary value problems of orders greater than two. The functional related to this variational formulation requires only \mathcal{H}^1 regularity in order to be well-defined. Using the finite element method based on this new formulation thus becomes simple even for domains in dimensions greater than one. We prove that a saddle-point solution to the new variational formulation is a weak solution to the associated boundary value problem. We also prove the convergence of the numerical methods used to find approximate solutions to the new formulation. We provide numerical tests to demonstrate the efficacy of this new paradigm.

Keywords: Functional minimization, Augmented Lagrangian methods.

1. Introduction

Many problems in physics and engineering are usually formulated in boundary value problems (BVPs). A weak solution to a BVP is usually associated with the minimization of some functional $I(u)$, where u represents some key feature of a system, and $I(u)$ represents the total potential energy of the system at the value u of the key feature. A minimum takes place at a stationary point of the functional $I(u)$. Thus to solve a BVP means to find stationary points of the associated functional $I(u)$.

BVPs of different orders usually have different regularity requirements for functional $I(u)$ to be well-defined. Consequently, we may need to apply different finite element methods (FEM) when solving for approximate solutions to BVPs of different orders.

As addressed by Ciarlet [1], in the “standard” variational formulations, a second order Laplace equation $\Delta u = 0$ requires an \mathcal{H}^1 regularity for the associated functional, whereas a fourth order biharmonic equation $\Delta^2 u = 0$ requires an \mathcal{H}^2 regularity. Regularity requirement of \mathcal{H}^k for $k > 1$ is notoriously unwieldy (Axelsson [2]) and poses serious computational difficulties (Ciarlet [1]), especially for BVPs in domains of dimensions greater than 1, when using FEM.

One way to avoid the high regularity requirement is to use the mixed FEM (Ciarlet [1]), where a fourth order BVP is decomposed into two second order ones along with new independent variables. See Oden [3], Babuska [4], Brezzi [5], Brezzi and Raviart [6], Raviart and Thomas [7], Falk [8], and more work cited in these papers for further details on how mixed FEM may be used to solve BVPs.

The mixed FEM have become one of the “standard” methods to handle BVPs, as demonstrated in the work by Han [9], Monk [10], Brenner [11], Figueroa, et al. [12], Camaño, et al. [13], Barnafi, et al. [14], Lee, et al. [15], Ambartsumyan, et al. [16], Carstensen and Ma [17].

The mixed FEM are highly flexible in the sense that there could be multiple schemes of decomposition to the same BVP. However, one must carefully design a unique decomposition scheme for every BVP in order to carry out the mixed FEM.

The goal of this paper is to provide a general purpose variational formulation to a BVP of order greater than two, whose weak solution is associated with the saddle-point of the variational formulation. In that sense, it is an extension to the mixed FEM, without having to carefully design a decomposition scheme for a BVP. In fact, the current formulation is algebraic in nature and is applicable to any existing variational formulation associated with a BVP of any order (e.g., $2k$ for a certain integer $k > 0$), regardless of the geometric or physical properties of the BVP.

This general purpose variational formulation has the following characteristics.

1. It requires only \mathcal{H}^1 regularity on the weak solution to the BVP, independent of the order of the BVP under consideration. That means Lagrange finite elements will be sufficient for solving the BVP of any order, over a domain of any dimension, under this new variational formulation.
2. When solving for weak solution to a BVP of order $2k$ using the new variational formulation, not only can we obtain a function that is a weak solution to the BVP, we obtain also functions that are *weak derivatives of the solution, up to order k* . These bonus functions enable us to compute for other quantities associated with a BVP without having to further process the solution itself.
3. We can apply this new variational formulation to any existing functional $I(u)$ associated with a BVP, regardless of whether $I(u)$ is linear or nonlinear in u .



In summary, this general purpose variational formulation provides a standard way to calculate numerical solution to a BVP of order $2k$, and produces estimates to partial derivatives, from 0-th up to k -th order, of the solution.

A successful application of this general purpose variational formulation thus depends on having a variational principle associated with a BVP. The semi-inverse method proposed by He [18], provides an excellent way to derive variational principles associated with BVPs. Even though the semi-inverse method was first demonstrated in fluid mechanics, it has since been widely applied to various problems, including but not limited to, elasticity (He [19]), nonlinear oscillators (He [20], He, et al. [21]), piezoelectric beams (He [22]), 3D unsteady flow (He [23]), plasma (EL-Kalaawy [24], He [25]), shallow water (He [26] with fractal derivatives, Cao, et al. [27], Cao, et al. [28]), and Schrödinger's equation (He [20], Liu, et al. [29]). We are very hopeful that we can use the versatile semi-inverse method to obtain variational principles for many more BVPs so that this general purpose variational formulation may be applied to obtain numerical solutions to these BVPs in the future.

The rest of the paper is organized as follows. In Section 2, we introduce the mathematical problems under consideration that is a weak formulation of a BVP. We then develop a new Lagrangian based on the Augmented Lagrangian Methods (ALM) by Fortin and Glowinski [30]. We prove the existence and uniqueness of the saddle-point solution of the new Lagrangian which induces a weak solution to the BVP. In Section 3, we introduce the saddle-point algorithm for finding saddle-points of the new Lagrangian, and prove the convergence of the algorithm. In Section 4, we solve the 4th order biharmonic equation to demonstrate the efficacy of this new paradigm.

2. The Original Problem and its Equivalency

We introduce notations, the general mathematical problem, and various equivalent forms of the problem in this section.

2.1 Notations and the Main Problem

The problem we're going to study relates to functions defined over an open bounded region $\Omega \subset \mathbb{R}^n$ with a Lipschitz-continuous boundary $\partial\Omega$.

For ease of presentation, given a suitable function u and integers $k, n \geq 1$, for $1 \leq l \leq k$, we define

$$\begin{aligned} j_l &\equiv (j_1, j_2, \dots, j_l), \quad 1 \leq j_i \leq n, \quad 1 \leq i \leq l, \\ \partial_{j_l}^l u &\equiv \partial_{j_1, j_2, \dots, j_l}^l u = \frac{\partial^l u}{\partial x_{j_1} \dots \partial x_{j_2} \partial x_{j_1}}. \end{aligned}$$

Notice that $\partial_{j_l}^l u \equiv u$ when $l = 0$ by convention.

We investigate the issue of finding approximate solution to minimization problem (1).

$$\text{Find } v \in \mathcal{V} \text{ such that } I(v) = \inf_{u \in \mathcal{V}} I(u), \quad (1)$$

over a certain appropriate set \mathcal{V} , where functional $I(u)$ is in the form of

$$I(u) = \int_{\Omega} \Phi(x, \langle \partial_{j_l}^l u \rangle) dx. \quad (2)$$

Notation $\langle \partial_{j_l}^l u \rangle$ represents a certain collection of l -th order partial derivatives of u that $\Phi()$ depends on explicitly, for l between 0 up to k . Let

$$\begin{cases} \mathcal{A} &\equiv \{j_l \mid \partial_{j_l}^l u \in \langle \partial_{j_l}^l u \rangle \text{ in functional (2), } 0 \leq l \leq k\}, \\ \mathcal{B}_T &\equiv \{j_k \in \mathcal{A}\} = \{j_k \mid \partial_{j_k}^k u \in \langle \partial_{j_l}^l u \rangle\}. \end{cases} \quad (3)$$

Notice that \mathcal{A} and \mathcal{B}_T are actually independent of u even though u appears in eq. (3). For example, if $\Phi()$ depends exactly on u and Δu , then $k = 2$, and

$$\langle \partial_{j_l}^l u \rangle = \{u, \partial_{ii}^2 u \mid 1 \leq i \leq n\}, \quad \mathcal{A} = \{(0), (i, i) \mid 1 \leq i \leq n\}, \quad \mathcal{B}_T = \{(i, i) \mid 1 \leq i \leq n\}.$$

We make some additional assumptions below.

- For ease of presentation, we assume that $\Phi()$ is a function with continuous partial derivatives of orders up to $k+1$. Therefore, functional $I(u)$ is well-defined for any $u \in C^k(\bar{\Omega}) \cap H^k(\Omega)$. Usually, functional $I(u)$ would be well-defined even for $\Phi()$ not satisfying this assumption. For example, Fortin and Glowinski [30] investigated functional $I(u)$ where

$$I(u) = \int_{\Omega} \Phi(x, \langle \partial_{j_l}^l u \rangle) dx = \int_{\Omega} f(x, \nabla u) dx + \int_{\Omega} u g(x) dx, \quad (4)$$

where functional $F(u) = \int_{\Omega} f(x, \nabla u) dx$ is assumed to be convex, lower semi-continuous but not necessarily differentiable with respect to u .

- \mathcal{V} is a closed convex subset of a certain Hilbert space, e.g.,

$$\mathcal{V} \subseteq \mathcal{H}^k(\Omega), \quad k > 0.$$

- We assume that subset \mathcal{V} enforces the Dirichlet boundary conditions for problem (1), e.g., $\forall x \in \partial\Omega$,

$$\partial_{\vec{N}^l}^l u = g_l(x), \quad 0 \leq l < k, \quad (5)$$

where $\vec{N} = (N_1, \dots, N_n)^T$ is the unit outward normal vector of $\partial\Omega$, $\partial_{\vec{N}^l}^l u = \frac{\partial^l u}{\partial \vec{N}^l}$ is the l -th order directional derivative of u in direction \vec{N} , for $0 \leq l < k$. These boundary conditions are homogeneous when $g_l(x) = 0$, for all $0 \leq l < k$.

- For brevity, we use $\|w\|$ to represent the norm of the space element w belongs to.



- We also assume that Φ is convex with respect to its arguments related to u . That is,

$$\Phi(x, \langle (1-t)\partial_{j_l}^l u + t\partial_{j_l}^l v \rangle) \leq (1-t)\Phi(x, \langle \partial_{j_l}^l u \rangle) + t\Phi(x, \langle \partial_{j_l}^l v \rangle), \\ \forall u, v \in \mathcal{V}, \forall t \in [0, 1].$$

If $v \in \mathcal{V}$ is a minimizer of problem (1), v must be a stationary point of the related functional. A stationary point is defined in Definition 1.

Definition 1. A stationary point $v \in \mathcal{V}$ of minimization problem (1) is defined as

$$\left. \frac{d}{dt} I(v + t(u - v)) \right|_{t=0} \geq 0, \forall u \in \mathcal{V}.$$

If

$$\exists U \subset \mathcal{V}, U \text{ is open and } v \in U, \quad (6)$$

then

$$\left. \frac{d}{dt} I(v + t(u - v)) \right|_{t=0} = 0, \forall u \in \mathcal{V}. \quad (7)$$

Therefore, when a stationary point v of functional (2) meets condition (6), it satisfies

$$\left. \frac{d}{dt} \int_{\Omega} \Phi(x, \langle \partial_{j_l}^l (v + t(u - v)) \rangle) dx \right|_{t=0} = 0, \forall u \in \mathcal{V}.$$

That is,

$$\sum_{j_l \in \mathcal{A}} \int_{\Omega} \partial_{j_l}^l (u - v) \frac{\partial \Phi(x, \langle \partial_{j_l}^l v \rangle)}{\partial (\partial_{j_l}^l u)} dx = 0, \forall u \in \mathcal{V}. \quad (8)$$

When condition (6) is not met, the above equations become inequalities where each “= 0” becomes “ ≥ 0 ”.

Due to the Dirichlet boundary conditions (5), $\forall u \in C^{2k}(\Omega)$, by applying Green's formula repeatedly for eq. (8), we arrive at the following Euler-Lagrange equation associated with functional (2).

$$\sum_{j_l \in \mathcal{A}} (-1)^l \partial_{j_l}^l \left(\frac{\partial \Phi(x, \langle \partial_{j_l}^l v \rangle)}{\partial (\partial_{j_l}^l u)} \right) = 0. \quad (9)$$

Because the maximum value of l is k , the above Euler-Lagrange is a differential equation of order $2k$. That is, minimization problem (1) with $I(u)$ in eq. (2) which is subject to boundary conditions (5), is naturally associated with the following $2k$ -th order BVP.

$$\begin{cases} \text{Find } v \in C^{2k}(\Omega) \text{ such that} \\ \sum_{j_l \in \mathcal{A}} (-1)^l \partial_{j_l}^l \left(\frac{\partial \Phi(x, \langle \partial_{j_l}^l v \rangle)}{\partial (\partial_{j_l}^l u)} \right) = 0, \forall x \in \Omega, \\ \frac{\partial^l v}{\partial \bar{N}^l} = g_l(x), 0 \leq l < k, \forall x \in \partial\Omega. \end{cases} \quad (10)$$

2.2 An Equivalent Lagrangian

For any $u \in \mathcal{V}$, $\forall j_l = (j_1, \dots, j_l) \in \mathcal{A}$, $\partial_{j_l}^l u$ corresponds to a hierarchical chain of partial derivatives.

$$\partial_{j_1, \dots, j_l}^l u = \partial_{j_l} (\partial_{j_1, \dots, j_{l-1}}^{l-1} u), \dots, \partial_{j_1, j_2}^2 u = \partial_{j_2} (\partial_{j_1} u), \partial_{j_1} u = \partial_{j_1} (u), \partial^0 u = u.$$

We therefore introduce a set of supplementary variables $p_{j_l}^{<u>}$ that corresponds to the chain of partial derivatives.

$$p_{j_l}^{<u>} \equiv \{p_{j_1, \dots, j_i}^{<u>} \mid 0 \leq i \leq l\} = \{u, p_{j_1}^{<u>}, p_{j_1, j_2}^{<u>}, \dots, p_{j_1, \dots, j_l}^{<u>}\}, \quad (11)$$

where

$$\begin{cases} p_{j_1, \dots, j_l}^{<u>} = \partial_{j_l} p_{j_1, \dots, j_{l-1}}^{<u>}, \dots, p_{j_1, j_2}^{<u>} = \partial_{j_2} p_{j_1}^{<u>}, p_{j_1}^{<u>} = \partial_{j_1} u, \text{ or} \\ p_{j_1, \dots, j_i}^{<u>} - \partial_{j_i} p_{j_1, \dots, j_{i-1}}^{<u>} = 0, 1 \leq i \leq l. \end{cases} \quad (12)$$

Here, we adopt the notation that

$$p_{j_0}^{<u>} \equiv \partial^0 u \equiv u. \quad (13)$$

Notice that $u \in p_{j_l}^{<u>}$, $\forall j_l \in \mathcal{A}$ by definition.

In equations (11), (12) and (13), superscript $<u>$ is used to indicate the dependence on u of the underlying variables. To avoid excessive use of superscripts, we'll drop this indication from now on so long as there is no ambiguity based on the context. We therefore rewrite equations (11), (12) and (13) as equations (14), (15) and (16), respectively.

$$p_{j_l} \equiv \{p_{j_1, \dots, j_i} \mid 0 \leq i \leq l\} = \{u, p_{j_1}, p_{j_1, j_2}, \dots, p_{j_1, \dots, j_l}\}, \quad (14)$$

$$\begin{cases} p_{j_1, \dots, j_l} = \partial_{j_l} p_{j_1, \dots, j_{l-1}}, \dots, p_{j_1, j_2} = \partial_{j_2} p_{j_1}, p_{j_1} = \partial_{j_1} u, \text{ or} \\ p_{j_1, \dots, j_i} - \partial_{j_i} p_{j_1, \dots, j_{i-1}} = 0, 1 \leq i \leq l, \end{cases} \quad (15)$$

$$p_{j_0} \equiv \partial^0 u \equiv u. \quad (16)$$



Relations in eq. (12) (and in eq. (15)) are referred to as *recursive linear equality relations*. We can see that $\forall j_l = (j_1, \dots, j_l) \in \mathcal{A}$,

$$p_{j_l} \equiv \partial_{j_l}^i u, \quad 1 \leq i \leq l, \quad (17)$$

so long as $u \in \mathcal{H}^l(\Omega)$.

Based on eq. (14), we introduce some more sets of supplementary variables.

$$\forall u \in \mathcal{V}, \quad \begin{cases} \mathfrak{p} \equiv (\cup_{j_l \in \mathcal{A}} \mathfrak{p}_{j_l}) \setminus \{u\}, \\ \mathfrak{p}_T = \{p_{j_k} \mid j_k \in \mathcal{B}_T\} = \{p_{j_k} \in \mathfrak{p}\}, \\ \mathfrak{p}_L = \mathfrak{p} \setminus \mathfrak{p}_T = \{p_{j_l} \in \mathfrak{p} \mid 1 \leq l < k\}, \\ \mathfrak{p} = (\mathfrak{p}_L, \mathfrak{p}_T), \end{cases}$$

where \mathcal{B}_T was defined in eq. (3). Correspondingly, we define sets of indexes

$$\mathcal{B} \equiv \{j_l \mid \text{if } p_{j_l} \in \mathfrak{p}\}, \quad \mathcal{B}_L \equiv \{j_l \mid \text{if } p_{j_l} \in \mathfrak{p}_L\}, \quad (18)$$

We denote the cardinality of each of the above sets as shown below.

$$\begin{aligned} N_L &\equiv \text{Card}(\mathfrak{p}_L) = \text{Card}(\mathcal{B}_L), \\ N_T &\equiv \text{Card}(\mathfrak{p}_T) = \text{Card}(\mathcal{B}_T), \\ N_C &\equiv \text{Card}(\mathfrak{p}) = \text{Card}(\mathcal{B}) = N_L + N_T. \end{aligned}$$

As a result, when substituting p_{j_l} for each derivative $\partial_{j_l}^i u$ in functional (2), we turn minimization problem (1) into an equivalent minimization problem (19).

$$\text{Find } (v, q_L, q_T) \in \mathcal{W} \text{ such that } \mathcal{I}(v, q_L, q_T) = \inf_{(u, \mathfrak{p}_L, \mathfrak{p}_T) \in \mathcal{W}} \mathcal{I}(u, \mathfrak{p}_L, \mathfrak{p}_T), \quad (19)$$

where

$$\mathcal{I}(u, \mathfrak{p}_L, \mathfrak{p}_T) = \int_{\Omega} \Phi(x, \langle p_{j_l} \rangle) dx, \quad \forall (u, \mathfrak{p}_L, \mathfrak{p}_T) \in \mathcal{W}, \quad (20)$$

and

$$\mathcal{W} \equiv \{(u, \mathfrak{p}_L, \mathfrak{p}_T) \mid \forall u \in \mathcal{V}, \forall p_{j_l} \in \mathfrak{p}_L \cup \mathfrak{p}_T \text{ satisfying (15)}\}. \quad (21)$$

In particular, $\langle p_{j_l} \rangle$ is an appropriate collection of p_{j_l} obtained from replacing each $\partial_{j_l}^i u$ in $\langle \partial_{j_l}^i u \rangle$ of functional (2) by p_{j_l} .

Regardless of whether $\Phi(\cdot)$ depends explicitly on u or not, we list u as an explicit independent variable for functional $\mathcal{I}(\cdot)$ in eq. (20) because $\mathcal{I}(\cdot)$ is related to u in eq. (21) through condition (15).

According to eq. (16), notation $(v, q_L, q_T) \in \mathcal{W}$ implies that $q_{j_0} = \partial^0 v = v$, and $(u, \mathfrak{p}_L, \mathfrak{p}_T) \in \mathcal{W}$ implies that $p_{j_0} = \partial^0 u = u$.

For example, in the case of $\Omega \subset \mathbb{R}^2$, and if $\Phi(\cdot)$ depends on u and Δu in the form of

$$\Phi(x, \langle \partial_{j_l}^i u \rangle) = \frac{1}{2} |\Delta u|^2 - uf(x) = \frac{1}{2} |\partial_{1,1}^2 u + \partial_{2,2}^2 u|^2 - uf(x),$$

in functional (2) where $f(x)$ is a known function, then in functional \mathcal{I} of (20),

$$\begin{cases} k = 2, \quad n = 2, \quad \langle \partial_{j_l}^i u \rangle = \{u, \partial_{1,1}^2 u, \partial_{2,2}^2 u\}, \quad \mathcal{A} = \{(0), (1, 1), (2, 2)\}, \\ \mathfrak{p}_0 = \{u\}, \quad \mathfrak{p}_{1,1} = \{u, p_{1,1}\}, \quad \mathfrak{p}_{2,2} = \{u, p_{2,2}\}, \quad \mathfrak{p} = \{p_{1,1}, p_{2,2}\}, \\ \mathfrak{p}_L = \{p_{1,1}, p_{2,2}\}, \quad \mathfrak{p}_T = \{p_{1,1}, p_{2,2}\}, \quad \langle p_{j_l} \rangle = \{u, p_{1,1}, p_{2,2}\}, \\ \mathcal{B} = \{(1), (2), (1, 1), (2, 2)\}, \quad \mathcal{B}_L = \{(1), (2)\}, \quad \mathcal{B}_T = \{(1, 1), (2, 2)\}, \\ N_L = 2, \quad N_T = 2, \quad N_C = 4, \\ \Phi(x, \langle p_{j_l} \rangle) = \frac{1}{2} |p_{1,1} + p_{2,2}|^2 - uf(x). \end{cases}$$

That is, we substitute $p_{1,1}$ and $p_{2,2}$ for $\partial_{1,1}^2 u$ and $\partial_{2,2}^2 u$, respectively. Due to eq. (17), functionals (2) and (20) are indeed equivalent so long as $u \in \mathcal{V} \subseteq \mathcal{H}^k(\Omega)$.

Minimization problem (19) is constrained through \mathcal{W} in association with recursive linear equality relations (15). To overcome the complexity involved in dealing with constraints, we introduce Lagrange multipliers, and convert minimization problem (19) into a saddle-point problem (22) of Lagrangian \mathcal{L} in eq. (23).

$$\begin{cases} \text{Find saddle-point } (v, q_L, q_T, \nu) \in \mathfrak{W} \text{ of } \mathcal{L}(u, \mathfrak{p}_L, \mathfrak{p}_T, \mu), \text{ such that} \\ \mathcal{L}(v, q_L, q_T, \mu) \leq \mathcal{L}(u, q_L, q_T, \nu) \leq \mathcal{L}(u, \mathfrak{p}_L, \mathfrak{p}_T, \nu), \quad \forall (u, \mathfrak{p}_L, \mathfrak{p}_T, \mu) \in \mathfrak{W}, \end{cases} \quad (22)$$

where

$$\mathcal{L}(u, \mathfrak{p}_L, \mathfrak{p}_T, \mu) \equiv \mathcal{I}(u, \mathfrak{p}_L, \mathfrak{p}_T) + \sum_{j_l \in \mathcal{B}} \int_{\Omega} \mu_{j_l} (p_{j_l} - \partial_{j_l} p_{j_l-1}) dx, \quad (23)$$

and

$$\begin{aligned} \mathfrak{W} &\equiv \mathfrak{U} \times \mathfrak{P}_L \times \mathfrak{P}_T \times \mathfrak{M}, \\ \mathfrak{U} &= \{u \in \mathcal{H}^1(\Omega) \mid u(x)|_{\partial\Omega} = b_0(x)\}, \end{aligned} \quad (24)$$

$$\mathfrak{P}_L = \{p_{j_l} \in \mathcal{H}^1(\Omega) \mid j_l \in \mathcal{B}_L, \quad p_{j_l}(x)|_{\partial\Omega} = b_{j_l}(x)\}, \quad (25)$$

$$\mathfrak{P}_T = \{p_{j_k} \in \mathcal{H}^0(\Omega) \mid j_k \in \mathcal{B}_T\} = (\mathcal{H}^0(\Omega))^{N_T},$$

$$\mathfrak{M} = \{\mu_{j_l} \in \mathcal{H}^0(\Omega) \mid j_l \in \mathcal{B}\} = (\mathcal{H}^0(\Omega))^{N_C},$$



for some boundary value functions $b_0(x)$ and $b_{j_l}(x)$, $j_l \in \mathcal{B}_L$. Notice that $b_0(x) \equiv g_0(x)$ in eq. (24). It is only a matter of algebra to solve for the boundary value functions $b_{j_l}(x)$ in eq. (25) using $g_l(x)$ from eq. (5), for $j_l \in \mathcal{B}_L$, $\forall x \in \partial\Omega$. We'll show specific examples in a later section.

Notice that according to assumption (16), $\partial_{j_l} p_{j_{l-1}} \equiv \partial_{j_l} u$ when $l = 1$ in Lagrangian \mathcal{L} defined in eq. (23).

Because $\Phi(\cdot)$ is continuously differentiable up to order $k + 1$, functional $\mathcal{I}(u, p_L, p_T)$ is well-defined $\forall (u, p_L, p_T) \in \mathcal{U} \times \mathcal{P}_L \times \mathcal{P}_T$. Hence Lagrangian $\mathcal{L}(u, p_L, p_T, \mu)$ is well-defined for all $(u, p_L, p_T, \mu) \in \mathcal{W}$.

Unlike minimization problem (1) which involves with partial derivatives of the unknown function up to k -th order, saddle-point problem (22) is well-defined so long as its variables belong to either $\mathcal{H}^1(\Omega)$ or $\mathcal{H}^0(\Omega)$. As a result, when finding solution to saddle-point problem (22) using finite element methods, we can meet the \mathcal{H}^1 regularity requirement for space R^n of arbitrary dimension n without needing any special treatment.

The equivalency of functionals $I(u)$ in (2) and $\mathcal{I}(u, p_L, p_T)$ in (20) is ensured so long as $u \in \mathcal{V} \subseteq \mathcal{H}^k(\Omega)$. To ensure the equivalency of functionals $I(u)$ and $\mathcal{L}(u, p_L, p_T, \mu)$, we need a lemma.

Lemma 1. Define a set of indexes

$$\mathcal{J}_l \equiv \{(j_1, \dots, j_l) \mid 1 \leq j_i \leq n, 1 \leq i \leq l\}, \quad (26)$$

for $1 \leq l \leq k$ where n is the dimension of the domain under consideration. Suppose that the index set \mathcal{B} as defined in eq. (18) is sufficiently large so that

$$\mathcal{J}_{k-1} \subset \mathcal{B}. \quad (27)$$

Then $(v, q_L, q_T) \in \mathcal{M} \times \mathcal{P}_L \times \mathcal{P}_T$ which satisfies the recursive linear equality relations (15), i.e., $\forall j_l \in \mathcal{B}$,

$$\begin{cases} q_{j_1, \dots, j_l} = \partial_{j_l} q_{j_1, \dots, j_{l-1}}, \dots, q_{j_1, j_2} = \partial_{j_2} q_{j_1}, q_{j_1} = \partial_{j_1} v, \text{ or} \\ q_{j_1, \dots, j_i} - \partial_{j_i} q_{j_1, \dots, j_{i-1}} = 0, 1 \leq i \leq l, \end{cases}$$

implies that $v \in \mathcal{H}^k(\Omega)$ and

$$q_{j_l} = \partial_{j_l}^l v, \forall j_l \in \mathcal{B}.$$

In other words, recursive linear equality relations for $(v, q_L, q_T) \in \mathcal{M} \times \mathcal{P}_L \times \mathcal{P}_T$ imply that $v \in \mathcal{H}^k(\Omega)$, and $q_{j_l} = \partial_{j_l}^l v$, $\forall j_l \in \mathcal{B}$, so long as condition (27) is met. Furthermore, because $v \in \mathcal{M} \subset \mathcal{H}^1(\Omega)$ by definition of \mathcal{M} , the conclusion of Lemma 1 is trivial for the case of $k = 1$.

We omit the proof of Lemma 1 because it is a simple manipulation of the recursive nature of the recursive linear equality relations (15).

The following theorem sums up the relation between minimization problem (1) and saddle-point problem (22).

Theorem 1. If $(v, q_L, q_T, \nu) \in \mathcal{W}$ is a saddle-point of Lagrangian \mathcal{L} of eq. (23), and boundary conditions (5) are homogeneous, then $v \in \mathcal{V}$, and v is a solution of minimization problem (1) that satisfies $q_{j_l} = \partial_{j_l}^l v$, $\forall j_l \in \mathcal{B}$.

Theorem 1 validates the fact that solving minimization problem (1) is equivalent to finding saddle-points of Lagrangian \mathcal{L} of eq. (23). We omit the proof of Theorem 1 because it again involves the manipulation of the recursive nature of the recursive linear equality relations (15).

2.3 The Augmented Lagrangian

To facilitate the numerical procedure for finding solutions to minimization problem (1), we propose an augmented Lagrangian \mathcal{L}_r based on ALM. $\forall (u, p_L, p_T, \mu) \in \mathcal{W}$,

$$\mathcal{L}_r(u, p_L, p_T, \mu) = \mathcal{L}(u, p_L, p_T, \mu) + \frac{1}{2} \sum_{j_l \in \mathcal{B}} r \int_{\Omega} (p_{j_l} - \partial_{j_l} p_{j_{l-1}})^2 dx, \quad (28)$$

where r is a pre-chosen positive constant. A saddle-point problem associated with the augmented Lagrangian $\mathcal{L}_r(u, p_L, p_T, \mu)$ is shown in eq. (29).

$$\begin{cases} \text{Find saddle-point } (v, q_L, q_T, \nu) \in \mathcal{W} \text{ of } \mathcal{L}_r, \text{ i.e., } \forall (u, p_L, p_T, \mu) \in \mathcal{W}, \\ \mathcal{L}_r(v, q_L, q_T, \mu) \leq \mathcal{L}_r(v, q_L, q_T, \nu) \leq \mathcal{L}_r(u, p_L, p_T, \nu). \end{cases} \quad (29)$$

Theorem 2. If $(v, q_L, q_T, \nu) \in \mathcal{W}$ is a saddle-point of Lagrangian \mathcal{L}_r of eq. (28), and boundary conditions (5) are homogeneous, then $v \in \mathcal{V}$, and it is a solution of minimization problem (1) that satisfies $q_{j_l} = \partial_{j_l}^l v$, $\forall j_l \in \mathcal{B}$.

We omit the proof of Theorem 2 because it is basically the same as that of Theorem 1.

According to Theorem 2, a saddle-point (v, q_L, q_T, ν) of the augmented Lagrangian \mathcal{L}_r also induces a solution v to the minimization problem (1). We'll focus on finding a saddle-point of the augmented Lagrangian \mathcal{L}_r in the next section.

3. The Saddle-Point Algorithm

Fortin and Glowinski [30] proposed two iterative methods, named ALG1 and ALG2, to be used with ALM for finding saddle-points of Lagrangian \mathcal{L}_r . The two methods may be combined into one method that uses ALG1 as an outer loop and ALG2 as an inner loop. Below is the outer loop related to the saddle-point problem (29).

Algorithm 1. ALG1 for finding saddle-point of problem (29).

1. Pick an arbitrary initial guess $\nu^{<0>} = \{\nu_{j_l}^{<0>} \mid j_l \in \mathcal{B}\} \in (\mathcal{H}^0(\Omega))^{N_C}$.
2. For $j \geq 0$, compute $(v^{<j>}, q_L^{<j>}, q_T^{<j>})$ so that $v^{<j>} = (v^{<j>}, q_L^{<j>}, q_T^{<j>}, \nu^{<j>}) \in \mathcal{W}$ is a solution of the minimization problem

$$\begin{cases} \mathcal{L}_r(v^{<j>}, q_L^{<j>}, q_T^{<j>}, \nu^{<j>}) \leq \mathcal{L}_r(u, p_L, p_T, \nu^{<j>}), \\ \forall u \in \mathcal{U}, \forall p_L \in \mathcal{P}_L, \forall p_T \in \mathcal{P}_T. \end{cases} \quad (30)$$



3. We compute update $\nu^{\prec j+1\rangle} = \{\nu_{j_l}^{\prec j+1\rangle}\} \in \mathfrak{M}$ by

$$\nu_{j_l}^{\prec j+1\rangle} = \nu_{j_l}^{\prec j\rangle} + \rho^{\prec j\rangle} (q_{j_l}^{\prec j\rangle} - \partial_{j_l} q_{j_{l-1}}^{\prec j\rangle}), \quad j_l \in \mathcal{B}, \quad (31)$$

where each $\rho^{\prec j\rangle}$ is a pre-chosen positive constant for $j \geq 0$.

4. Repeat steps 2 and 3 until the following convergence criteria are met for a pre-chosen relative tolerance ε_r .

$$\forall j_l \in \mathcal{B}, \quad \begin{cases} \|v^{\prec j+1\rangle} - v^{\prec j\rangle}\|_{0,\Omega} & \leq \varepsilon_r \|v^{\prec j\rangle}\|_{0,\Omega}, \\ \|q_{j_l}^{\prec j+1\rangle} - q_{j_l}^{\prec j\rangle}\|_{0,\Omega} & \leq \varepsilon_r \|q_{j_l}^{\prec j\rangle}\|_{0,\Omega}, \\ \|\nu_{j_l}^{\prec j+1\rangle} - \nu_{j_l}^{\prec j\rangle}\|_{0,\Omega} & \leq \varepsilon_r \|\nu_{j_l}^{\prec j\rangle}\|_{0,\Omega}. \end{cases}$$

Minimization problem (30) is a cornerstone for the numerical algorithms discussed in this paper. We therefore introduce a lemma concerning additional relations associated with minimization problem (30).

Lemma 2. If $(v, q_L, q_T) \in \mathfrak{U} \times \mathfrak{P}_L \times \mathfrak{P}_T$ is a solution of the minimization problem (32),

$$\mathcal{L}_r(v, q_L, q_T, \nu) \leq \mathcal{L}_r(u, p_L, p_T, \nu), \quad \forall u \in \mathfrak{U}, \quad \forall p_L \in \mathfrak{P}_L, \quad \forall p_T \in \mathfrak{P}_T, \quad (32)$$

for some $\nu \in \mathfrak{M}$, then (v, q_L, q_T) satisfies the following additional relations.

- Under the assumption that functional $\mathcal{I}(u, p_L, p_T)$ is convex with respect to (u, p_L, p_T) , then $\forall u \in \mathfrak{U}, \forall p_L \in \mathfrak{P}_L, \forall p_T \in \mathfrak{P}_T$,

$$\begin{aligned} 0 & \leq \mathcal{I}(u, p_L, p_T) - \mathcal{I}(v, q_L, q_T) + \sum_{j_l \in \mathcal{B}} \int_{\Omega} \nu_{j_l} (p_{j_l} - \partial_{j_l} p_{j_{l-1}} - (q_{j_l} - \partial_{j_l} q_{j_{l-1}})) dx \\ & + \sum_{j_l \in \mathcal{B}} r \int_{\Omega} (q_{j_l} - \partial_{j_l} q_{j_{l-1}}) (p_{j_l} - \partial_{j_l} p_{j_{l-1}} - (q_{j_l} - \partial_{j_l} q_{j_{l-1}})) dx. \end{aligned} \quad (33)$$

- Under the assumption that $\Phi(x, \langle p_{j_l} \rangle)$ is differentiable (so is functional $\mathcal{I}(u, p_L, p_T)$) with respect to p_{j_l} , $\forall j_l \in \mathcal{A}$, then $\forall u \in \mathfrak{U}, \forall p_L \in \mathfrak{P}_L, \forall p_T \in \mathfrak{P}_T$,

$$\begin{aligned} 0 & \leq \sum_{j_l \in \mathcal{A}} \int_{\Omega} \frac{\partial \Phi(x, \langle p_{j_l} \rangle)}{\partial p_{j_l}} (p_{j_l} - q_{j_l}) dx + \sum_{j_l \in \mathcal{B}} \int_{\Omega} \nu_{j_l} (p_{j_l} - \partial_{j_l} p_{j_{l-1}} - (q_{j_l} - \partial_{j_l} q_{j_{l-1}})) dx \\ & + \sum_{j_l \in \mathcal{B}} r \int_{\Omega} (q_{j_l} - \partial_{j_l} q_{j_{l-1}}) (p_{j_l} - \partial_{j_l} p_{j_{l-1}} - (q_{j_l} - \partial_{j_l} q_{j_{l-1}})) dx. \end{aligned} \quad (34)$$

We omit the proof of Lemma 2 because it is a simple application of the definition of a saddle-point of a Lagrangian that is either convex and/or differentiable.

In order to prove the convergence of Algorithm 1, we'll need to make further assumptions, as shown in equations (35), (36) and (37).

1. We assume that functional $\mathcal{I}(u, p_L, p_T)$ is unbounded in (u, p_L, p_T) . That is,

$$\begin{aligned} \sup_{\|u\| \rightarrow +\infty} |\mathcal{I}(u, p_L, p_T)| &= +\infty, \text{ or} \\ \sup_{\|p_L\| \rightarrow +\infty} |\mathcal{I}(u, p_L, p_T)| &= +\infty, \text{ or} \\ \sup_{\|p_T\| \rightarrow +\infty} |\mathcal{I}(u, p_L, p_T)| &= +\infty. \end{aligned} \quad (35)$$

2. We assume that functional \mathcal{I} satisfies the following condition. That is,

$$\begin{aligned} \sum_{j_l \in \mathcal{A}} \int_{\Omega} \left(\frac{\partial \Phi(x, \langle p_{j_l} \rangle)}{\partial p_{j_l}} \Big|_{(u_2, p_{L,2}, p_{T,2})} - \frac{\partial \Phi(x, \langle p_{j_l} \rangle)}{\partial p_{j_l}} \Big|_{(u_1, p_{L,1}, p_{T,1})} \right) (p_{j_l,2} - p_{j_l,1}) dx &\geq 0, \\ \forall (u_1, p_{L,1}, p_{T,1}), (u_2, p_{L,2}, p_{T,2}) \in \mathfrak{U} \times \mathfrak{P}_L \times \mathfrak{P}_T. \end{aligned} \quad (36)$$

Furthermore, if $(u_1, p_{L,1}, p_{T,1})$ and $(u_2, p_{L,2}, p_{T,2}) \in \mathfrak{U} \times \mathfrak{P}_L \times \mathfrak{P}_T$, and both satisfy the recursive linear equality relations (15), then

$$\begin{aligned} \sum_{j_l \in \mathcal{A}} \int_{\Omega} \left(\frac{\partial \Phi(x, \langle p_{j_l} \rangle)}{\partial p_{j_l}} \Big|_{(u_2, p_{L,2}, p_{T,2})} - \frac{\partial \Phi(x, \langle p_{j_l} \rangle)}{\partial p_{j_l}} \Big|_{(u_1, p_{L,1}, p_{T,1})} \right) (p_{j_l,2} - p_{j_l,1}) dx &= 0 \\ \text{if and only if } (u_1, p_{L,1}, p_{T,1}) &= (u_2, p_{L,2}, p_{T,2}). \end{aligned} \quad (37)$$

Conditions (36) and (37) are the counterpart to the uniformly convex condition assumed in Fortin and Glowinski [30] (page 114).

We present the convergence of Algorithm 1 in the following theorem.



Theorem 3. Suppose $v = (v, q_L, q_T, \nu) \in \mathfrak{M}$ is a saddle-point of Lagrangian \mathcal{L}_r of eq. (28). Assume that constant $\rho^{\prec j \succ}$ in Algorithm 1 satisfies

$$0 < \rho^{\prec j \succ} < 2r, \quad \forall j \geq 0, \quad (38)$$

and functional \mathcal{I} satisfies conditions (35), (36) and (37). Then the iterate from Algorithm 1, $v^{\prec j \succ} = (v^{\prec j \succ}, q_L^{\prec j \succ}, q_T^{\prec j \succ}, \nu^{\prec j \succ}) \in \mathfrak{M}$ satisfy

$$\lim_{j \rightarrow +\infty} \|v^{\prec j \succ} - v\|_{1,\Omega} = 0, \quad (39)$$

$$\lim_{j \rightarrow +\infty} \|q_{j_l}^{\prec j \succ} - q_{j_l}\|_{1,\Omega} = 0, \quad \forall j_l \in \mathcal{B}_L, \quad (40)$$

$$\lim_{j \rightarrow +\infty} \|q_{j_l}^{\prec j \succ} - q_{j_l}\|_{0,\Omega} = 0, \quad \forall j_l \in \mathcal{B}_T, \quad (41)$$

$$\lim_{j \rightarrow +\infty} \|\nu_{j_l}^{\prec j+1 \succ} - \nu_{j_l}^{\prec j \succ}\|_{0,\Omega} = 0, \quad \forall j_l \in \mathcal{B}, \quad (42)$$

$$\{\nu_{j_l}^{\prec j \succ} \mid \forall j_l \in \mathcal{B}\} \text{ is bounded.} \quad (43)$$

Furthermore, if $\nu^* \in \mathfrak{M}$ is a cluster point of $\{\nu_{j_l}^{\prec j \succ} \mid \forall j_l \in \mathcal{B}\}$, then (v, q_L, q_T, ν^*) is a saddle-point of \mathcal{L}_r .

Theorems 1 and 2 establish the fact that finding a solution of minimization problem (1) is equivalent to finding saddle-points of Lagrangian \mathcal{L} of eq. (23) and the augmented Lagrangian \mathcal{L}_r of eq. (28). Theorem 3 ensures that by following Algorithm 1, one will be able to compute numerical solutions by iteration that converge to a saddle-point of augmented Lagrangian \mathcal{L}_r . Due to space limitation, we omit the proof of Theorem 3 in this manuscript.

To find solution to minimization problem (30), under condition (6), according to equations (7),

$$\begin{cases} \frac{d}{dt} \mathcal{L}_r(v^{\prec j \succ} + t(u - v^{\prec j \succ}), q_L^{\prec j \succ} + t(p_L - q_L^{\prec j \succ}), \\ q_T^{\prec j \succ} + t(p_T - q_T^{\prec j \succ}), \nu^{\prec j \succ}) \Big|_{t=0} = 0, \quad \forall u \in \mathfrak{U}, \quad \forall p_L \in \mathfrak{P}_L, \quad \forall p_T \in \mathfrak{P}_T. \end{cases}$$

That simplifies into three equations (44), (45) and (46).

$$\begin{aligned} & \int_{\Omega} (u - v^{\prec j \succ}) \frac{\partial \Phi(x, \langle q_{j_l}^{\prec j \succ} \rangle)}{\partial u} dx - \sum_{j_1 \in \mathcal{B}} \int_{\Omega} \partial_{j_1} (u - v^{\prec j \succ}) \nu_{j_1}^{\prec j \succ} dx \\ & - \sum_{j_1 \in \mathcal{B}} r \int_{\Omega} \partial_{j_1} (u - v^{\prec j \succ}) (q_{j_1}^{\prec j \succ} - \partial_{j_1} v^{\prec j \succ}) dx = 0, \quad \forall u \in \mathfrak{U}. \end{aligned} \quad (44)$$

$$\begin{cases} \forall j_l \in \mathcal{B}_L, & \int_{\Omega} (p_{j_l} - q_{j_l}^{\prec j \succ}) \frac{\partial \Phi(x, \langle q_{j_l}^{\prec j \succ} \rangle)}{\partial p_{j_l}} dx + \int_{\Omega} (p_{j_l} - q_{j_l}^{\prec j \succ}) \nu_{j_l}^{\prec j \succ} dx \\ & - \sum_{(j_l, j_{l+1}) \in \mathcal{B}} \int_{\Omega} \partial_{j_{l+1}} (p_{j_l} - q_{j_l}^{\prec j \succ}) \nu_{j_{l+1}}^{\prec j \succ} dx \\ & + r \int_{\Omega} (p_{j_l} - q_{j_l}^{\prec j \succ}) (q_{j_l}^{\prec j \succ} - \partial_{j_l} q_{j_{l-1}}^{\prec j \succ}) dx \\ & - \sum_{(j_l, j_{l+1}) \in \mathcal{B}} r \int_{\Omega} \partial_{j_{l+1}} (p_{j_l} - q_{j_l}^{\prec j \succ}) (q_{j_{l+1}}^{\prec j \succ} - \partial_{j_{l+1}} q_{j_l}^{\prec j \succ}) dx = 0, \end{cases} \quad (45)$$

where $\sum_{(j_l, j_{l+1}) \in \mathcal{B}}$ is the summation over all possible j_{l+1} such that $(j_l, j_{l+1}) \in \mathcal{B}$ for the given $j_l \in \mathcal{B}$.

$$\begin{aligned} & \int_{\Omega} (p_{j_k} - q_{j_k}^{\prec j \succ}) \frac{\partial \Phi(x, \langle q_{j_k}^{\prec j \succ} \rangle)}{\partial p_{j_k}} dx + \int_{\Omega} (p_{j_k} - q_{j_k}^{\prec j \succ}) \nu_{j_k}^{\prec j \succ} dx \\ & + r \int_{\Omega} (p_{j_k} - q_{j_k}^{\prec j \succ}) (q_{j_k}^{\prec j \succ} - \partial_{j_k} q_{j_{k-1}}^{\prec j \succ}) dx = 0, \quad \forall j_k \in \mathcal{B}_T. \end{aligned} \quad (46)$$

We therefore solve minimization problem (30) for $v^{\prec j \succ}$, $q_L^{\prec j \succ}$ and $q_T^{\prec j \succ}$ based on equations (44), (45) and (46), as shown in Algorithm 2.

Algorithm 2. ALG2 for finding saddle-point of problem (30).

1. Pick arbitrary initial guesses $q_L^{\prec 0 \succ}$ and $q_T^{\prec 0 \succ}$.
2. For a fixed $j \geq 1$, let $q_L^{\prec j, 0 \succ} = q_L^{\prec j-1 \succ}$ and $q_T^{\prec j, 0 \succ} = q_T^{\prec j-1 \succ}$.
3. For $m \geq 1$,

(a) Based on eq. (44), we solve for $v^{\prec j, m \succ} \in \mathfrak{U}$ from eq. (47).

$$\begin{aligned} & \int_{\Omega} (u - v^{\prec j, m \succ}) \frac{\partial \Phi(x, \langle q_{j_l}^{\prec j, m-1 \succ} \rangle)}{\partial u} dx - \sum_{j_1 \in \mathcal{B}} \int_{\Omega} \partial_{j_1} (u - v^{\prec j, m \succ}) \nu_{j_1} dx \\ & - \sum_{j_1 \in \mathcal{B}} r \int_{\Omega} \partial_{j_1} (u - v^{\prec j, m \succ}) (q_{j_1}^{\prec j, m-1 \succ} - \partial_{j_1} v^{\prec j, m \succ}) dx = 0, \quad \forall u \in \mathfrak{U}. \end{aligned} \quad (47)$$



(b) Based on eq. (45), we solve for $q_L^{\prec j, m \succ} \in \mathfrak{P}_L$, from system of equations (48).

$$\begin{aligned} \forall j_l \in \mathcal{B}_L, \int_{\Omega} (p_{j_l} - q_{j_l}^{\prec j, m \succ}) \left(\frac{\partial \Phi(x, \langle q_{j_l}^{\prec j, m \succ} \rangle)}{\partial p_{j_l}} + \nu_{j_l}^{\prec j \succ} \right) dx \\ - \sum_{(j_l, j_{l+1}) \in \mathcal{B}} \int_{\Omega} \partial_{j_{l+1}} (p_{j_l} - q_{j_l}^{\prec j, m \succ}) \nu_{j_{l+1}}^{\prec j \succ} dx \\ + r \int_{\Omega} (p_{j_l} - q_{j_l}^{\prec j, m \succ}) (q_{j_l}^{\prec j, m \succ} - \partial_{j_l} q_{j_{l-1}}^{\prec j, m \succ}) dx \\ - \sum_{(j_l, j_{l+1}) \in \mathcal{B}} r \int_{\Omega} \partial_{j_{l+1}} (p_{j_l} - q_{j_l}^{\prec j, m \succ}) (q_{j_{l+1}}^{\prec j, m \succ} - \partial_{j_{l+1}} q_{j_l}^{\prec j, m \succ}) dx = 0. \end{aligned} \quad (48)$$

At this stage, because we have not yet solved for $q_{j_k}^{\prec j, m \succ}$, any such item that may be involved in eq. (48) is substituted by $q_{j_k}^{\prec j, m-1 \succ}$.

(c) Based on eq. (46), we solve for $q_T^{\prec j, m \succ} \in \mathfrak{P}_T$, from system of equations (49).

$$\begin{aligned} \int_{\Omega} (p_{j_k} - q_{j_k}^{\prec j, m \succ}) \frac{\partial \Phi(x, \langle q_{j_k}^{\prec j, m \succ} \rangle)}{\partial p_{j_k}} dx + \int_{\Omega} (p_{j_k} - q_{j_k}^{\prec j, m \succ}) \nu_{j_k}^{\prec j \succ} dx \\ + r \int_{\Omega} (p_{j_k} - q_{j_k}^{\prec j, m \succ}) (q_{j_k}^{\prec j, m \succ} - \partial_{j_k} q_{j_{k-1}}^{\prec j, m \succ}) dx = 0, \forall j_k \in \mathcal{B}_T. \end{aligned} \quad (49)$$

4. Repeat step 3 for a certain number of times or until convergence. Then,

$$\begin{cases} v^{\prec j \succ} &= \lim_{m \geq 1} v^{\prec j, m \succ}, \\ q_L^{\prec j \succ} &= \lim_{m \geq 1} q_L^{\prec j, m \succ}, \\ q_T^{\prec j \succ} &= \lim_{m \geq 1} q_T^{\prec j, m \succ}. \end{cases}$$

Fortin and Glowinski [30] provided the convergence proof of Algorithm 2 for the limiting case when step 3 in Algorithm 2 is performed only once, for a special case as defined in eq. (4). Effectively, Algorithm 2 uses the block relaxation method sequentially to find solutions to minimization problem (30). That is only one of the many ways that one can find solutions of minimization problem (30). Using parallel computation will be another great endeavor, which would be investigated in the future.

To find numerical approximations to the solution of minimization problem (30), we apply to equations (47), (48) and (49) the Ritz-Galerkin methods (finite element methods in case the equations are linear).

3.1 The Phenomenon of Lagrange Crises

We use the Lagrange multiplier method in saddle-point problem (22) to overcome the complexity involved in dealing with constraints (15). However, when using the Lagrange multiplier method, one must take efforts to avoid the phenomenon of Lagrange crises (Chien [31], He [18, 19, 23]). In fact, a purpose of the semi-inverse method is to overcome the phenomenon of Lagrange crises when using the Lagrange multiplier method. Due to the use of augmented Lagrangian \mathcal{L}_r in eq. (28) instead of Lagrangian \mathcal{L} in eq. (23), we are able to avoid the phenomenon of Lagrange crises.

According to He [18], a Lagrange crisis arises when

1. an independent variable associated with a Lagrange multiplier is missing from the original functional, resulting in a Lagrange multiplier function to become a zero function.

In the case of functional (28), a zero Lagrange multiplier cannot be part of a saddle-point due to the augmented term as $\frac{1}{2} \sum_{j_l \in \mathcal{B}} r \int_{\Omega} (p_{j_l} - \partial_{j_l} p_{j_{l-1}})^2 dx$ with parameter r . According to stationary condition (46), $\forall j_k \in \mathcal{B}_T$,

$$\nu_{j_k}^{\prec j \succ} = - \frac{\partial \Phi(x, \langle q_{j_l}^{\prec j \succ} \rangle)}{\partial p_{j_k}} - r(q_{j_k}^{\prec j \succ} - \partial_{j_k} q_{j_{k-1}}^{\prec j \succ}),$$

which is linear in r . That implies that $\nu_{j_k}^{\prec j \succ}$ could only become 0 for at most one single value of r , and $\nu_{j_k}^{\prec j \succ}$ is a non-zero function for any value other than possibly that single value.

Similarly, according to stationary condition (45), $\forall j_l \in \mathcal{B}_L$,

$$\begin{aligned} \nu_{j_l}^{\prec j \succ} &= - \frac{\partial \Phi(x, \langle q_{j_l}^{\prec j \succ} \rangle)}{\partial p_{j_l}} - \sum_{(j_l, j_{l+1}) \in \mathcal{B}} \partial_{j_{l+1}} \nu_{j_{l+1}}^{\prec j \succ} \\ &\quad - r(q_{j_l}^{\prec j \succ} - \partial_{j_l} q_{j_{l-1}}^{\prec j \succ}) - r \sum_{(j_l, j_{l+1}) \in \mathcal{B}} \partial_{j_{l+1}} (q_{j_{l+1}}^{\prec j \succ} - \partial_{j_{l+1}} q_{j_l}^{\prec j \succ}), \end{aligned}$$

which is also linear in r . We conclude that $\nu_{j_l}^{\prec j \succ}$ will be non-zero for almost all values of r .

2. The Euler-Lagrange equation of the original functional yields only a trivial identity.

In the case of functional (2), its Euler-Lagrange eq. (9) is the BVP (10), which is non-trivial by choice.

4. Numerical Tests

We use some problems to test the general purpose variational formulation in this section.



4.1 Test Case of 1-dimensional Problem

Wei and Li [32] applied successfully the current augmented Lagrangian paradigm to the 1-dimensional Euler-Bernoulli beam equation

$$(\tilde{E}Iu'')'' - (T_r + T_a)u'' = \frac{\varepsilon_0 w U^2}{2(g - u(x))^2}, \quad 0 < x < L,$$

where $u(x)$ is the deflection of the beam, $T_a \approx (\tilde{E}wt/(2L)) \int_0^L |u'|^2 dx$, and \tilde{E} , I , T_r , w , t , L , ε_0 , U and g are constants associated with a beam. The boundary conditions considered are:

$$u(0) = 0, \quad u'(0) = 0; \quad u''(L) = 0, \quad u'''(L) = 0,$$

for fixed-free cantilever beams, and

$$u(0) = 0, \quad u'(0) = 0; \quad u(L) = 0, \quad u'(L) = 0,$$

for fixed-fixed beams. After non-dimensionalization of all variables, an associated variational principle is

$$I(u) = \int_0^1 \frac{1}{2} |u''|^2 d\xi + \beta_1 \int_0^1 |u'|^2 d\xi + \beta_2 \left(\int_0^1 |u'|^2 d\xi \right)^2 - \beta_3 \int_0^1 F(u) d\xi,$$

where β_1 , β_2 and β_3 are constants related to the beam, and $F(u) = \frac{1}{1-u} - \frac{0.65g}{w} \ln(1-u)$. In notations consistent with the current manuscript, the associated augmented Lagrangian is effectively

$$\begin{aligned} \mathcal{L}_r(u, p_1, p_{1,1}, \mu_1, \mu_{1,1}) &= \int_0^1 \frac{1}{2} |p_{1,1}|^2 d\xi + \beta_1 \int_0^1 |p_1|^2 d\xi + \beta_2 \left(\int_0^1 |p_1|^2 d\xi \right)^2 \\ &\quad - \beta_3 \int_0^1 F(u) d\xi + \int_0^1 \mu_1 (p_1 - u') d\xi + \int_0^1 \mu_{1,1} (p_{1,1} - p_1') d\xi \\ &\quad + \frac{r}{2} \int_0^1 (p_1 - u')^2 d\xi + \frac{r}{2} \int_0^1 (p_{1,1} - p_1')^2 d\xi. \end{aligned}$$

We were able to obtain numerical solutions with comparable or better accuracy than those reported in prior literature.

4.2 Test Case of 2-dimensional Steady State Stokes Equation

The steady state Stokes equation may be expressed as

$$\begin{cases} \frac{1}{R} \Delta^2 \psi(x) = f(x), & x \in \Omega, \\ \psi(x) = g_0(x), \quad \frac{\partial \psi(x)}{\partial \vec{N}} = g_1(x), & x \in \partial\Omega. \end{cases}$$

Here, ψ is the stream function for the flow, R is the Reynold's number, $f(x)$ is an external force, and $g_0(x)$, $g_1(x)$ are two prescribed functions on the boundary of the domain. Once we use augmented Lagrangian to compute for an approximate solution to the stream function $\psi(x)$, we also have approximate solutions to $\partial_j \psi(x)$ and $\partial_{j,j}^2 \psi(x)$ for $1 \leq j \leq 2$. Consequently, flow related quantities such as

$$\begin{cases} \text{velocity} &= (u, v) = (\partial_2 \psi(x), -\partial_1 \psi(x)), \\ \text{vorticity} &= \xi = \partial_1 v - \partial_2 u = -\partial_{1,1}^2 \psi - \partial_{2,2}^2 \psi, \end{cases}$$

are available at no extra cost.

In this particular case, if we let $F(x) \equiv Rf(x)$, then the stream function $\psi(x)$ satisfies the following biharmonic equation.

$$\begin{cases} \Delta^2 \psi(x) = F(x), & x \in \Omega, \\ \psi(x) = g_0(x), \quad \frac{\partial \psi(x)}{\partial \vec{N}} = g_1(x), & x \in \partial\Omega. \end{cases}$$

We therefore will focus on the biharmonic equation in the next subsection.

4.3 Test Case of 2-dimensional Biharmonic Equation

The boundary value problem for the biharmonic operator is the following 4-th order differential equation,

$$\Delta^2 u(x) = f(x), \quad x \in \Omega, \quad (50)$$

subject to boundary conditions

$$u(x) = g_0(x), \quad \frac{\partial u(x)}{\partial \vec{N}} = g_1(x), \quad x \in \partial\Omega. \quad (51)$$

We mean to find a weak solution to the above boundary value problem over a set

$$\mathcal{V} = \{ u \in \mathcal{H}^2(\Omega) \mid u(x)|_{\partial\Omega} = g_0(x), \quad \frac{\partial u(x)}{\partial \vec{N}}|_{\partial\Omega} = g_1(x) \}. \quad (52)$$

Equation (50) is associated with the bilinear form

$$a(u, v) = \int_{\Omega} \Delta u \Delta v dx,$$

and eq. (50) along with boundary conditions (51) corresponds to the following minimization problem.

$$\text{Find } v \in \mathcal{V} \text{ such that } I(v) = \inf_{u \in \mathcal{V}} I(u), \quad (53)$$

where

$$I(u) = \frac{1}{2} a(u, u) - \int_{\Omega} u f(x) dx = \int_{\Omega} \left(\frac{1}{2} |\Delta u|^2 dx - u f(x) \right) dx, \quad \forall u \in \mathcal{V}. \quad (54)$$



Even though Dirichlet boundary conditions (51) are inhomogeneous, we can convert the inhomogeneous boundary value problem into a homogeneous one. As a result, conclusions from Theorems 2 and 3 will apply.

We assume that $\exists u^* \in \mathcal{V}$. If $u \in \mathcal{V}$ is the solution to eq. (50), then $w = u - u^* \in \mathcal{H}_0^2(\Omega)$ satisfies the following homogeneous boundary value problem.

$$\Delta^2 w(x) = f(x) - \Delta^2 u^*, \quad x \in \Omega,$$

subject to boundary conditions

$$w(x) = 0, \quad \frac{\partial w(x)}{\partial \vec{N}} = 0, \quad x \in \partial\Omega.$$

We further define

$$\begin{aligned} I^*(w) &\equiv I(w + u^*) - I(u^*) \\ &= \frac{1}{2}a(w + u^*, w + u^*) - \int_{\Omega} (w + u^*)f(x)dx - \frac{1}{2}a(u^*, u^*) + \int_{\Omega} u^*f(x)dx \\ &= \frac{1}{2}a(w, w) - \left(\int_{\Omega} wf(x)dx - a(w, u^*) \right). \end{aligned}$$

Applying Lax-Milgram Theorem to functional $I^*(w)$ over $w \in \mathcal{H}_0^2(\Omega)$, we conclude that $\exists w_* \in \mathcal{H}_0^2(\Omega)$, such that

$$\begin{cases} I^*(w_*) = \min_{w \in \mathcal{H}_0^2(\Omega)} I^*(w). \\ \text{And } u_* = w_* + u^* \in \mathcal{V} \\ \text{minimizes } I(u) \text{ over } u \in \mathcal{V}. \end{cases} \quad (55)$$

In other words, we can find a solution u_* to an inhomogeneous boundary value problem so long as we can find a solution w_* to a corresponding homogeneous boundary value problem.

We'll explain how the augmented Lagrangian (28) can be applied to find the solution to problem (53) next.

For ease of exposition, we'll consider the biharmonic problem in two-dimensional space, i.e., $\Omega \subset \mathcal{R}^2, n = 2$. $\forall u \in \mathcal{V}$, by making the substitutions as shown in eq. (56), known as the recursive linear equality relations,

$$p_1 = \partial_1 u, \quad p_2 = \partial_2 u, \quad p_{1,1} = \partial_1 p_1, \quad p_{2,2} = \partial_2 p_2, \quad (56)$$

we turn the minimization problem (53) into the following equivalent problem.

$$\text{Find } (v, \mathbf{q}) \in \mathcal{W} \text{ such that } \mathcal{I}(v, \mathbf{q}) = \inf_{(u, \mathbf{p}) \in \mathcal{W}} \mathcal{I}(u, \mathbf{p}),$$

where

$$\mathcal{I}(u, \mathbf{p}) = \int_{\Omega} \left(\frac{1}{2} |p_{1,1} + p_{2,2}|^2 dx - uf(x) \right) dx, \quad \forall (u, \mathbf{p}) \in \mathcal{W},$$

and

$$\mathcal{W} \equiv \{(u, \mathbf{p}) = (u, \{p_1, p_2, p_{1,1}, p_{2,2}\}) \mid u \in \mathcal{V}, \mathbf{p} \text{ satisfies (56)}\}$$

Thus functional (54) corresponds to eq. (2) with $k = 2$ and

$$\begin{aligned} \Phi(x, \langle \partial_{i_l}^l u \rangle) &= \frac{1}{2} |\Delta u|^2 - uf(x) = \frac{1}{2} |\partial_{1,1}^2 u + \partial_{2,2}^2 u|^2 - uf(x) \\ &= \Phi(x, u, \partial_{1,1}^2 u, \partial_{2,2}^2 u), \end{aligned} \quad (57)$$

where $\langle \partial_{i_l}^l u \rangle = \{u, \partial_{1,1}^2 u, \partial_{2,2}^2 u\}$, and $\mathcal{A} = \{(0), (1, 1), (2, 2)\}$. By definition,

$$\Phi(x, \langle p_{i_l} \rangle) = \Phi(x, u, p_{1,1}, p_{2,2}) = \frac{1}{2} |p_{1,1} + p_{2,2}|^2 - uf(x), \quad (58)$$

where we substitute $p_{1,1}$ and $p_{2,2}$ for $\partial_{1,1}^2 u$ and $\partial_{2,2}^2 u$ in eq. (57), respectively.

In particular,

- $\{p_{i_l}\} \equiv \{p_1, p_2, p_{1,1}, p_{2,2}\}$ are functions over Ω called supplementary variables.
- $\{\mu_{i_l}\} \equiv \{\mu_1, \mu_2, \mu_{1,1}, \mu_{2,2}\}$ are functions over Ω called Lagrangian multipliers.

Partial derivatives of $\Phi(x, u, p_{1,1}, p_{2,2})$ with respect to its variables related to u are listed below for easy references.

$$\begin{aligned} \frac{\partial \Phi(x, u, p_{1,1}, p_{2,2})}{\partial u} &= -f(x), \quad \frac{\partial \Phi(x, u, p_{1,1}, p_{2,2})}{\partial p_1} = 0, \quad \frac{\partial \Phi(x, u, p_{1,1}, p_{2,2})}{\partial p_2} = 0, \\ \frac{\partial \Phi(x, u, p_{1,1}, p_{2,2})}{\partial p_{1,1}} &= p_{1,1} + p_{2,2}, \quad \frac{\partial \Phi(x, u, p_{1,1}, p_{2,2})}{\partial p_{2,2}} = p_{1,1} + p_{2,2}. \end{aligned}$$

For functional (54), the associated index set $\mathcal{B} = \{(1), (2), (1, 1), (2, 2)\}$, and $\mathcal{I}_{k-1} = \mathcal{I}_1 = \{(1), (2)\} \subset \mathcal{B}$. So assumption (26) is met.

$$\begin{aligned} &\sum_{i_l \in \mathcal{A}} \int_{\Omega} \left(\frac{\partial \Phi(x, \langle p_{i_l} \rangle)}{\partial p_{i_l}} \Big|_{(u_2, \mathbf{p}_{L,2}, \mathbf{p}_{T,2})} - \frac{\partial \Phi(x, \langle p_{i_l} \rangle)}{\partial p_{i_l}} \Big|_{(u_1, \mathbf{p}_{L,1}, \mathbf{p}_{T,1})} \right) (p_{i_l,2} - p_{i_l,1}) dx \\ &= \int_{\Omega} ((p_{(1,1),2} + p_{(2,2),2}) - (p_{(1,1),1} + p_{(2,2),1})) (p_{(1,1),2} - p_{(1,1),1}) dx \\ &\quad + \int_{\Omega} ((p_{(1,1),2} + p_{(2,2),2}) - (p_{(1,1),1} + p_{(2,2),1})) (p_{(2,2),2} - p_{(2,2),1}) dx \\ &= \int_{\Omega} ((p_{(1,1),2} + p_{(2,2),2}) - (p_{(1,1),1} + p_{(2,2),1}))^2 dx \geq 0, \\ &\forall (u_1, \mathbf{p}_{L,1}, \mathbf{p}_{T,1}), (u_2, \mathbf{p}_{L,2}, \mathbf{p}_{T,2}) \in \mathcal{U} \times \mathcal{P}_L \times \mathcal{P}_T. \end{aligned}$$



So $\Phi(\cdot)$ in equations (57) and (58) meets condition (36). Furthermore, if $(u_1, \mathbf{p}_{L,1}, \mathbf{p}_{T,1})$ and $(u_2, \mathbf{p}_{L,2}, \mathbf{p}_{T,2})$ satisfy the recursive linear equality relations, $p_{(1,1),2} + p_{(2,2),2} = \partial_{1,1}^2 u_2 + \partial_{2,2}^2 u_2 = \Delta u_2$. Similarly, $p_{(1,1),1} + p_{(2,2),1} = \partial_{1,1}^2 u_1 + \partial_{2,2}^2 u_1 = \Delta u_1$. So

$$\sum_{j_l \in \mathcal{A}} \int_{\Omega} \left(\frac{\partial \Phi(x, \langle p_{j_l} \rangle)}{\partial p_{j_l}} \Big|_{(u_2, \mathbf{p}_{L,2}, \mathbf{p}_{T,2})} - \frac{\partial \Phi(x, \langle p_{j_l} \rangle)}{\partial p_{j_l}} \Big|_{(u_1, \mathbf{p}_{L,1}, \mathbf{p}_{T,1})} \right) (p_{j_l,2} - p_{j_l,1}) dx = 0$$

implies that $\Delta(u_2 - u_1) = 0$, subject to homogeneous boundary condition $(u_2 - u_1)|_{\partial\Omega} = 0$. We therefore conclude that $u_2 - u_1 = 0$. So condition (37) is met, which implies that Algorithm 1 converges when applied to the biharmonic equation (50) to find approximate solutions.

The augmented Lagrangian $\mathcal{L}_r(u, \mathbf{p}_L, \mathbf{p}_T, \mu)$ associated with functional (54) is in the form shown below.

$$\mathcal{L}_r(u, \mathbf{p}_L, \mathbf{p}_T, \mu) \equiv \mathcal{L}_r(u, p_1, p_2, p_{1,1}, p_{2,2}, \mu_1, \mu_2, \mu_{1,1}, \mu_{2,2}) : \mathfrak{W} \mapsto R,$$

where

$$\begin{aligned} \mathfrak{W} &\equiv \mathfrak{U} \times \mathfrak{P}_L \times \mathfrak{P}_T \times \mathfrak{M}, \\ \mathfrak{U} &= \{u \in \mathcal{H}^1(\Omega) \mid u(x)|_{\partial\Omega} = b_0(x)\}, \\ \mathfrak{P}_L &= \mathfrak{P}_1 \times \mathfrak{P}_2 = \{p_1 \in \mathcal{H}^1(\Omega) \mid p_1|_{\partial\Omega} = b_1\} \times \{p_2 \in \mathcal{H}^1(\Omega) \mid p_2|_{\partial\Omega} = b_2\}, \\ \mathfrak{P}_T &= \mathfrak{P}_{1,1} \times \mathfrak{P}_{2,2} = \{p_{1,1} \in \mathcal{H}^0(\Omega)\} \times \{p_{2,2} \in \mathcal{H}^0(\Omega)\} = (\mathcal{H}^0(\Omega))^2, \\ \mathfrak{M} &= \{\mu_{j_l} \in \mathcal{H}^0(\Omega) \mid j_l = (1), (2), (1,1), (2,2)\} = (\mathcal{H}^0(\Omega))^4. \end{aligned} \quad (59)$$

The expression for augmented Lagrangian $\mathcal{L}_r(u, \mathbf{p}_L, \mathbf{p}_T, \mu)$ is shown in eq. (60).

$$\begin{aligned} \mathcal{L}_r(u, p_1, p_2, p_{1,1}, p_{2,2}, \mu_1, \mu_2, \mu_{1,1}, \mu_{2,2}) &= \int_{\Omega} \left(\frac{1}{2} |p_{1,1} + p_{2,2}|^2 - u f(x) \right) dx \\ &+ \int_{\Omega} \mu_1 (p_1 - \partial_1 u) dx + \int_{\Omega} \mu_2 (p_2 - \partial_2 u) dx \\ &+ \int_{\Omega} \mu_{1,1} (p_{1,1} - \partial_1 p_1) dx + \int_{\Omega} \mu_{2,2} (p_{2,2} - \partial_2 p_2) dx \\ &+ \frac{1}{2} r \int_{\Omega} (p_1 - \partial_1 u)^2 dx + \frac{1}{2} r \int_{\Omega} (p_2 - \partial_2 u)^2 dx \\ &+ \frac{1}{2} r \int_{\Omega} (p_{1,1} - \partial_1 p_1)^2 dx + \frac{1}{2} r \int_{\Omega} (p_{2,2} - \partial_2 p_2)^2 dx. \end{aligned} \quad (60)$$

4.4 Choosing Parameter r

For a solution $(v^{\prec j \succ}, \mathbf{q}_L^{\prec j \succ}, \mathbf{q}_T^{\prec j \succ})$ of minimization problem (30),

$$\begin{aligned} \mathcal{L}_r(u, \mathbf{p}_L, \mathbf{p}_T, \nu^{\prec j \succ}) &= \mathcal{L}_r(v^{\prec j \succ}, \mathbf{q}_L^{\prec j \succ}, \mathbf{q}_T^{\prec j \succ}, \nu^{\prec j \succ}) \\ &+ \left\langle \frac{\partial^2 \mathcal{L}_r}{\partial (u, \mathbf{p}_L, \mathbf{p}_T)^2} \Big|_{(v^{\prec j \succ}, \mathbf{q}_L^{\prec j \succ}, \mathbf{q}_T^{\prec j \succ})}, \delta(u, \mathbf{p}_L, \mathbf{p}_T), \delta(u, \mathbf{p}_L, \mathbf{p}_T) \right\rangle + o(\|\delta(u, \mathbf{p}_L, \mathbf{p}_T)\|^2), \end{aligned} \quad (61)$$

where $\frac{\partial^2 \mathcal{L}_r}{\partial (u, \mathbf{p}_L, \mathbf{p}_T)^2}$ is the Hessian of the \mathcal{L}_r (a bilinear form) when restricted for a given $\nu^{\prec j \succ}$, and $\delta(u, \mathbf{p}_L, \mathbf{p}_T)$ is equal to $(u - v^{\prec j \succ}, \mathbf{p}_L - \mathbf{q}_L^{\prec j \succ}, \mathbf{p}_T - \mathbf{q}_T^{\prec j \succ})$, and $\langle \cdot \rangle$ denotes the value of the Hessian of \mathcal{L}_r at $(\delta(u, \mathbf{p}_L, \mathbf{p}_T), \delta(u, \mathbf{p}_L, \mathbf{p}_T))$.

Because of the term $\frac{1}{2} \sum_{j_l \in \mathcal{B}} r \int_{\Omega} (p_{j_l} - \partial_{j_l} p_{j_l-1})^2 dx$ in eq. (28), the value of Hessian (61) will have some terms proportional to r . In other words, parameter r in augmented Lagrangian (28) affects the eigenvalues of the Hessian matrix of \mathcal{L}_r . In turn, it affects the speed of convergence of Algorithm 1. We'll elaborate on this issue now for the particular Lagrangian (60).

It is easy to compute the Hessian of the minimization problem (30) for Lagrangian (60) at $(v^{\prec j \succ}, \mathbf{q}_L^{\prec j \succ}, \mathbf{q}_T^{\prec j \succ})$ for a given $\nu^{\prec j \succ}$, which is

$$\begin{aligned} &\left\langle \frac{\partial^2 \mathcal{L}_r}{\partial u^2}, u - v^{\prec j \succ}, u - v^{\prec j \succ} \right\rangle + \left\langle \frac{\partial^2 \mathcal{L}_r}{\partial \mathbf{p}_L^2}, \mathbf{p}_L - \mathbf{q}_L^{\prec j \succ}, \mathbf{p}_L - \mathbf{q}_L^{\prec j \succ} \right\rangle + \left\langle \frac{\partial^2 \mathcal{L}_r}{\partial \mathbf{p}_T^2}, \mathbf{p}_T - \mathbf{q}_T^{\prec j \succ}, \mathbf{p}_T - \mathbf{q}_T^{\prec j \succ} \right\rangle \\ &= \int_{\Omega} |(p_{1,1} - q_{1,1}^{\prec j \succ}) + (p_{2,2} - q_{2,2}^{\prec j \succ})|^2 dx \\ &+ r \int_{\Omega} |(p_1 - q_1^{\prec j \succ}) - \partial_1(u - v^{\prec j \succ})|^2 dx + r \int_{\Omega} |(p_2 - q_2^{\prec j \succ}) - \partial_2(u - v^{\prec j \succ})|^2 dx \\ &+ r \int_{\Omega} |(p_{1,1} - q_{1,1}^{\prec j \succ}) - \partial_1(p_1 - q_1^{\prec j \succ})|^2 dx + r \int_{\Omega} |(p_{2,2} - q_{2,2}^{\prec j \succ}) - \partial_2(p_2 - q_2^{\prec j \succ})|^2 dx. \end{aligned} \quad (62)$$

In the case of biharmonic equations, if r is too big, iterate $(v^{\prec j \succ}, \mathbf{q}_L^{\prec j \succ}, \mathbf{q}_T^{\prec j \succ})$ may converge to satisfy the recursive linear equality relations too quickly before iterate $\nu^{\prec j \succ}$ converges. Conversely, if r is not big enough, iterate $\nu^{\prec j \succ}$ may converge too quickly before iterate $(v^{\prec j \succ}, \mathbf{q}_L^{\prec j \succ}, \mathbf{q}_T^{\prec j \succ})$ converges to meet the recursive linear equality relations. Therefore, we should choose r so that all of the terms in eq. (62) would be approximately of the same magnitude.

4.5 Boundary Value Functions for the Augmented Lagrangian

Because of the inhomogeneous boundary conditions in eq. (52), we'll determine $b_{j_l}(x)$ as introduced in equations (24) and (25) for j_l for $0 \leq l < k$, i.e., $j_l = (0), (1), (2)$ for $l = 0, 1$ and $k = 2$ next.

Because of eq. (24), $b_0(x) \equiv g_0(x)$, $\forall x \in \partial\Omega$.



Let $\vec{T} = (T_1, T_2)^T$ be the unit tangent vector to $\partial\Omega$ in counterclockwise direction. Because of boundary conditions in eq. (52), $\forall x \in \partial\Omega$,

$$\begin{aligned}\frac{\partial u(x)}{\partial \vec{T}} &= T_1 \partial_1 u + T_2 \partial_2 u = \frac{\partial g_0(x)}{\partial \vec{T}}, \\ \frac{\partial u(x)}{\partial \vec{N}} &= N_1 \partial_1 u + N_2 \partial_2 u = g_1(x),\end{aligned}$$

we can solve for $\partial_1 u$ and $\partial_2 u$ by Cramer's rule on $\partial\Omega$.

$$\partial_1 u = \frac{N_2 \frac{\partial g_0(x)}{\partial \vec{T}} - T_2 g_1(x)}{T_1 N_2 - T_2 N_1} \equiv b_1(x), \quad (63)$$

$$\partial_2 u = \frac{T_1 g_1(x) - N_1 \frac{\partial g_0(x)}{\partial \vec{T}}}{T_1 N_2 - T_2 N_1} \equiv b_2(x). \quad (64)$$

That is, $b_1(x)$ and $b_2(x)$ that are involved in eq. (59) are determined in equations (63) and (64), respectively, in terms of boundary value functions $g_0(x)$ and $g_1(x)$.

4.6 Numerical Results

Due to eq. (55), we'll focus on biharmonic equations with homogeneous boundary conditions, i.e., $g_0(x) = g_1(x) = 0$, for our numerical tests.

For brevity, we test Algorithm 1 on the biharmonic equation (50) with a manufactured solution. First, we define a simple polynomial $h_0(x)$ over the domain $\Omega = [-1, 1] \times [-1, 1]$,

$$\begin{cases} h_0(x) &\equiv \prod_{j=1}^n (x_j^2 - 1)^2, \quad \forall x \in \Omega, \\ &= (x_1^2 - 1)^2 (x_2^2 - 1)^2, \quad \text{for } n = 2, \end{cases} \quad (65)$$

that satisfies the homogeneous boundary conditions $h_0(x) = \frac{\partial h_0(x)}{\partial \vec{N}} = 0, \forall x \in \partial\Omega$. We introduce another "sophisticated" function $h_1(x)$,

$$h_1(x) = \sin(K\pi\|x\|^2), \quad (66)$$

where K is a positive integer that controls how "wavy" the function behaves with respect to the center of the domain Ω . If we define

$$f(x) \equiv \Delta^2(h_0(x)h_1(x)), \quad (67)$$

we can see that $u(x) \equiv h_0(x)h_1(x)$ is a manufactured solution to the following biharmonic equation with the homogeneous Dirichlet boundary conditions.

$$\begin{cases} \Delta^2 u = f(x), & x \in \Omega, \\ u(x) = \frac{\partial u(x)}{\partial \vec{N}} = 0, & x \in \partial\Omega. \end{cases}$$

Because $h_1(x)$ is a bounded function, and different orders of its derivatives are differed by a constant K in magnitude. According to eq. (62), an optimal choice of parameters for Algorithm 1 will be $\rho^{\prec j \succ} \equiv r = K$. We choose relative tolerance $\varepsilon_r = 10^{-3}$ in all of our calculations.

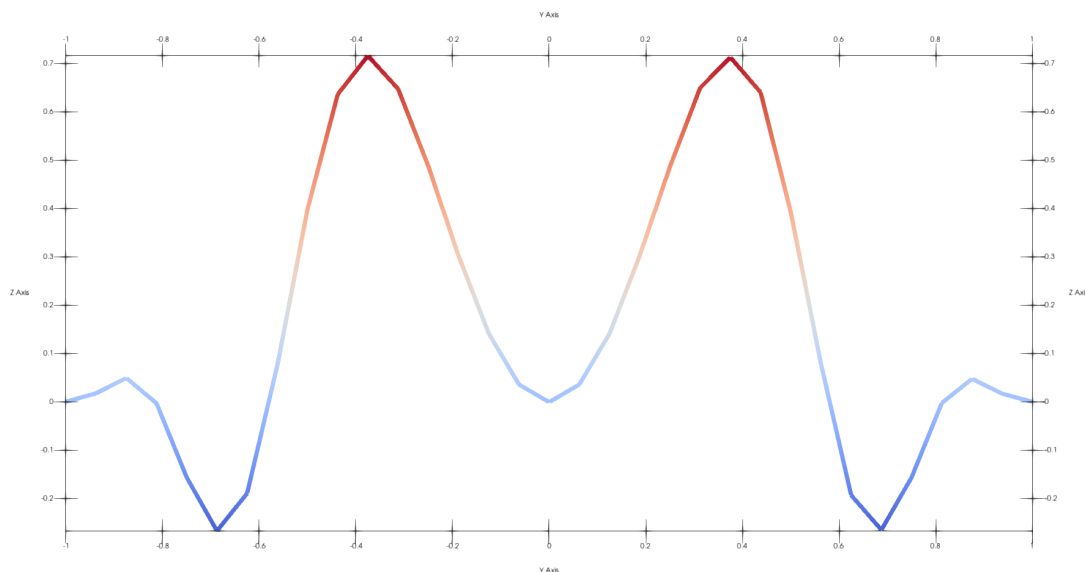
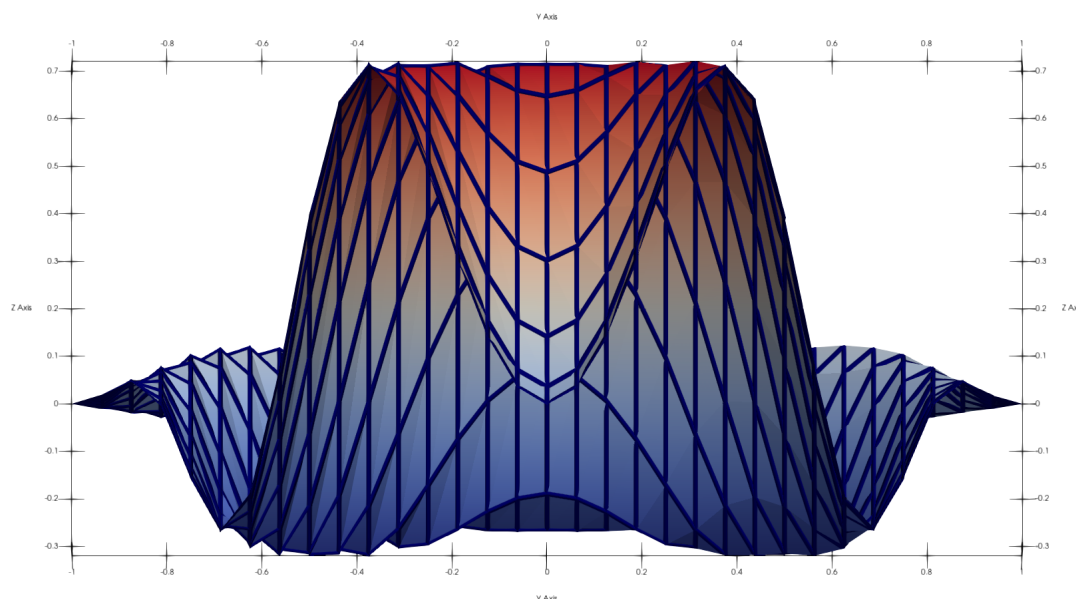


Fig. 1. A slice of numerical solution, $K = 3$.

Figures 1 and 2 show plots of the numerical solution, with a triangulation of 32×32 equal rectangles for the domain Ω . We use Lagrange finite element of degree 3 in the calculation.

Figure 1 shows a profile of the numerical solution, which is symmetric with respect to the x and y axes. The "wavy" feature of function $h_1(x)$ is resolved adequately with only a triangulation of 32×32 equal rectangles.



Fig. 2. Cross-sectional views of numerical solution, $K = 3$.

	L^2 error	CPU time	$\nu^{<j>}$ converges after	Total # of iteration
$r = 0.3 = \frac{1}{10}K$	0.0176459	46m36s	70 iterations	727
$r = 3 = K$	0.0097166	21m49s	80 iterations	351
$r = 30 = 10K$	0.0132300	13m50s	549 iterations	549

Table 1. Performance comparison on 16×16 triangulation and 3rd degree Lagrange finite elements.

Figure 2 shows a cross-sectional view of the numerical solution of the solution.

Table 1 demonstrates that $\rho^{<j>} \equiv r = K$ is indeed the optimal choice of parameters to balance the convergence between $\nu^{<j>}$ (numerical solution) and $\nu^{<j>}$ (Lagrange multipliers).

Next, we test the efficacy of Algorithm 1 on different triangulations and different degree of Lagrange finite elements. Because the domain is a square, the triangulations used in the runs are obtained by simply subdividing each dimension on $[-1, 1]$ into certain number of equal parts. In particular, a 16×16 triangulation means that we subdivide $[-1, 1]$ into 16 equal subintervals in each of the two dimensions.

As shown in Table 2, the errors become smaller when we approximate the domain with finer triangulations. Similarly, the errors become smaller when we use Lagrange finite elements with higher degree. However, the price to pay for higher accuracy is longer CPU time.

Triangulation	Degree of Lagrange finite element					
	2	3	4	2	3	4
	Solution error in L^2 -norm			CPU time		
16×16	0.0900811	0.00971658	0.00525816	10m41s	21m50s	18m07s
32×32	0.0126101	0.00485926	0.00518511	42m38s	35m20s	91m45s

Table 2. Comparisons with $\rho^{<j>} \equiv r = K = 3$, $\varepsilon_r = 10^{-3}$.

We carry out all of the computations on an ordinary stock computer with a 9th Gen Intel® Core™ i9 9900 (8-Core, 16MB Cache, 5GHz) with 10GB DDR4 RAM at 2666Mhz that runs Ubuntu 18 (64-bit).

5. Further Discussions

We've applied the proposed general purpose variational formulation to the 4th order biharmonic equation with a manufactured solution. As a result, we are able to compute errors between the exact solution and numerical solutions as shown in Table 2.

On the other hand, one could use the Adomian Decomposition Method (ADM) developed by Adomian [33, 34] to find exact solutions to a wide class of differential equations of different orders. We are hopeful that ADM would further widen the applicability of the current general purpose variational formulation to even more types of differential equations beyond BVPs. One may find more interesting applications of ADM to problems other than BVPs in the work by Zeidan, et al. [35], Sil, et al. [36] and Zeidan, et al. [37].

6. Conclusion

We develop a new general purpose variational formulation for solving BVPs of any order. The regularity requirement for this new Lagrangian is always \mathcal{H}^1 regardless of the order of the BVP. We prove that solution to the saddle-point problem of the new Lagrangian



is a weak solution to the BVP. Furthermore, we prove the convergence of numerical algorithm based on ALM. Numerical results for problems in multi-dimensional spaces are computed with great accuracy using only stock computer hardware.

Author Contributions

The author contributed all the work in preparation of this manuscript, and approved the final version of the manuscript.

Acknowledgments

The author would like to express his deep appreciation to reviewers for their helpful comments. Their suggestions have made this manuscript a better publication.

Conflict of Interest

The author(s) declared no potential conflicts of interest with respect to the research, authorship and publication of this article.

Funding

The author(s) received no financial support for the research, authorship and publication of this article.

References

- [1] Ciarlet, P.G., *The Finite Element Method for Elliptic Problems*, Elsevier North-Holland, Inc., 1st ed., 1978.
- [2] Axelsson, O., Barker, V.A., *Finite Element Solution of Boundary Value Problems. Theory and Computation*, SIAM, 2001.
- [3] Oden, J.T., Generalized conjugate functions for mixed finite element approximations of boundary value problems, *The Mathematical Foundations of the Finite Element Method with Applications to Partial Differential Equations*, 1972, 629–669.
- [4] Babuska, I., Finite element method with lagrangian multipliers, *Numer. Math.*, 1973, 20, 179–192.
- [5] Brezzi, F., On the existence, uniqueness and approximation of saddle-point problems arising from lagrangian multipliers, *Rev. Française Automat. Informat. Recherche Opérationnelle Sér. Rouge Anal. Numér.*, 1974, R-2, 129–151.
- [6] Brezzi, F., Raviart, P.A., Mixed finite element methods for 4th order elliptic equations, *Topics in numerical analysis III: proceedings of the Royal Irish Academy Conference on Numerical Analysis*, 1976, 33–56.
- [7] Raviart, P.A., Thomas, J.M., A mixed finite element method for 2nd order elliptic problems, *Mathematical aspects of finite element methods: proceedings of the conference held in Rome, 10-12 December 1975*, 292–315.
- [8] Falk, R.S., Approximation of the biharmonic equation by a mixed finite element method, *SIAM J. Numer. Anal.*, 1978, 15(2), 556–567.
- [9] Han, H.D., Nonconfirming elements in the mixed finite element method, *Journal of Computational Mathematics*, 1984, 2(3), 223–233.
- [10] Monk, P., A mixed finite element method for the biharmonic equation, *SIAM J. NUMER. ANAL.*, 1987, 24(4), 737–749.
- [11] Brenner, S.C., A multigrid algorithm for the lowest-order raviart-thomas mixed triangular finite element method, *SIAM J. NUMER. ANAL.*, 1992, 29(3), 647–678.
- [12] Figueroa, L.E., Gatica, G.N., Márquez, A., Augmented mixed finite element methods for the stationary stokes equations, *SIAM J. SCI. COMPUT.*, 2008, 31(2), 1082–1119.
- [13] Camaño, J., Gatica, G.N., Oyarzúa, R., Tierra, G., An augmented mixed finite element method for the navier-stokes equations with variable viscosity, *SIAM J. NUMER. ANAL.*, 2016, 54(2), 1069–1092.
- [14] Barnafi, N., Gatica, G.N., Hurtado, D.E., Primal and mixed finite element methods for deformable image registration problems, *SIAM Journal on Imaging Sciences*, 2018, 11(4), 2529–2567.
- [15] Lee, J.J., Piersanti, E., Mardal, K.A., Rognes, M.E., A mixed finite element method for nearly incompressible multiple-network poroelasticity, *SIAM Journal on Scientific Computing*, 2019, 41(2), A722–A747.
- [16] Ambartsumyan, I., Khattatov, E., Nordbotten, J.M., Yotov, I., A multipoint stress mixed finite element method for elasticity on simplicial grids, *SIAM Journal on Numerical Analysis*, 2020, 58(1), 630–656.
- [17] Carstensen, C., Ma, R., Adaptive mixed finite element methods for non-self-adjoint indefinite second-order elliptic pdes with optimal rates, *SIAM Journal on Numerical Analysis*, 2021, 59(2), 955–982.
- [18] He, J.H., Modified lagrange multiplier method and generalized variational principle in fluid mechanics, *JOURNAL OF SHANGHAI UNIVERSITY*, 1997, 1(2), 117–122.
- [19] He, J.H., Semi-inverse method and generalized variational principles with multi-variables in elasticity, *Applied Mathematics and Mechanics*, 2000, 21(7), 797–808.
- [20] He, J.H., Variational principles for some nonlinear partial differential equations with variable coefficients, *Chaos, Solitons and Fractals*, 2004, 19, 847–851.
- [21] He, J.H., Anjum, N., Skrzypacz, P.S., A variational principle for a nonlinear oscillator arising in the microelectromechanical system, *Journal of Applied and Computational Mechanics*, 2021, 7(1), 78–83.
- [22] He, J.H., An alternative approach to establishment of a variational principle for the torsional problem of piezoelectric beams, *Applied Mathematics Letters*, 2016, 52, 1–3.
- [23] He, J.H., Lagrange crisis and generalized variational principle for 3d unsteady flow, *International Journal of Numerical Methods for Heat & Fluid Flow*, 2020, 30(3), 1189–1196.
- [24] EL-Kalaawy, O.H., New variational principle–exact solutions and conservation laws for modified ion-acoustic shock waves and double layers with electron degenerate in plasma, *Physics of Plasmas*, 2017, 24, 032308.
- [25] He, J.H., A modified li-he's variational principle for plasma, *International Journal of Numerical Methods for Heat & Fluid Flow*, 2021, 31(5), 1369–1372.
- [26] He, J.H., Variational principle for the generalized kdv-burgers equation with fractal derivatives for shallow water waves, *Journal of Applied and Computational Mechanics*, 2020, 6(4), 735–740.
- [27] Cao, X.Q., Guo, Y.N., Zhang, C.Z., Hou, S.C., Peng, K.C., Different groups of variational principles for whitam-broer-kaup equations in shallow water, *Journal of Applied and Computational Mechanics*, 2020, 6(Special Issue), 1178–1183.
- [28] Cao, X.Q., Peng, K.C., Liu, M.Z., Zhang, C.Z., Guo, Y.N., Variational principles for two compound nonlinear equations with variable coefficients, *Journal of Applied and Computational Mechanics*, 2021, 7(2), 415–421.
- [29] Liu, M.Z., Cao, X.Q., Zhu, X.Q., Liu, B.N., Peng, K.C., Variational principles and solitary wave solutions of generalized nonlinear schrödinger equation in the ocean, *Journal of Applied and Computational Mechanics*, 2021, –.
- [30] Fortin, M., Glowinski, R., *Augmented Lagrangian Methods: Applications to the Numerical Solution of Boundary-Value Problems*, NORTH-HOLLAND, 1st ed., 1983.
- [31] Chien, W.Z., Method of high-order lagrange multiplier and generalized variational principles of elasticity with more general forms of functionals, *Applied Mechanics and Mechanics*, 1983, 4(2), 137–150.
- [32] Wei, D., Li, X., Finite element solutions of cantilever and fixed actuator beams using augmented lagrangian methods, *Journal of Applied and Computational Mechanics*, 2018, 4, 125–132.
- [33] Adomian, G., A review of the decomposition method in applied mathematics, *JOURNAL OF MATHEMATICAL ANALYSIS AND APPLICATIONS*, 1988, 135, 501–544.
- [34] Adomian, G., A review of the decomposition method and some recent results for nonlinear equations, *Computers & Mathematics with Applications*, 1991, 21(5), 101–127.



- [35] Zeidan, D., Chau, C.K., Lu, T.T., On the characteristic adomian decomposition method for the riemann problem, *Math Meth Appl Sci.*, 2019, special issue, 1–16.
- [36] Sil, S., Sekhar, T.R., Zeidan, D., Nonlocal conservation laws, nonlocal symmetries and exact solutions of an integrable soliton equation, *Chaos, Solitons and Fractals*, 2020, 139, 1–9.
- [37] Zeidan, D., Chau, C.K., Lu, T.T., Zheng, W.Q., Mathematical studies of the solution of burgers' equations by adomian decomposition method, *Math Meth Appl Sci.*, 2020, 43, 2171–2188.

ORCID iD

Xuefeng Li  <https://orcid.org/0000-0002-5462-6274>



© 2021 Shahid Chamran University of Ahvaz, Ahvaz, Iran. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution-NonCommercial 4.0 International (CC BY-NC 4.0 license) (<http://creativecommons.org/licenses/by-nc/4.0/>)

How to cite this article: Xuefeng Li. A General Purpose Variational Formulation for Boundary Value Problems of Orders Greater than Two, *J. Appl. Comput. Mech.*, 7(3), 2021, 1788-1802. <https://doi.org/10.22055/JACM.2021.37244.2987>

