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On the Physical Interpretation of Adjoint Methods for Sensitivity Analysis, Part I:

Self-Adjoint Linear Systems

Vijay Srinivasan

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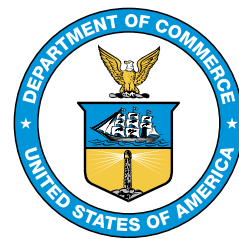
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Methods for Sensitivity Analysis, Part I:
*Self-Adjoint Linear Systems***

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Abstract

Engineers and scientists rely on computational models not just to predict outcomes, but to understand which input parameters most influence those outcomes. However, answering this question for models involving thousands of inputs is computationally prohibitive using standard brute-force perturbation methods. Adjoint methods provide an efficient means for such local sensitivity analysis, which is a critical component of uncertainty quantification for complex computational modeling and simulation. While powerful, their application is often masked by a purely mathematical presentation that obscures the underlying physical principles. This report, the first in a series, aims to demystify the adjoint method by grounding it in physical principles, such as that of structural mechanics. Using a simple Warren truss as a recurring example, we demonstrate that the adjoint vector has profound physical interpretations: acting as a “receptivity map,” a discrete Green’s function, a row of the flexibility matrix, or a linear combination thereof. This perspective unifies the stiffness-based formulation (from the principle of virtual work) with the flexibility-based formulation (from the complementary energy principle). This mechanical analogy provides a tangible basis for understanding the adjoint vector in a broader class of self-adjoint physical systems. Furthermore, we extend the analysis using the principles of similitude, developing dimensionless Pi groups to create a more general methodology for comparing parameter sensitivities. Ultimately, this report clarifies how the adjoint method serves as more than a computational shortcut; it is an analytical tool that elegantly combines various physical principles, making it attractive for insightful uncertainty quantification.

Keywords

Adjoint Method; Flexibility Method; Green’s Function; Physical Interpretation; Sensitivity Analysis; Structural Mechanics; Uncertainty Quantification.

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1. Introduction

Computational modeling and simulation are indispensable tools for predicting the behavior of complex physical and engineered systems. Our focus in this report is specifically on *mechanistic models*—those governed by fundamental physical laws such as the conservation of mass, momentum, and energy—as opposed to purely empirical or data-driven statistical models. The reliability of predictions from these mechanistic models depends critically on the input parameters, which are often subject to uncertainty. To this end, *sensitivity analysis* (SA) and *uncertainty quantification* (UQ) are essential practices. Sensitivity analysis identifies which parameters most significantly influence a model’s output, while uncertainty quantification propagates input uncertainties to determine the confidence in the model’s predictions.

A primary challenge in performing comprehensive SA is computational cost. When a model depends on a large number of parameters, traditional methods that require re-solving the governing equations for each parameter become prohibitively expensive. The *adjoint method* offers an elegant and remarkably efficient solution to this problem, allowing the local sensitivity of a single scalar output with respect to hundreds of parameters to be computed with just two solves of a linear system. Even though our ultimate goal is to quantify uncertainties in this exposition, the utility of adjoint-based sensitivity analysis extends beyond UQ. It is fundamental to gradient-based design optimization, where sensitivities serve as the search directions for optimization algorithms. Furthermore, it is critical for creating surrogate models (reduced-order models), where derivatives enable Taylor series expansions to construct compact, efficient approximations of high-fidelity simulations.

Despite their power, adjoint methods are often perceived as a purely mathematical “trick,” obscuring the physical intuition that is vital for engineering insight. As Albert Einstein suggested, it is useful to ask what is the physical meaning of a given mathematical expression [1]. This report is written in that spirit and serves as the foundational first installment in a series dedicated to the physical interpretation of adjoint methods. Its primary purpose is to develop a conceptual understanding of adjoint methods by exploring their underlying physical principles. We interpret “physics” broadly to mean the fundamental laws governing state evolution and equilibrium, whether the domain is mechanics, chemistry, or biology.

This report unfolds this physical interpretation in several stages. We begin by introducing the method in the context of linear self-adjoint algebraic equations. While the condition of self-adjointness is mathematically synonymous with matrix symmetry ($K = K^T$) in real variables, we adopt the operator-theoretic term “self-adjoint” throughout this series. This choice aligns with the standard nomenclature of the literature on *Adjoint Methods* and provides a consistent vocabulary that generalizes seamlessly to the non-symmetric operators discussed in subsequent reports. We then ground these concepts in the tangible world of structural mechanics, using a simple Warren truss as a recurring example. Through this lens, we demonstrate that the adjoint vector corresponds to concrete physical concepts: a *discrete Green’s function* and the rows of the structure’s *flexibility matrix*. This exploration reveals a powerful duality between stiffness and flexibility methods. To generalize these

findings, we then apply the principles of dimensional analysis and similitude, reformulating the problem in terms of dimensionless Pi groups that provide a more general basis for comparing sensitivities. Finally, we place the discrete algebraic formulation in its broader context, discussing its connection to continuous differential equations and the practical implications of different discretization paradigms. Ultimately, this report aims to show that the adjoint method is not just a computational shortcut but a powerful analytical tool rooted in fundamental physical principles.

2. Linear Algebraic Equations

It is prudent to begin with linear algebraic equations, as Courant and Hilbert [2] observed that more intricate functional equations, such as differential and integral equations, can be viewed as their limiting cases. This analogy serves as a powerful heuristic principle, suggesting that phenomena observed in linear algebra will have direct counterparts in continuous systems.

2.1. Sensitivity Analysis

A detailed account of sensitivity analysis can be found in [3], which is adapted here with a slight change in notation. Let a governing system of linear algebraic equations be given by:

$$\mathbf{A}\mathbf{u} = \mathbf{f} \quad (1)$$

where $\mathbf{A} \in \mathbb{R}^{n \times n}$, $\mathbf{u} \in \mathbb{R}^n$, and $\mathbf{f} \in \mathbb{R}^n$. In this context, the matrix \mathbf{A} serves as a *linear algebraic operator* mapping the state vector \mathbf{u} to the forcing vector \mathbf{f} . The system depends on a vector of k parameters, $\mathbf{p} = [p_1, \dots, p_k]^T$, drawn from the set \mathcal{P} . The matrix \mathbf{A} and vector \mathbf{f} are explicit functions of these parameters, denoted $\mathbf{A}(\mathbf{p})$ and $\mathbf{f}(\mathbf{p})$, while the solution vector \mathbf{u} depends on them implicitly.

We assume that for a given set of nominal parameter values, the matrix $\mathbf{A}(\mathbf{p})$ is invertible. In many physical systems, \mathbf{A} is also *symmetric and positive definite* (SPD), a property we will assume hereafter unless stated otherwise. In effect, we assume that the governing Eq. (1) describes a linear *self-adjoint* system because $\mathbf{A}^T = \mathbf{A}$.

We define the partial derivative of a vector or matrix with respect to a parameter as an element-wise operation. That is, the resulting object is a vector or matrix whose components are the partial derivatives of the original components with respect to that parameter. This means that the partial derivative of a vector $\mathbf{u} = [u_1, \dots, u_n]^T$ with respect to a parameter p_i is defined as:

$$\frac{\partial \mathbf{u}}{\partial p_i} = \left[\frac{\partial u_1}{\partial p_i}, \dots, \frac{\partial u_n}{\partial p_i} \right]^T$$

A similar element-wise definition applies to matrices.

Differentiating Eq. (1) with respect to a parameter p_i yields the *sensitivity equation*:

$$\mathbf{A} \frac{\partial \mathbf{u}}{\partial p_i} = \frac{\partial \mathbf{f}}{\partial p_i} - \frac{\partial \mathbf{A}}{\partial p_i} \mathbf{u} \quad (2)$$

where \mathbf{u} is the solution to the original governing equation. To find the sensitivity of the entire solution vector \mathbf{u} with respect to all k parameters, one must construct the $n \times k$ sensitivity matrix \mathcal{M} :

$$\mathcal{M} = \begin{bmatrix} \partial u_1 / \partial p_1 & \dots & \partial u_1 / \partial p_k \\ \vdots & \ddots & \vdots \\ \partial u_n / \partial p_1 & \dots & \partial u_n / \partial p_k \end{bmatrix} \quad (3)$$

Determining all the k columns of this matrix requires solving the linear system in Eq. (2) k times, one for each column. This “brute-force” approach can be computationally prohibitive when k is large.

2.2. The Adjoint Method

An economical solution exists when the *quantity of interest*, Q , is a scalar function of the parameters and the solution vector, $Q = Q(\mathbf{p}, \mathbf{u})$. The sensitivity of Q with respect to p_i , denoted $S_{p_i}(Q)$, is found using the chain rule:

$$S_{p_i}(Q) = \frac{\partial Q}{\partial p_i} + \sum_{j=1}^n \frac{\partial Q}{\partial u_j} \frac{\partial u_j}{\partial p_i} = \frac{\partial Q}{\partial p_i} + \left\langle \mathbf{c}, \frac{\partial \mathbf{u}}{\partial p_i} \right\rangle \quad (4)$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product, and \mathbf{c} is the gradient of Q with respect to \mathbf{u} :

$$\mathbf{c} = \left[\frac{\partial Q}{\partial u_1}, \dots, \frac{\partial Q}{\partial u_n} \right]^T \quad (5)$$

Calculating $S_{p_i}(Q)$ for all k parameters still appears to require solving Eq. (2) k times to find each $\partial \mathbf{u} / \partial p_i$ vector. The adjoint method elegantly circumvents this.

Let \mathbf{v} be an arbitrary vector. Taking the inner product of \mathbf{v} with the sensitivity Eq. (2) gives:

$$\left\langle \mathbf{v}, \mathbf{A} \frac{\partial \mathbf{u}}{\partial p_i} \right\rangle = \left\langle \mathbf{v}, \frac{\partial \mathbf{f}}{\partial p_i} - \frac{\partial \mathbf{A}}{\partial p_i} \mathbf{u} \right\rangle \quad (6)$$

Using the commutativity property of the inner product, the left-hand side can be rewritten as $\left\langle \mathbf{A}^T \mathbf{v}, \frac{\partial \mathbf{u}}{\partial p_i} \right\rangle$. The core idea is to choose the arbitrary vector \mathbf{v} such that it satisfies the *adjoint equation*:

$$\mathbf{A}^T \mathbf{v} = \mathbf{c} \quad (7)$$

With this choice, \mathbf{v} is now defined as the *adjoint vector*. Substituting this result back into the sensitivity formulation yields the final expression for the sensitivity of Q :

$$S_{p_i}(Q) = \frac{\partial Q}{\partial p_i} + \left\langle \mathbf{v}, \frac{\partial \mathbf{f}}{\partial p_i} - \frac{\partial \mathbf{A}}{\partial p_i} \mathbf{u} \right\rangle \quad (8)$$

The sensitivity analysis procedure can be summarized in the following steps:

1. **Solve Governing Equation:** Solve Eq. (1) for the primary vector \mathbf{u} using nominal parameter values.
2. **Compute Gradient \mathbf{c} :** Evaluate the gradient vector \mathbf{c} from Eq. (5) using the computed \mathbf{u} and nominal parameter values. This step results in a purely numerical vector \mathbf{c} .
3. **Solve Adjoint Equation:** Solve Eq. (7) for the adjoint vector \mathbf{v} . In this step, the matrix \mathbf{A}^T is numerically instantiated using the nominal parameter values and the computed \mathbf{u} from the first step.
4. **Compute Sensitivities:** Calculate $S_{p_i}(Q)$ for each parameter p_i using Eq. (8) with the same vectors \mathbf{u} and \mathbf{v} .

The key advantage of the adjoint method is its efficiency: only two major linear systems must be solved, one for \mathbf{u} and one for \mathbf{v} . Since all subsequent calculations for each of the k parameters are merely vector inner products, the method is substantially more economical than the brute-force approach when k is large.

The adjoint formulation presented thus far can also be viewed as a “weighted sum” operation. Equation (8) reveals that the total sensitivity of Q is the sum of its direct partial derivative, $\frac{\partial Q}{\partial p_i}$, and the sensitivity terms, $\frac{\partial \mathbf{f}}{\partial p_i} - \frac{\partial \mathbf{A}}{\partial p_i} \mathbf{u}$, weighted by the adjoint vector \mathbf{v} . This weighting role justifies referring to \mathbf{v} as an “influence map”: its elements assign a precise numerical importance to each local perturbation in the system’s residual (represented by $\frac{\partial \mathbf{f}}{\partial p_i} - \frac{\partial \mathbf{A}}{\partial p_i} \mathbf{u}$), determining how strongly that local change affects the final global quantity of interest.

3. Physical Interpretations of the Adjoint Method

The adjoint method has been presented thus far from a primarily mathematical perspective. However, since the governing equations describe physical phenomena, their mathematical components often have meaningful physical interpretations. This section explores these interpretations to provide deeper insight into the adjoint method.

3.1. The Adjoint Vector as a Discrete Green’s Function

A powerful insight emerges when the quantity of interest is a single component of the solution vector, $Q = u_i$. In this case, the gradient vector \mathbf{c} from Eq. (5) becomes the standard basis vector $\hat{\mathbf{e}}_i$ (a vector of zeros with a 1 in the i^{th} position). The adjoint equation (7) then becomes:

$$\mathbf{A}^T \mathbf{v} = \hat{\mathbf{e}}_i \tag{9}$$

Here, $\hat{\mathbf{e}}_i$ can be seen as a *discrete Dirac delta function* — a unit concentrated load applied at location i . The solution, the adjoint vector \mathbf{v} , is therefore the system’s response to this load. This is precisely the definition of the *discrete Green’s function* for the linear algebraic operator \mathbf{A}^T [4].

This concept can be visualized in the context of structural mechanics. Consider the simple Warren truss shown in Fig. 1. This structure consists of five nodes (joints) and seven elements (rods), with nodes L0 and L2 fixed. It is subjected to external nodal forces \mathbf{f} , resulting in nodal deflections \mathbf{u} .

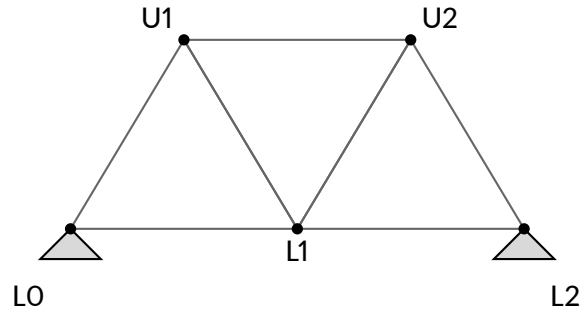


Fig. 1. A simple Warren truss example.

In this context, the matrix \mathbf{A} is the structural *stiffness matrix*, typically denoted \mathbf{K} , after proper boundary conditions are enforced. If the quantity of interest is the deflection at a specific node in a specific direction ($Q = u_i$), then the vector $\mathbf{c} = \hat{\mathbf{e}}_i$ represents a *unit virtual load* applied at that degree of freedom. As illustrated in Fig. 2, the solution to the adjoint equation, \mathbf{v} , is the vector of nodal deflections caused by this unit load. Due to the symmetry of the stiffness matrix ($\mathbf{K}^T = \mathbf{K}$), the adjoint vector \mathbf{v} is identical to the physical displacement field caused by the unit load. In mathematical physics literature, this is also known as the *influence function* [2]. In the engineering literature on dynamic systems, this is referred to as the *impulse response function* [5].

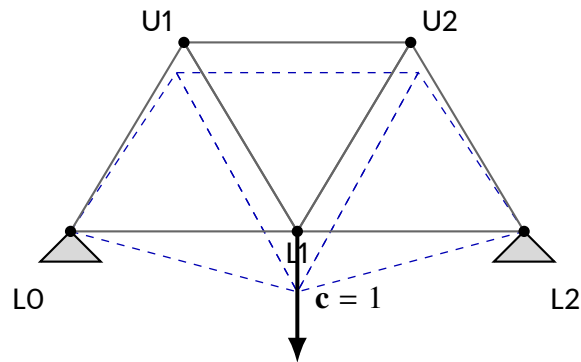


Fig. 2. Illustration of the Green's function for the simple Warren truss, representing the deflection field (\mathbf{v}) due to a unit virtual load (\mathbf{c}) at node L1.

3.2. The Adjoint Vector as a Row of the Flexibility Matrix

An alternative interpretation arises from directly examining the sensitivity equation (2). Since $\partial \mathbf{u} / \partial p_j = \mathbf{A}^{-1} \left(\frac{\partial \mathbf{f}}{\partial p_j} - \frac{\partial \mathbf{A}}{\partial p_j} \mathbf{u} \right)$, its i^{th} component is:

$$\frac{\partial u_i}{\partial p_j} = \left\langle \text{row}_i(\mathbf{A}^{-1}), \left(\frac{\partial \mathbf{f}}{\partial p_j} - \frac{\partial \mathbf{A}}{\partial p_j} \mathbf{u} \right) \right\rangle \quad (10)$$

Comparing this to the final adjoint sensitivity formula (Eq. (8) specialized for $Q = u_i$), we see that the adjoint vector \mathbf{v} is precisely the i^{th} row of the inverse matrix \mathbf{A}^{-1} .

In structural mechanics, the inverse of the stiffness matrix \mathbf{K} is the *flexibility matrix* $\mathbf{F} = \mathbf{K}^{-1}$. Therefore, for a quantity of interest $Q = u_i$, the adjoint vector \mathbf{v} is the i^{th} row (or column, by symmetry) of the flexibility matrix.

3.3. The Adjoint Vector for a General Quantity of Interest

For a more general quantity of interest, such as the stress in a specific element, we can show that Q can often be expressed as a linear combination of nodal displacements, $Q = \langle \mathbf{c}, \mathbf{u} \rangle$. For example, the stress in the top horizontal member (Element 3) of our Warren truss (Fig. 3 and Table 1) is derived as follows.

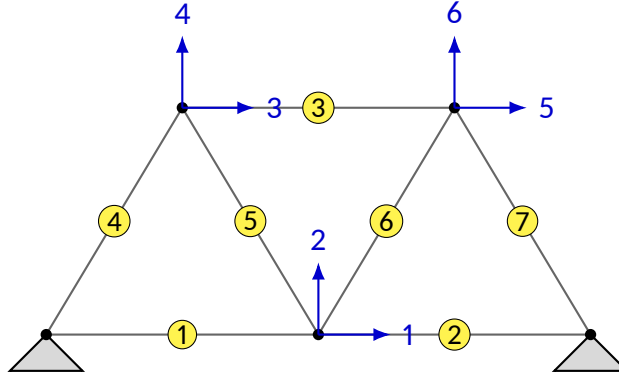


Fig. 3. Warren truss with numbered elements and nodal degrees of freedom. The nodes are labeled in Fig. 1.

The axial stress $\sigma_3 = E_3 \epsilon_3$. The axial strain ϵ_3 is related to the element's local nodal displacements $\mathbf{d}_3 = [u_3, u_4, u_5, u_6]^T$ through the strain-displacement matrix $\mathbf{B}_3 = \frac{1}{L_3} [-1, 0, 1, 0]$. This yields:

$$\begin{aligned} \epsilon_3 &= \mathbf{B}_3 \mathbf{d}_3 = \frac{1}{L_3} (-u_3 + u_5) \\ \sigma_3 &= E_3 \epsilon_3 = \frac{E_3}{L_3} (u_5 - u_3) \end{aligned}$$

Table 1. Symbolic Properties of Truss Elements

Element (j)	Connected Nodes	Length (L_j)	Area (A_j)	Modulus (E_j)
1	L0 - L1	L_1	A_1	E_1
2	L1 - L2	L_2	A_2	E_2
3	U1 - U2	L_3	A_3	E_3
4	L0 - U1	L_4	A_4	E_4
5	U1 - L1	L_5	A_5	E_5
6	L1 - U2	L_6	A_6	E_6
7	U2 - L2	L_7	A_7	E_7

Since $Q = \sigma_3$, we can write $Q = \langle \mathbf{c}, \mathbf{u} \rangle$ with $\mathbf{c} = \frac{E_3}{L_3} [0, 0, -1, 0, 1, 0]^T$. The adjoint vector is then $\mathbf{v} = \mathbf{K}^{-1}\mathbf{c}$. This shows that for a general linear quantity of interest, the adjoint vector \mathbf{v} is a *linear combination of the columns (equivalently, rows) of the flexibility matrix*.

Even when Q is not linear, Eq. (5) shows that the vector \mathbf{c} is numerically instantiated from the derivatives of Q . Therefore, the adjoint vector \mathbf{v} computed from the solution of Eq. (7) is still a linear combination of the columns of $[\mathbf{A}^T]^{-1} = \mathbf{K}^{-1}$.

4. Adjoint Method and the Duality of Formulations

The governing equation (1) can be viewed as representing a simple static force balance principle in the context of structural mechanics. However, a richer set of concepts and understanding arise when the same equation emerges from the energy methods in applied mechanics [6].

Relating the adjoint vector to the flexibility matrix highlights a fundamental duality in mechanics. The stiffness-based governing equation $\mathbf{K}\mathbf{u} = \mathbf{f}$ can be derived from the *principle of minimum potential energy*, which is a specialization of the *principle of virtual displacement* (also referred to as the *principle of virtual work*) [6, 7]. Conversely, the flexibility formulation, $\mathbf{F}\mathbf{f} = \mathbf{u}$, can be derived from Castigliano's second theorem, which is a specialization of the *complementary energy principle* [6].

If such a flexibility matrix $\mathbf{F}(\mathbf{p})$ were available at the outset, the governing equation $\mathbf{u} = \mathbf{F}\mathbf{f}$ could be differentiated directly with respect to p_i :

$$\frac{\partial \mathbf{u}}{\partial p_i} = \mathbf{F} \frac{\partial \mathbf{f}}{\partial p_i} + \frac{\partial \mathbf{F}}{\partial p_i} \mathbf{f}$$

This provides the sensitivity of \mathbf{u} without resorting to solving a matrix equation.

While the flexibility formulation offers direct paths to sensitivity analysis, stiffness methods dominate computational mechanics for practical reasons, such as ease of assembly for complex geometries. Moreover, deriving the symbolic flexibility matrix \mathbf{F} is notoriously difficult, either by direct application of Castigliano's second theorem to statically indeterminate structures or by symbolic inversion of the stiffness matrix \mathbf{K} . We examine these two involved approaches below to highlight the difficulty.

4.1. Symbolic Inversion of the Stiffness Matrix

A direct approach is to find $\mathbf{F}(\mathbf{p})$ by symbolically inverting $\mathbf{K}(\mathbf{p})$. For our simple Warren truss, we first assemble the 6×6 symbolic stiffness matrix \mathbf{K} from its 7 elemental contributions, assuming equilateral triangle geometry (Table 2). Each node has two degrees of freedom (DOF). The components of \mathbf{K} are functions of the stiffness coefficients $S_j = A_j E_j / L_j$ (see Table 1).

Table 2. Angles for the Warren truss elements.

Element (j)	Angle (θ_j)	c_j	s_j	Connects DOFs
1	0°	1	0	(Fixed) to (1, 2)
2	0°	1	0	(1, 2) to (Fixed)
3	0°	1	0	(3, 4) to (5, 6)
4	60°	$1/2$	$\sqrt{3}/2$	(Fixed) to (3, 4)
5	-60°	$1/2$	$-\sqrt{3}/2$	(3, 4) to (1, 2)
6	60°	$1/2$	$\sqrt{3}/2$	(1, 2) to (5, 6)
7	-60°	$1/2$	$-\sqrt{3}/2$	(5, 6) to (Fixed)

The resulting stiffness matrix components are shown in Table 3. The stiffness coefficients, which have the unit of force per unit length, are equivalent to the classical spring constants if the truss elements were treated simply as springs. To find the symbolic flexibility matrix, we must compute $\mathbf{F} = \mathbf{K}^{-1} = \frac{1}{\det(\mathbf{K})} \text{adj}(\mathbf{K})$. Let us elaborate on the components of this formula. The term $\text{adj}(\mathbf{K})$ is the *adjugate* (or classical adjoint) of \mathbf{K} , which is defined as the *transpose of its cofactor matrix*, \mathbf{C} .

First, we construct the cofactor matrix \mathbf{C} , which has the same dimensions as \mathbf{K} . Each element C_{ij} in this matrix is the cofactor corresponding to the element K_{ij} from the original stiffness matrix:

$$\mathbf{C} = \begin{bmatrix} C_{11} & C_{12} & \dots & C_{16} \\ C_{21} & C_{22} & \dots & C_{26} \\ \vdots & \vdots & \ddots & \vdots \\ C_{61} & C_{62} & \dots & C_{66} \end{bmatrix}$$

Then, the adjugate matrix is simply the transpose of \mathbf{C} :

$$\text{adj}(\mathbf{K}) = \mathbf{C}^T = \begin{bmatrix} C_{11} & C_{21} & \dots & C_{61} \\ C_{12} & C_{22} & \dots & C_{62} \\ \vdots & \vdots & \ddots & \vdots \\ C_{16} & C_{26} & \dots & C_{66} \end{bmatrix}$$

Each cofactor is calculated as $C_{ij} = (-1)^{i+j} M_{ij}$, where M_{ij} (the minor) is the determinant of the submatrix formed by removing the i -th row and j -th column of \mathbf{K} . This means that to

construct the full adjugate matrix for our 6×6 system, we would need to calculate the determinants of 36 different 5×5 submatrices. Each of these, along with the main determinant $\det(\mathbf{K})$, is an elaborate polynomial of the seven stiffness parameters (S_1, \dots, S_7).

Table 3. Components of the Global Stiffness Matrix \mathbf{K} (Upper Triangle)

		$j=1$	$j=2$		
$i=1$		$S_1 + S_2 + \frac{1}{4}(S_5 + S_6)$	$-\frac{\sqrt{3}}{4}(S_5 - S_6)$		
$i=2$			$\frac{3}{4}(S_5 + S_6)$		
		$j=3$	$j=4$	$j=5$	$j=6$
$i=1$		$-\frac{1}{4}S_5$	$\frac{\sqrt{3}}{4}S_5$	$-\frac{1}{4}S_6$	$-\frac{\sqrt{3}}{4}S_6$
$i=2$		$\frac{\sqrt{3}}{4}S_5$	$-\frac{3}{4}S_5$	$\frac{\sqrt{3}}{4}S_6$	$-\frac{3}{4}S_6$
$i=3$		$S_3 + \frac{1}{4}(S_4 + S_5)$	$\frac{\sqrt{3}}{4}(S_4 - S_5)$	$-S_3$	0
$i=4$			$\frac{3}{4}(S_4 + S_5)$	0	0
$i=5$				$S_3 + \frac{1}{4}(S_6 + S_7)$	$-\frac{\sqrt{3}}{4}(S_6 - S_7)$
$i=6$					$\frac{3}{4}(S_6 + S_7)$

Finally, each element of the flexibility matrix, F_{ij} , is given by the corresponding element of the adjugate matrix divided by the determinant:

$$F_{ij} = \frac{(\text{adj}(\mathbf{K}))_{ij}}{\det(\mathbf{K})} = \frac{C_{ji}}{\det(\mathbf{K})}$$

This explicit relationship makes it clear that deriving a closed-form symbolic expression for any single element of \mathbf{F} is a monumental task, as it requires the symbolic evaluation of two large determinants. The structure of the resulting symbolic matrix is shown conceptually in Table 4.

Table 4. Structure of the Symbolic Flexibility Matrix $\mathbf{F} = [F_{ij}]$

	$j=1$	$j=2$...
$i=1$	$\frac{C_{11}}{\det(\mathbf{K})}$	$\frac{C_{21}}{\det(\mathbf{K})}$...
$i=2$	$\frac{C_{12}}{\det(\mathbf{K})}$	$\frac{C_{22}}{\det(\mathbf{K})}$...
\vdots	\vdots	\vdots	\ddots

4.2. Direct Derivation of the Symbolic Flexibility Matrix

Alternatively, one can derive \mathbf{F} using Castigliano’s second theorem. For a statically indeterminate structure, this is a non-trivial task. The key challenge is that the internal forces P_j cannot be expressed as a function of only the external forces \mathbf{f} using static equilibrium alone [8]. We must first solve for redundant forces using the Method of Consistent Deformations. The core idea is to break the intricate problem into simpler, statically determinate ones and then enforce geometric compatibility to find the unknown forces.

1. Create a Statically Determinate “Primary Structure”

A structure is *statically indeterminate* if its internal forces cannot be found using only the equations of static equilibrium ($\sum F_x = 0$, $\sum F_y = 0$, $\sum M = 0$). Our truss has more members than necessary for stability, making it indeterminate. To make it solvable, we temporarily remove a “redundant” member (in this case, Element 6). The structure that remains is called the *primary structure*, as shown in Fig. 4, and it is designed to be statically determinate. We replace the removed member with the unknown internal force it was carrying. This force, which acts to pull the two nodes (L1 and U2) together, is called the *redundant force*, denoted by X . Our goal is to find the value of X .

It should be noted that the force \mathbf{f} indicated in the figure is a conceptual illustration; the external load \mathbf{f} in the analysis is a symbolic vector containing six components, $\mathbf{f} = [f_1, f_2, \dots, f_6]^T$. Each component corresponds to a force applied in one of the two directions (horizontal or vertical) at one of the three free nodes (L1, U1, or U2).

2. Express Internal Forces via Superposition

Because the primary structure is linear, we can analyze the effects of the loads separately and add them up (the principle of superposition). The total internal force,

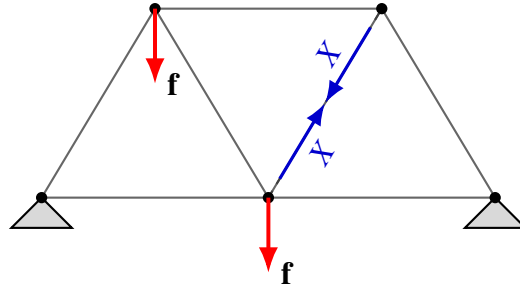


Fig. 4. The primary structure of Fig. 3 with the redundant member 6 replaced by the force X .

P_j , in any member j of the primary structure is the sum of two contributions:

$$P_j(\mathbf{f}, X) = P'_j(\mathbf{f}) + n_j X$$

where:

- $P'_j(\mathbf{f})$ is the internal force in member j due *only to the external loads* \mathbf{f} applied to the primary structure (assuming $X = 0$).
- n_j is the internal force in member j due *only to a unit redundant load* ($X = 1$) applied where the member was removed (assuming $\mathbf{f} = 0$). The term $n_j X$ scales this unit response by the actual (but still unknown) value of X .

3. Apply the Compatibility Condition

This is the physical heart of the method. In the real, intact truss, there is no gap where member 6 is. We must enforce this geometric fact, known as the *compatibility condition*.

- In the primary structure, the loads cause the gap between nodes L1 and U2 to change. We call this change in the gap's length Δ_6 .
- Meanwhile, the actual redundant member (Element 6) experiences the internal force X and will stretch or compress by an amount δ_6 . According to Hooke's Law, this deformation is $\delta_6 = (P_6 L_6)/(A_6 E_6)$. Since the force in member 6 is simply X , this becomes $\delta_6 = (X L_6)/(A_6 E_6)$.

For the structure to be compatible (i.e., for the gap to be closed by the member), the gap that opens in the primary structure (Δ_6) must be exactly closed by the deformation of the member (δ_6). This means $\Delta_6 = -\delta_6$, which is commonly written as:

$$\Delta_6 + \delta_6 = 0$$

4. Use Castigliano's Second Theorem to Find Relative Displacement

To use our compatibility equation, we need a way to calculate the gap Δ_6 . Castigliano's second theorem provides the perfect tool. It states that the displacement of a structure at the point of application of a force, in the direction of that force, is equal to the partial derivative of the structure's complementary strain energy (U^*) with respect to that force.

Here, the "force" is the redundant force X , and the "displacement" is the gap Δ_6 . The complementary energy of the primary structure is $U_{\text{primary}}^* = \sum_{j \neq 6} \frac{P_j^2 L_j}{2A_j E_j}$. Applying the theorem:

$$\Delta_6 = \frac{\partial U_{\text{primary}}^*}{\partial X} = \sum_{j \neq 6} \frac{\partial}{\partial X} \left(\frac{P_j^2 L_j}{2A_j E_j} \right)$$

Using the chain rule, this becomes:

$$\Delta_6 = \sum_{j \neq 6} \frac{P_j L_j}{A_j E_j} \frac{\partial P_j}{\partial X}$$

From our superposition equation in Step 2, we know that $\frac{\partial P_j}{\partial X} = n_j$.

5. Solve the Full Compatibility Equation

Now we substitute our expressions for Δ_6 (from Step 4) and δ_6 (from Step 3) into the compatibility equation:

$$\underbrace{\sum_{j \neq 6} \frac{(P'_j + n_j X) n_j L_j}{A_j E_j}}_{\Delta_6} + \underbrace{\frac{X L_6}{A_6 E_6}}_{\delta_6} = 0$$

This is a linear equation with only one unknown, X . All other terms are known constants or functions of the external loads \mathbf{f} . We can now algebraically solve for X in terms of \mathbf{f} .

6. Derive the Flexibility Matrix

Once we have the expression $X(\mathbf{f})$, the problem is essentially solved.

- We can write the total internal force P_j in any member of the original, indeterminate structure purely as a function of the external loads \mathbf{f} .
- With these forces, we write the total complementary energy U^* for the *entire* original structure, now also purely as a function of \mathbf{f} .

- Finally, we apply Castigliano's second theorem one last time. To find the displacement u_i at a specific degree of freedom, we take the partial derivative of the total complementary energy with respect to the force f_i applied at that location:

$$u_i = \frac{\partial U^*}{\partial f_i}$$

By performing this differentiation for each DOF $i = 1, \dots, 6$, we systematically generate the expressions that define the rows of the global flexibility matrix \mathbf{F} .

The intensive nature of this derivation of the symbolic flexibility matrix for statically indeterminate structures stands in sharp contrast to the stiffness matrix's simple direct assembly. This highlights the computational elegance of the adjoint method, which avoids a symbolic flexibility matrix or a full symbolic inversion of a stiffness matrix by instead computing required components of the inverse of a *numerically instantiated* stiffness matrix "on demand."

5. Uncertainty Quantification

Sensitivity analysis is an important part of uncertainty quantification. The parameter sensitivities, $S_{p_i}(Q)$, can be used to propagate input uncertainties to the quantity of interest. Following the methodology of standardized metrology guides [9, 10], we can ensure that uncertainties from computational models are directly comparable to those from physical experiments. This is crucial for the validation step in the ASME VVUQ (Verification, Validation, and Uncertainty Quantification) process [11], as illustrated in Fig. 5. More details on the role of uncertainty quantification in verification and validation of computational solid mechanics models can be found in [12, 13].

Let the input parameters \mathbf{p} be random variables with known mean values (the nominal values used in the SA) and a known covariance matrix Σ :

$$\Sigma = \begin{bmatrix} \text{Var}(p_1) & \dots & \text{Covar}(p_1, p_k) \\ \vdots & \ddots & \vdots \\ \text{Covar}(p_k, p_1) & \dots & \text{Var}(p_k) \end{bmatrix} \quad (11)$$

Let the sensitivity vector for the quantity of interest Q be $\mathbf{S} = [S_{p_1}(Q), \dots, S_{p_k}(Q)]^T$. Using a first-order Taylor series expansion, the variance of Q is given by the well-known "law of propagation of uncertainty":

$$\text{Var}(Q) = \mathbf{S}^T \Sigma \mathbf{S} \quad (12)$$

The standard uncertainty of the output is $u(Q) = \sqrt{\text{Var}(Q)}$, and the result of the simulation can be presented as $Q_0 \pm k \cdot u(Q)$, where Q_0 is the predicted mean value and k is a coverage factor (typically 2 or 3). The efficiency of the adjoint method in computing the sensitivity

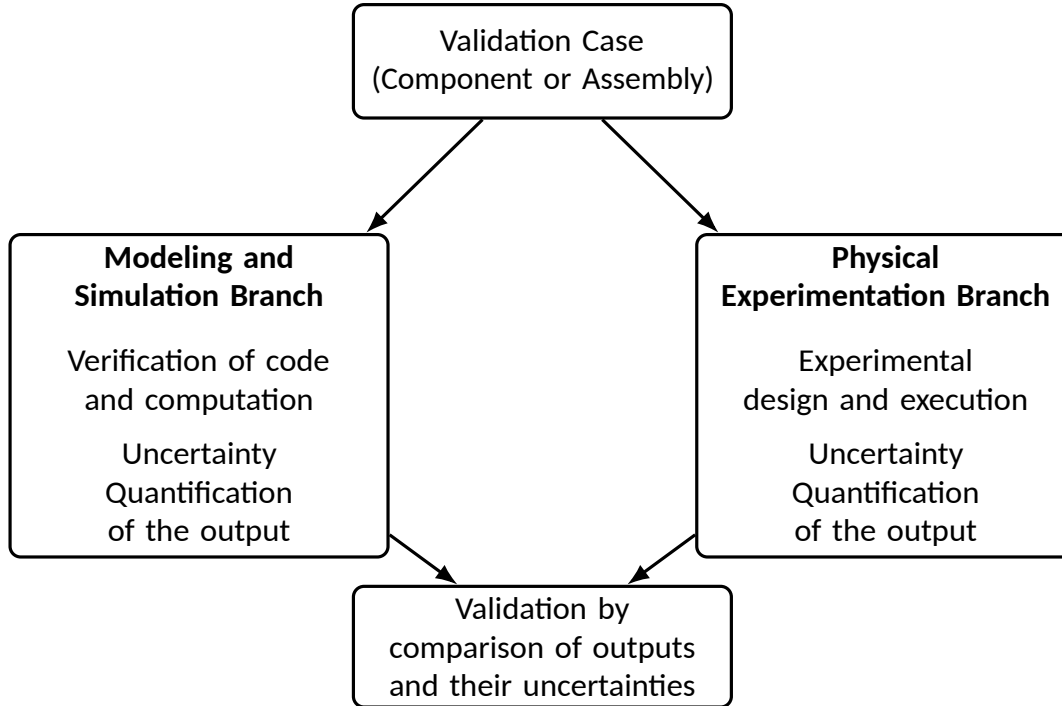


Fig. 5. A simplified version of the ASME VVUQ process.

vector \mathbf{S} makes this approach feasible even for models with a very large number of uncertain parameters.

It is worth noting that adjoint-based *local* sensitivity analysis is a key component of one powerful approach to uncertainty quantification [14, 15]. This approach is distinct from other methods, such as sampling-based techniques like Monte Carlo simulation [15, 16], which are often more general but computationally expensive. Even within the broad field of sensitivity analysis itself, adjoint methods form a specific subset, focusing on derivative-based local rates of change rather than global measures. Figure 6 illustrates the role of adjoint methods within the broader landscape of UQ techniques.

6. Non-Dimensional Analysis and Similitude

Thus far, our analysis has used dimensional quantities (e.g., L_j, E_j, A_j), which makes comparing the sensitivities of different parameter types challenging. To create a more general basis and gain deeper physical insight, we can non-dimensionalize the governing equations [17–19]. A useful approach, analogous to methods in thermal and fluid mechanics [20, 21], is to define dimensionless groups that represent ratios of competing physical effects. This aligns with the principles of *similitude*, where two systems are considered physically similar if their governing dimensionless parameters are identical.

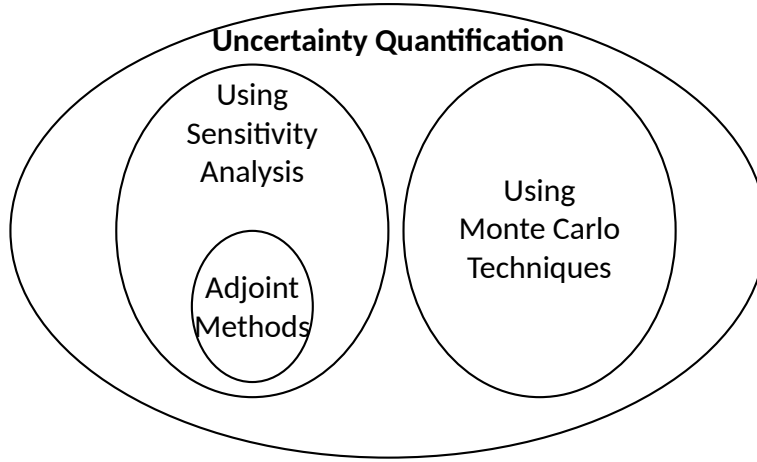


Fig. 6. Role of adjoint methods for uncertainty quantification in computational modeling and simulation.

6.1. Dimensionless Π Groups

For a structural system, the competing effects are the relative stiffness of its components and the relative magnitudes of applied loads. We can capture these effects in dimensionless Π (Π) groups, in accordance with the Buckingham Π theorem.

First, we select a reference stiffness, such as that of Element 1, to be the *characteristic stiffness*: $S^* = S_1 = (A_1 E_1)/L_1$. We then define dimensionless stiffness ratios for the other elements:

$$\Pi_{S_j} = \frac{S_j}{S^*} = \frac{A_j E_j / L_j}{A_1 E_1 / L_1} \quad \text{for } j = 2, \dots, 7$$

Similarly, we select a *characteristic force*, such as $f^* = f_1$, and define dimensionless force ratios, treating each force component f_i as a parameter:

$$\Pi_{f_i} = \frac{f_i}{f^*} \quad \text{for } i = 2, \dots, 6$$

This process reduces the parameter space significantly. The system is no longer described by up to 27 individual dimensional parameters but by a smaller set of physically meaningful ratios and a few characteristic scales (S^* and f^*).

6.2. Dimensionless Governing Equation

Using these Π groups, the dimensional stiffness matrix and force vector can be factored:

$$\mathbf{K} = S^* \hat{\mathbf{K}}(\Pi_{S_j}) \quad \text{and} \quad \mathbf{f} = f^* \hat{\mathbf{f}}(\Pi_{f_i})$$

where $\hat{\mathbf{K}}$ and $\hat{\mathbf{f}}$ are dimensionless and depend only on the Π groups. Substituting these into the original governing equation, $\mathbf{K}\mathbf{u} = \mathbf{f}$, gives:

$$S^* \hat{\mathbf{K}}\mathbf{u} = f^* \hat{\mathbf{f}}$$

By defining a characteristic displacement $u^* = f^*/S^*$ and a dimensionless displacement vector $\hat{\mathbf{u}} = \mathbf{u}/u^*$, the equation simplifies to the elegant, fully dimensionless form:

$$\hat{\mathbf{K}}\hat{\mathbf{u}} = \hat{\mathbf{f}}$$

This result reveals a key principle of similitude: the *dimensionless shape of the deformation*, $\hat{\mathbf{u}}$, depends *only* on the dimensionless stiffness and force ratios. The overall dimensional magnitude of the displacement is then found by simply scaling this result by u^* .

6.3. Implications for Sensitivity and Uncertainty Analysis

This non-dimensional formulation offers several advantages. A key practical benefit is improved *numerical stability*, as it prevents artificially large or small numbers from arising due to the choice of units. Beyond this, it provides two profound benefits for the analysis itself:

First, it allows for a *fair comparison of sensitivities*. The sensitivity of a dimensionless quantity (e.g., dimensionless stress, $\hat{\sigma}_3$) with respect to a dimensionless parameter (e.g., a stiffness ratio, Π_{S_j}) is inherently scaled. Because all quantities are ratios, the resulting sensitivities are not artificially inflated or deflated by the choice of units. This enables a direct, apples-to-apples comparison of which physical effects — be they geometric, material, or load-based — most dominate the system’s response.

Second, this leads to more *insightful sensitivity questions*. For example, we can compute $S_{\Pi_{S_j}}(\hat{\sigma}_3)$, which answers the key design question: “What is the percentage change in stress if we make Element j 1% stiffer relative to Element 1?”

The main practical challenge lies in uncertainty quantification. Experimental uncertainty data is typically provided for dimensional parameters (e.g., L_j, E_j, f_i) in a covariance matrix Σ_p . To be used with our dimensionless model, this matrix must be transformed to the basis of the Π group parameters. This requires a formal *covariance transformation*:

$$\Sigma_{\Pi} \approx \mathbf{J}\Sigma_p\mathbf{J}^T$$

where \mathbf{J} is the *Jacobian matrix* of the transformation, with elements $J_{ij} = \partial\Pi_i/\partial p_j$. Constructing this Jacobian is a necessary but non-trivial step. Furthermore, this transformation can introduce *induced correlations* in the new covariance matrix Σ_{Π} , even if the original physical parameters were uncorrelated. This is because multiple Π groups may depend on the same reference parameters (e.g., S_1 and f_1), creating statistical dependencies that must be accounted for.

7. Broader Context and Extension to Continuous Systems

The linear algebraic system discussed thus far provides a foundational basis. This section places that formulation into a broader physical and computational context, discussing the nature of the system and its extension to problems governed by differential and integral equations.

7.1. Cause, Effect, and System Properties

The governing equation, $\mathbf{A} \mathbf{u} = \mathbf{f}$, is a discrete representation of a physical system. For the systems considered here, the matrix \mathbf{A} is assumed to be *Symmetric Positive-Definite (SPD)*. The symmetry ($\mathbf{A} = \mathbf{A}^T$) implies that the system is *self-adjoint*, a property reflecting a reciprocal relationship between sources and responses, which is common in physics. In structural mechanics, this is known as *Maxwell's reciprocal theorem*. For problems in linear static elasticity, it states that the displacement at point i in the direction d_i due to a unit load at point j applied in the direction d_j is identical to the displacement at j in the direction d_j due to a unit load at i applied in the direction d_i . It is a direct consequence of the principle of complementary energy and its specialization in Castigliano's second theorem, as detailed in Section 4.2 [6].

From this perspective, we can establish a clear analogy of cause and effect:

- The vector \mathbf{f} represents the known *cause* or external stimulus.
- The vector \mathbf{u} represents the unknown *effect* or the system's response.

This cause-and-effect relationship manifests across various domains of science and engineering, as illustrated in the following table:

Domain	Cause (\mathbf{f})	Effect (\mathbf{u})
Structural/Mechanical	Applied Forces	Displacements
Electrical	Voltages	Currents
Fluid Dynamics	Pressure Gradients	Fluid Velocities
Thermal	Heat Sources/Work	Temperatures

To illustrate this concretely, consider the thermal domain (the last entry in the table). Imagine a simple, insulated metal rod discretized into finite segments.

- The Cause vector (\mathbf{f}) represents local heat sources — for example, a heater injecting thermal energy (Watts) at specific nodes along the rod.
- The Effect vector (\mathbf{u}) represents the resulting steady-state temperature (Kelvin) at each node.
- The Operator (\mathbf{A}), which links them via $\mathbf{A} \mathbf{u} = \mathbf{f}$, is the *thermal conductivity matrix*.

Just as a mechanical force applied to a single truss node causes displacements to propagate throughout the structure based on its stiffness, a localized heat source applied to one segment of the rod causes a temperature distribution to spread throughout the material based on its conductivity. In this analogy, the inverse operator (the flexibility equivalent) represents the *thermal influence function*, quantifying how a heat source at one location impacts the temperature at any other location.

7.2. Forward and Inverse Methods in System Analysis

In most engineering analyses, the problem is to determine the effect \mathbf{u} for a given cause \mathbf{f} . The stiffness and flexibility methods offer two different perspectives on solving this problem.

The stiffness formulation, $\mathbf{A}\mathbf{u} = \mathbf{f}$, can be viewed as an *inverse method* in the context of analysis. The stiffness matrix \mathbf{A} (or \mathbf{K}) inherently describes an “effect-to-cause” relationship, defining the forces \mathbf{f} required to produce a given displacement \mathbf{u} . Since we typically know the cause (\mathbf{f}) and want to find the effect (\mathbf{u}), we must *invert* this natural relationship by solving the linear system, which is mathematically equivalent to $\mathbf{u} = \mathbf{A}^{-1}\mathbf{f}$.

Conversely, the flexibility formulation, $\mathbf{u} = \mathbf{F}\mathbf{f}$, represents a *direct method*. The flexibility matrix \mathbf{F} acts as a direct “cause-to-effect” operator. Once \mathbf{F} is known, finding the displacement for any given set of forces is a simple matrix-vector multiplication. The primary challenge of this method lies in constructing the matrix \mathbf{F} itself for statically indeterminate structures.

While the structural example provided a convenient means to discuss these interpretations, the same formulation applies to other self-adjoint linear systems. The physical meaning will depend on what each system matrix (\mathbf{A} or its inverse \mathbf{F}) naturally describes in its respective domain.

7.3. Extension to Continuous Systems and Discretization Paradigms

As noted by Courant and Hilbert, self-adjoint linear algebraic systems are often discrete approximations of continuous self-adjoint linear differential and integral equations. When performing sensitivity analysis on these continuous systems, two competing philosophies emerge.

Discretize-then-Differentiate (the Discrete Adjoint): In this paradigm, the continuous governing equation (e.g., a Partial Differential Equation, PDE) is first discretized to produce the algebraic system $\mathbf{A}\mathbf{u} = \mathbf{f}$. The adjoint equation is then derived by differentiating this discrete system, as has been done throughout this report.

Differentiate-then-Discretize (the Continuous Adjoint): In this approach, the continuous governing equations are first differentiated using functional analysis to derive a new, continuous *adjoint PDE*. This new adjoint PDE is then discretized separately.

For sensitivity analysis, particularly within a UQ context, we can draw from the precedent set in gradient-based optimization, where the discretize-then-differentiate (discrete adjoint) approach is overwhelmingly preferred [22, 23]. The reason is a crucial property known as *gradient consistency*. A numerical optimizer operates on the discrete model, not the underlying continuous physics. The discrete adjoint method provides the *exact analytical gradient* of the discrete objective function. In contrast, the continuous adjoint method yields a *discrete approximation* of the continuous gradient, which is not, in general, identical

to the exact discrete gradient. Feeding this slightly inconsistent gradient to an optimizer can lead to slower convergence or even a complete stall of the optimization process [24].

Regardless of the paradigm chosen, discretization introduces numerical errors that must be quantified and accounted for in the overall UQ, which remains a major challenge in computational modeling.

7.4. The Adjoint System: Operators and Boundary Conditions

To place the work of this report in a broader context, it is beneficial to define a full *adjoint system* as comprising both an adjoint operator and a specific set of adjoint boundary conditions.

For example, the matrix \mathbf{A} in Eq. (1) functions as a linear operator encoding the physical laws of the phenomenon. It maps the unknown state vector \mathbf{u} to the known source (or force) vector \mathbf{f} . In this discrete formulation, the essential boundary conditions (such as the zero displacements at nodes L0 and L2 in Fig. 1) are implicitly incorporated into the matrix structure itself, ensuring that \mathbf{A} is invertible.

In the self-adjoint cases considered here, the adjoint problem $\mathbf{A}^T \mathbf{v} = \mathbf{c}$ inherits these same boundary constraints while $\mathbf{A}^T = \mathbf{A}$ acts as the adjoint operator. However, in the broader context of non-conservative or transport-driven physical problems, this symmetry does not hold. The adjoint system will require the explicit derivation of distinct *adjoint boundary conditions* that may differ from those of the primal problem. We will rigorously develop this distinction between the operator and its boundary constraints in future reports.

8. Summary and Concluding Remarks

The primary goal of this report was to demystify the adjoint method for sensitivity analysis by grounding its mathematical formulation in a tangible physical context. By using a simple, self-adjoint linear system represented by a Warren truss, we have demonstrated that the adjoint vector is not merely an abstract mathematical construct. Instead, it has profound physical interpretations: it can be viewed as a *discrete Green's function* representing the system's response to a unit impulse, as a *row of the flexibility matrix*, or as a linear combination thereof for more general quantities of interest. This perspective successfully unifies the stiffness-based formulation (derived from the principle of minimum potential energy) with the flexibility-based formulation (derived from the complementary energy principle), clarifying how the adjoint method elegantly combines the computational convenience of the former with the analytical power of the latter.

The analysis herein was intentionally confined to linear, self-adjoint systems, which represent an important but idealized class of physical problems. Future reports in this series will extend this interpretive approach to non-self-adjoint and non-linear systems. Beyond these planned extensions, we also identify over- and under-determined systems as a fertile ground for broader investigation. Key areas include:

- **Non-Self-Adjoint Linear Systems:** Many physical systems, particularly those involving convective transport or damping, are described by non-symmetric matrices where $\mathbf{A} \neq \mathbf{A}^T$. In such cases, the adjoint operator is mathematically distinct from the original forward operator. Exploring the physical meaning of the adjoint vector in this context is the primary focus of the next report in this series.
- **Non-Linear Systems:** The vast majority of real-world engineering problems are non-linear. While the adjoint method is widely used for such problems, the resulting adjoint system is linear with respect to a specific operating point. A detailed investigation into the physical interpretation of the adjoint vector in this case—where it represents the sensitivity of a quantity of interest to a local source term in the *linearized* system—is planned for a future installment.
- **Over- and Under-Determined Systems:** Many problems, particularly in data assimilation and machine learning, result in non-square systems where the number of equations does not equal the number of unknowns. Extending the physical interpretation of the adjoint method to these systems, where solutions are often found in a least-squares or other minimum-norm sense, is a fascinating area for further research. This is particularly relevant as the *backpropagation algorithm*, the cornerstone of training modern artificial neural networks, can be elegantly formulated as an application of the adjoint method to a large-scale learning system.

By continuing to connect the mathematics of the adjoint method to underlying physical principles, it is envisioned that its power as a tool for both efficient computation and insightful scientific and engineering analysis can be fully realized. Such a focus on conceptual understanding and physical insight is becoming increasingly vital. In an era where AI (Artificial Intelligence) and automated systems can perform many routine computational tasks, the human role shifts toward supervision and strategy. Consequently, developing deep physical intuition is essential for scientists and engineers to effectively guide these systems and rigorously evaluate their outputs.

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