NIST Advanced Manufacturing Series
NIST AMS 100-79

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

Non-Self-Adjoint Linear Systems

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https://doi.org/10.6028/NIST.AMS.100-79

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
U.S. DEPARTMENT OF COMMERCE

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Vijay Srinivasan
Systems Integration Division
Engineering Laboratory

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May 2026

U.S. Department of Commerce
Howard Lutnick, Secretary

National Institute of Standards and Technology
Craig Burkhardt, Acting Under Secretary of Commerce for Standards and Technology and Acting NIST Director

Publication History
Approved by the NIST Editorial Review Board on 2026-05-28

How to cite this NIST Technical Series Publication:
Vijay Srinivasan (2026) On the Physical Interpretation of Adjoint Methods for Sensitivity Analysis, ParII: Non-Self-Adjoint Linear Systems. (National Institute of Standards and Technology, Gaithersburg, MD), NIST Advanced Manufacturing Series (AMS) NIST AMS 100-79. https://doi.org/10.6028/NIST .AMS.100-79

Author ORCID iDs
Vijay Srinivasan: 0000-0002-4653-8821

Contact Information
vijay.srinivasan@nist.gov

Abstract

Adjoint methods have gained prominence in science and engineering as the preferred approach for sensitivity analysis of mechanistic models involving a large number of pa-rameters. Part I of this series explored adjoint methods for self-adjoint (symmetric) linear systems, which possess a mathematically symmetric structure. In such systems, the adjoint vector has a direct physical interpretation as a system response (e.g., a displacement field), and the mathematical symmetry is a manifestation of the physical concept of reciprocity. This direct interpretation is lost in non-self-adjoint (non-symmetric) linear systems, where the matrix operat or ($\mathbf{A}$) and its tr anspose ($\mathbf{A}^T$) are distinct. Such syst ems, common in engineering, are charact erized by *directional transport* in space and *directional evolution* in time. This report, the second in the series, explores the physical meaning of the adjoint vect or in these non-self-adjoint syst ems by analyzing tw o fundament al examples: (1) a one-dimensional convection-diffusion problem, which exhibits *spatial asymmetry*, and (2) a one-dimensional damped structur al dynamics problem, which exhibits *temporal asym-metry*. We demonstr at e tha t in both cases, the adjoint operat or represents a *reversed* physical syst em. The adjoint equation for convection reverses the flow velocit y, while the adjoint equation for dynamics reverses the direction of time (solving backward from a final condition). Consequent ly, the adjoint v ect or $\mathbf{v}$ is int erpret ed not as a physical response of the original syst em, but as a general *influence map* representing *receptivity*. It quantifies how a local perturba tion in space or time affects the final quantity of int erest, providing a unified principle for sensitivity analysis and uncert ainty quan tification.

Keywords

Adjoint Method; Calibration; Digit al Twin; Influence Map; Non-Self-Adjoint Syst ems; Opti-mization; Receptivity; Reversed Syst em; Sensitivity Analysis; Verification, Validation, and Uncert ainty Quan tification (VVUQ).

Acknowledgments

This manuscript was edited with the assistance of Gemini, a large language model developed by Google. Gemini was used to refine language, improve clarity, and enhance readability in accordance with the author’s instructions. All content, scientific claims, and conclusions have been reviewed and verified by the author to ensure accuracy and originality.

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1. Introduction

The adjoint method is a powerful tool for computing sensitivities in computational models, which can then be used for uncertainty quantification [1]. For self-adjoint linear systems, such as those in structural mechanics or pure diffusion, the mathematical structure is underpinned by a strong physical intuition. As explored in Part I [2], for self-adjoint systems
where the linear algebraic operator satisfies $\mathbf{A} = \mathbf{A}^T$, this matrix symmetry is a manifestation of the physical principle of reciprocity. Consequently, the adjoint vector ($\mathbf{v}$) has a direct physical meaning: it *is* the physical response (e.g., displacement) to a virtual load, subject to the same boundary conditions as the original forward problem.

This direct physical interpretation is lost in many real-world systems that are not self-adjoint. We interpret "physics" broadly to mean the fundamental laws governing state evolution and equilibrium, whether the domain is mechanics, chemistry, or biology. The introduction of non-reciprocal physical processes breaks the symmetry of the linear operator. Key examples include:

- **Spatial Asymmetry:** Caused by *directional transport*, like the convective term $\rho c_p V \frac{dT}{dx}$ in a fluid flow studied in Section 4.
- **Temporal Asymmetry:** While dissipative effects (like the term $C\dot{\mathbf{u}}$ studied in Section 5) break time-reversal symmetry, a fundamental asymmetry exists even in their absence due to *causality*. Since sources that occur later in time cannot cause earlier events, the influence map must strictly propagate backward, regardless of whether the system is damped or conservative.

For these systems, $\mathbf{A} \neq \mathbf{A}^T$. While the mathematical formalism of the adjoint method for linear algebraic operators remains valid, the *direct* intuitive link is obscured. The adjoint equation $\mathbf{A}^T\mathbf{v} = \mathbf{c}$ involves a different mathematical operator from the forward problem, and it may also have different boundary conditions. We will define a full *adjoint system* as comprising both an adjoint operator and a specific set of adjoint boundary conditions.

The central question of this report is: What, then, *is* the physical meaning of the adjoint vector $\mathbf{v}$ in a non-self-adjoint linear system? Answering this question is not merely an academic exercise; it provides a vital conceptual foundation for advanced engineering and manufacturing applications. In the context of industrial digital twins, accurately computing sensitivities for physical systems involving transport and dissipation is critical for process optimization, model calibration, and Verification, Validation, and Uncertainty Quantification (VVUQ). While the mathematical machinery of the adjoint method functions perfectly well as an algebraic "black box," relying solely on abstract equations deprives the analyst of crucial engineering intuition. A rigorous physical interpretation demystifies how these abstract systems behave, enabling engineers to reason intuitively about structural vulnerabilities, optimal sensor placement, and active control limits. Furthermore, establishing this physical baseline for linear non-self-adjoint systems paves the way for extending the adjoint method to nonlinear and nonsquare systems. By understanding the linear non-self-adjoint case as a map of physical receptivity, we establish the interpretive lens required to make sense of highly complex, state-dependent environments—and even to understand the physical analogues of backpropagation in modern machine learning.

To answer this central question, we build the interpretation from its foundations. We first review the universal algebraic paradigm of the "discretize-then-differentiate" method. We then introduce the formal "differentiate-then-discretize" approach by deriving the continuous adjoint differential operator, $\mathcal{L}^*$, from Lagrange's identity. This theoretical foun-dation allows us to see precisely *how* the adjoint operator is mathematically constructed.

With this foundation, we analyze two simple non-self-adjoint models to build a unified physical interpretation. First, we examine a *one-dimensional convection-diffusion problem* and show that its spatial asymmetry leads to an adjoint operator with a *reversed spatial flow*. Second, we examine a *one-dimensional damped structural dynamics problem* and show that its temporal asymmetry leads to an adjoint operator that must be solved *backward in time*.

In both cases, we will demonstrate that the adjoint vector $\mathbf{v}$ can be viewed not as a *physical* entity but rather as a non-physical *informational* entity in the form of an *influence map* that quantifies the *receptivity* of the quantity of interest to local perturbations, thereby providing a powerful and general interpretation for linear systems.

While we continue to prioritize the development of conceptual understanding and physical intuition as we did in Part I [2], the nature of non-self-adjoint systems inherently demands a closer inspection of their mathematical machinery. Therefore, we will not shy away from detailed mathematical derivations or the specifics of discrete computational implementations, especially within our Model Problems. We engage with these details not for the sake of rigor alone, but because the physical interpretation—the concepts of "reversed flow," "information transport," and "receptivity"—is often most clearly revealed in the precise differential and algebraic details of the adjoint operator's construction.

2. Adjoint Method for Linear Algebraic Operators

We first establish the core mathematical formulation for adjoint sensitivity analysis of linear algebraic systems. Even if one starts with a differential or integral form of the governing equations, they can be turned into a system of algebraic equations by proper discretization of the domain over which they are defined. These algebraic equations still contain the parameters symbolically, and the algebraic equations themselves can be differentiated with respect to these parameters for sensitivity analysis. This is often called the "discretize-then-differentiate" approach. The resulting mathematical procedure given below is independent of the algebraic system symmetry.

2.1. Forward and Sensitivity Problems

We begin with the primary governing equation, or "forward problem," as a system of linear algebraic equations:

$$\mathbf{A}\mathbf{u} = \mathbf{f} \tag{1}$$

where $\mathbf{A} \in \mathbb{R}^{n\times n}$ is the invertible system matrix, $\mathbf{f} \in \mathbb{R}^n$ is the source vector, and $\mathbf{u} \in \mathbb{R}^n$ is the unknown state vector. The linear operator $\mathbf{A}$ captures the "physics" of the system under investigation. The system depends on a vector of k parameters, $\mathbf{p} = [p_1, \ldots, p_k]^T$, drawn from the set $\mathscr{P}$. The matrix $\mathbf{A}$ and vector $\mathbf{f}$ are explicit functions of these parameters, $\mathbf{A}(\mathbf{p})$ and $\mathbf{f}(\mathbf{p})$, while $\mathbf{u}$ depends on them implicitly.

Our goal is to find the sensitivity of a scalar *quantity of interest*, $Q = Q(\mathbf{u}, \mathbf{p})$, with respect to any parameter p_i. A "brute-force" or "forward sensitivity" approach involves first finding the sensitivity of the entire state, $\frac{\partial \mathbf{u}}{\partial p_i}$. We can find this by differentiating the governing equation (Eq. (1)):

$$\mathbf{A}\frac{\partial \mathbf{u}}{\partial p_i} = \frac{\partial \mathbf{f}}{\partial p_i} - \frac{\partial \mathbf{A}}{\partial p_i}\mathbf{u} \tag{2}$$

Solving this *sensitivity equation* for $\frac{\partial \mathbf{u}}{\partial p_i}$ requires one full $n \times n$ system solve. To find the sensitivities for all k parameters, this equation must be solved k times. This is computationally prohibitive when k is large.

2.2. Adjoint Formulation

The adjoint method provides an economical solution when we only need the sensitivity of the scalar Q. The total sensitivity of Q with respect to p_i, denoted $S_{p_i}(Q)$, is found using the chain rule:

$$S_{p_i}(Q) = \frac{\partial Q}{\partial p_i} + \left\langle \mathbf{c}, \frac{\partial \mathbf{u}}{\partial p_i} \right\rangle \tag{3}$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product, and

$$\mathbf{c} = \nabla_{\mathbf{u}} Q = \left[\frac{\partial Q}{\partial u_1}, \ldots, \frac{\partial Q}{\partial u_n}\right]^T$$

is the gradient of Q with respect to the state vector $\mathbf{u}$.

The term $\left\langle \mathbf{c}, \frac{\partial \mathbf{u}}{\partial p_i} \right\rangle$ is the problematic one, as it still requires $\frac{\partial \mathbf{u}}{\partial p_i}$. To get around this problem, we introduce an arbitrary vector $\mathbf{v}$. We take the inner product of $\mathbf{v}$ with the sensitivity equation (Eq. (2)):

$$\left\langle \mathbf{v}, \mathbf{A}\frac{\partial \mathbf{u}}{\partial p_i} \right\rangle = \left\langle \mathbf{v}, \frac{\partial \mathbf{f}}{\partial p_i} - \frac{\partial \mathbf{A}}{\partial p_i}\mathbf{u} \right\rangle \tag{4}$$

The left-hand side can be transformed using the definition of the matrix transpose: $\langle \mathbf{v}, \mathbf{A}\mathbf{x} \rangle = \langle \mathbf{A}^T\mathbf{v}, \mathbf{x} \rangle$. Applying this gives:

$$\left\langle \mathbf{A}^T\mathbf{v}, \frac{\partial \mathbf{u}}{\partial p_i} \right\rangle = \left\langle \mathbf{v}, \frac{\partial \mathbf{f}}{\partial p_i} - \frac{\partial \mathbf{A}}{\partial p_i}\mathbf{u} \right\rangle \tag{5}$$

Now, we make a clever choice. Since $\mathbf{v}$ is arbitrary, we specifically choose it to be an *adjoint vector* that satisfies the *adjoint equation*:

$$\mathbf{A}^T\mathbf{v} = \mathbf{c} \tag{6}$$

By making this substitution, Eq. (5) becomes:

$$\left\langle \mathbf{c}, \frac{\partial \mathbf{u}}{\partial p_i} \right\rangle = \left\langle \mathbf{v}, \frac{\partial \mathbf{f}}{\partial p_i} - \frac{\partial \mathbf{A}}{\partial p_i}\mathbf{u} \right\rangle$$

This gives us an expression for the problematic term in the chain rule (Eq. (3)). Substituting this back, we arrive at the final adjoint sensitivity formula:

$$S_{p_i}(Q) = \frac{\partial Q}{\partial p_i} + \left\langle \mathbf{v}, \frac{\partial \mathbf{f}}{\partial p_i} - \frac{\partial \mathbf{A}}{\partial p_i}\mathbf{u} \right\rangle \tag{7}$$

This procedure is mathematically valid for *any* invertible, square matrix $\mathbf{A}$. Its computational advantage is immense: we solve the forward problem (Eq. (1)) once for $\mathbf{u}$, solve the adjoint problem (Eq. (6)) once for $\mathbf{v}$, and then compute all k sensitivities using the simple inner product in Eq. (7).

The adjoint formulation presented thus far can also be viewed as a "weighted sum" operation. Equation (7) 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.

2.3. Physical Interpretation: Self-Adjoint vs. Non-Self-Adjoint

The physical meaning of the adjoint vector $\mathbf{v}$ depends crucially on the symmetry properties of the matrix $\mathbf{A}$ and the quantity of interest Q.

- **Case 1: Self-Adjoint Systems ($\mathbf{A} = \mathbf{A}^T$)**

  In many physical systems (like linear structural mechanics or pure heat conduction), the matrix $\mathbf{A}$ is symmetric. This symmetry is not a mathematical convenience; it is the discrete representation of a fundamental physical property: *reciprocity*. 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. In Part I [2] it was shown that this symmetric reciprocity is a direct consequence of the principle of complementary energy and its specialization in Castigliano's second theorem.

  In this case, the adjoint equation $\mathbf{A}^T\mathbf{v} = \mathbf{c}$ becomes $\mathbf{A}\mathbf{v} = \mathbf{c}$, with the same boundary conditions. This is a critical point: the adjoint problem is governed by the *exact same physical operator and the same boundary conditions* as the forward problem. The "adjoint load" $\mathbf{c}$ (which can be viewed as a virtual load as opposed to a real load) is applied to the original, physical system. This is why, in this case, the adjoint vector $\mathbf{v}$ has a direct physical interpretation as the system's physical response (e.g., a displacement field) to a virtual load.

- **Case 2: Non-Self-Adjoint Systems ($\mathbf{A} \neq \mathbf{A}^T$)**

  When processes like convection or damping are introduced, the physical reciprocity is broken. The resulting discretized matrix $\mathbf{A}$ is no longer symmetric. The mathematical formalism of the adjoint method (Eqs. (1)-(7)) is, however, still perfectly valid.

  In this case, the adjoint equation $\mathbf{A}^T\mathbf{v} = \mathbf{c}$ still holds, but $\mathbf{A}^T$ is now a *different mathematical operator* from $\mathbf{A}$. The goal of this report is to find the new physical meaning of $\mathbf{v}$ in this non-symmetric context. We will show that $\mathbf{A}^T$ mathematically represents a *reversed* physical system, and $\mathbf{v}$ represents an informational entity in the form of an *influence map* that quantifies *receptivity*. The notion of receptivity generalizes the notion of reciprocity to non-symmetric cases.

3. Adjoint Method for Linear Differential Operators

In their classical book on methods of mathematical physics, Courant and Hilbert advanced the heuristic principle that continuous functional equations (such as differential equations) can be understood as the limit of discrete algebraic systems [3]. This was the motivator for the detailed study of the algebraic system in the previous section. Following this same principle, we observe that the discrete adjoint equation $\mathbf{A}^T\mathbf{v} = \mathbf{c}$ is the algebraic analogue of a continuous adjoint differential equation. It turns out that this continuous formulation, which underpins the "differentiate-then-discretize" paradigm, provides deep physical insight into the nature of the adjoint operator, as we will now demonstrate.

3.1. Formal Adjoint Operator ($\mathcal{L}^*$)

Just as the discrete system in Section 2 is defined by the matrix operator $\mathbf{A}$, a continuous linear physical system is defined by a *linear differential operator*, which we will denote as $\mathcal{L}$. This operator $\mathcal{L}$ is simply the mathematical representation of the governing equation's physics. For instance, in the convection-diffusion problem we will explore in Section 4, the operator is $\mathcal{L} = -k\frac{d^2}{dx^2} + V\frac{d}{dx}$.

In the discrete case, the adjoint operator was easy to find: it was the matrix transpose, $\mathbf{A}^T$. To find the continuous analogue, the *adjoint operator* $\mathcal{L}^*$, we must use a more general definition based on an inner product. For two functions u and v (and a suitable inner product, e.g., $\langle f, g\rangle = \int_a^b f(x)g(x)dx$), we use integration by parts to derive the following fundamental relationship, which is known as *Lagrange's identity* [4]:

$$\langle v, \mathcal{L}u\rangle = \langle \mathcal{L}^*v, u\rangle + \mathcal{B}(u, v) \tag{8}$$

This relationship is also referred to, particularly in the context of boundary value problems, as *extended Green's identity* [5]. Here, $\mathcal{L}^*$ is the formal adjoint operator, and $\mathcal{B}(u, v)$ is known as the "bilinear concomitant" or simply as the "boundary term."

The continuous adjoint problem is constructed by choosing an adjoint function v and a set of adjoint boundary conditions such that the boundary term $\mathcal{B}(u, v)$ vanishes. This simplifies the relationship to $\langle v, \mathcal{L}u \rangle = \langle \mathcal{L}^* v, u \rangle$, which is the continuous analogue of the discrete inner product property $\langle \mathbf{v}, \mathbf{A}\mathbf{u} \rangle = \langle \mathbf{A}^T \mathbf{v}, \mathbf{u} \rangle$.

We can now see the formal definitions:

- **Self-Adjoint Operator:** An operator is formally self-adjoint if $\mathcal{L} = \mathcal{L}^*$. This is the case for pure steady-state diffusion or static elasticity. For such systems, the boundary term $\mathcal{B}(u, v)$ in Eq. (8) vanishes if v satisfies the same boundary conditions as u.
- **Non-Self-Adjoint Operator:** An operator is non-self-adjoint if $\mathcal{L} \neq \mathcal{L}^*$. In this case, the adjoint problem involves a different operator and typically requires boundary conditions that differ from those of the original forward problem (e.g., final conditions instead of initial conditions).

To make this concrete, consider the most general equation involving a linear second-order ordinary differential operator that can be expressed as:

$$\mathcal{L}u(x) = a(x)u''(x) + b(x)u'(x) + c(x)u(x) \tag{9}$$

whose adjoint operator (derived from Lagrange's identity) is:

$$\mathcal{L}^* v(x) = a(x)v''(x) + [2a'(x) - b(x)]v'(x) + [a''(x) - b'(x) + c(x)]v(x) \tag{10}$$

where the prime indicates differentiation with respect to the independent variable x [4, 5].

From this, we can conclude that the operator is self-adjoint ($\mathcal{L} = \mathcal{L}^*$) if and only if its coefficients satisfy $b(x) = a'(x)$. Substituting this condition into Eq. (9) reveals that the most general self-adjoint linear differential operator of the second order is given by:

$$\mathcal{L}u(x) = [a(x)u'(x)]' + c(x)u(x). \tag{11}$$

As we will demonstrate, the operators for convection and damping are non-self-adjoint because they do not satisfy this condition. The physical interpretation of $\mathcal{L}^*$ as a "reversed" physical system will provide the key insight in these cases.

Mathematical Note: The Independence of the Adjoint Operator

Consider the primary (forward) problem governed by the linear equation:

$$\mathcal{L}(u) = f(x) \tag{12}$$

where $\mathcal{L}$ is the differential operator representing the physics, and $f(x)$ is the external forcing function.

It is crucial to observe that the derivation of the adjoint operator $\mathcal{L}^*$ depends *only* on the operator $\mathcal{L}$ and the inner product definition. It is completely independent of the forcing function $f(x)$. This is evident from Lagrange's identity, which defines $\mathcal{L}^*$:

$$\langle v, \mathcal{L}u \rangle = \langle \mathcal{L}^* v, u \rangle + \text{Boundary Terms} \tag{13}$$

This identity must hold for *any* arbitrary test functions u and v. The specific forcing $f(x)$ that drives the physical system does not appear in this definition.

Physical Interpretation: Physically, $\mathcal{L}$ and $\mathcal{L}^*$ describe the *intrinsic properties of the medium* (e.g., conductivity , flow velocity, stiffness), whereas $f(x)$ describes a specific *externalInput*. Just as the transpose of a matrix $\mathbf{A}^T$ is determined solely by the matrix $\mathbf{A}$ and ignores the vector $\mathbf{b}$ in the linear system $\mathbf{Ax} = \mathbf{b}$, the adjoint operator $\mathcal{L}^*$ is a structural property of the physics itself .

While the adjoint *operator* is independent of $f(x)$, the adjoint *solution* $v(x)$ will even-tually require a source term. However, the source for the adjoint equation is derived not from the physical forcing $f(x)$, but from the *sensitivity objective* (the Quantity of Interest) defined by the analyst.

3.2. Continuous Adjoint Sensitivity Formulation

We can now derive the continuous sensitivity formula in the “differentiate-then-discretize” spirit. We start with the continuous governing equation, $\mathcal{L}u = f$, and a quantity of interest Q defined as a functional over the domain Ω:

$$Q(u,p) = \int_\Omega g(u,p)\,d\Omega$$

Our goal is to find the total derivative of Q with respect to a parameter p, denoted $\frac{dQ}{dp}$.

To circumvent the need for the unknown sensitivity $\frac{du}{dp}$, we employ the *Lagrangian method*. We define an augmented functional, $\mathcal{J}$, by adding the governing equation (weighted by an arbitrary function v) to the quantity of interest Q:

$$\mathcal{J}(u,v,p) = Q(u,p) - \langle v, \mathcal{L}u - f\rangle \tag{14}$$

Since the governing equation $\mathcal{L}u - f = 0$ is satisfied by the physical solution u, the term $\langle v, \mathcal{L}u - f\rangle$ is identically zero. Therefore, $\mathcal{J} = Q$, and their total derivatives with respect to p are equal: $\frac{d\mathcal{J}}{dp} = \frac{dQ}{dp}$.

We now differentiate $\mathcal{J}$ in Eq. (14) with respect to p. For the first term (Q), we apply the chain rule inside the integral:

$$\frac{d}{dp}\int_\Omega g(u,p)\,d\Omega = \int_\Omega \frac{\partial g}{\partial p}d\Omega + \int_\Omega \frac{\partial g}{\partial u}\frac{du}{dp}d\Omega$$

Identifying the first integral as the partial derivative $\frac{\partial Q}{\partial p}$ and the second integral as the inner product $\left\langle \frac{\partial g}{\partial u}, \frac{du}{dp}\right\rangle$, we can write the full derivative of the Lagrangian as:

$$\frac{dQ}{dp} = \underbrace{\frac{\partial Q}{\partial p} + \left\langle \frac{\partial g}{\partial u}, \frac{du}{dp}\right\rangle}_{\text{Derivative of } Q} - \underbrace{\left\langle v, \frac{d}{dp}(\mathcal{L}u - f)\right\rangle}_{\text{Derivative of Constraint}} \tag{15}$$

Expanding the total derivative in the constraint term gives:

$$\frac{d}{dp}(\mathcal{L}u - f) = \frac{\partial \mathcal{L}}{\partial p}u + \mathcal{L}\frac{du}{dp} - \frac{\partial f}{\partial p}$$

Substituting this back into the Eq. (15) for $\frac{dQ}{dp}$ and regrouping terms by those that contain the unknown $\frac{du}{dp}$ and those that do not:

$$\frac{dQ}{dp} = \underbrace{\left(\frac{\partial Q}{\partial p} + \left\langle v, \frac{\partial f}{\partial p} - \frac{\partial \mathcal{L}}{\partial p}u \right\rangle\right)}_{\text{Explicit Parameter Dependence}} + \underbrace{\left(\left\langle \frac{\partial g}{\partial u}, \frac{du}{dp} \right\rangle - \left\langle v, \mathcal{L}\frac{du}{dp} \right\rangle\right)}_{\text{Implicit Dependence via } \frac{du}{dp}} \tag{16}$$

The second group of terms that depend on $\frac{du}{dp}$ is the obstacle. To eliminate it, we use the *Lagrange's identity* (Eq. (8)) to move the operator $\mathcal{L}$ from the unknown sensitivity $\frac{du}{dp}$ onto the arbitrary function v:

$$\left\langle v, \mathcal{L}\frac{du}{dp} \right\rangle = \left\langle \mathcal{L}^* v, \frac{du}{dp} \right\rangle + \mathcal{B}\left(\frac{du}{dp}, v\right)$$

Substituting this adjoint relationship into the sensitivity equation (16) allows us to factor out $\frac{du}{dp}$:

$$\text{Implicit Term} = \left\langle \frac{\partial g}{\partial u} - \mathcal{L}^* v, \frac{du}{dp} \right\rangle - \mathcal{B}\left(\frac{du}{dp}, v\right)$$

Now comes the crucial step. Since v is an arbitrary function, we are free to *choose* it specifically to make this entire implicit term vanish. We do this by enforcing two conditions:

1. **The Continuous Adjoint Equation:** We choose v to satisfy $\mathcal{L}^* v = \frac{\partial g}{\partial u}$ in the domain Ω.

2. **The Adjoint Boundary Conditions:** We select boundary conditions for v such that the boundary term $\mathcal{B}(\frac{du}{dp}, v)$ equals zero.

By solving this continuous adjoint equation $\mathcal{L}^* v = \frac{\partial g}{\partial u}$ for v, the dependence on $\frac{du}{dp}$ is eliminated. The total sensitivity is now given by the remaining explicit terms:

$$\frac{dQ}{dp} = \frac{\partial Q}{\partial p} + \left\langle v, \frac{\partial f}{\partial p} - \frac{\partial \mathcal{L}}{\partial p}u \right\rangle \tag{17}$$

This final result is the continuous-field equivalent of the discrete sensitivity formula derived in Section 2 (Eq. (7)). It allows us to compute the sensitivity of Q with respect to *any* number of parameters by solving only two systems of equations: the forward problem for u and the adjoint problem for v.

The continuous adjoint formulation can also be viewed as a "weighted integral" operation. Equation (17) reveals that the total sensitivity of Q is the sum of its direct partial derivative, $\frac{\partial Q}{\partial p}$, and the sensitivity terms, $\frac{\partial f}{\partial p} - \frac{\partial \mathcal{L}}{\partial p}u$, weighted by the adjoint function v in the inner product integral given by:

$$\left\langle v, \frac{\partial f}{\partial p} - \frac{\partial \mathcal{L}}{\partial p}u \right\rangle = \int_{\Omega} v \left(\frac{\partial f}{\partial p} - \frac{\partial \mathcal{L}}{\partial p}u \right) d\Omega$$

In the language of functional analysis, v acts as the *kernel* of this integral operation. This weighting role justifies referring to v as an *influence map*: it assigns a precise numerical importance to each local perturbation in the system's residual (represented by $\frac{\partial f}{\partial p} - \frac{\partial \mathcal{L}}{\partial p}u$), determining how strongly that local change affects the final global quantity of interest.

4. Model Problem 1: Spatial Asymmetry (Convection-Diffusion)

To build intuition for spatial asymmetry, we select a canonical non-self-adjoint problem: steady-state heat transfer in a one-dimensional pipe with both diffusion and convection [6]. This problem clearly demonstrates how a directional physical process breaks reciprocity.

4.1. Forward (Physical) Problem

We consider the temperature $T(x)$ in a one-dimensional fluid flow in a *pipe* of length L, with a constant fluid velocity V_{fluid} flowing from left to right as shown in Fig. 1. The governing equation for this system is a direct expression of the *First Law of Thermodynamics* (Conservation of Energy) applied to a differential control volume at steady state.

This law states that the net rate of energy entering the control volume, plus the rate of energy generated within it, must be zero at steady state. The total energy flux, $j(x)$ (in W/m^2), has two components:

1. **Conduction (j_{cond}):** Heat transfer due to molecular motion, governed by *Fourier's Law of Conduction*: $j_{\text{cond}} = -k\frac{dT}{dx}$. Here, k is the *thermal conductivity*, representing the material's ability to conduct heat.

2. **Convection (j_{conv}):** Heat transfer due to the bulk motion of the fluid carrying its internal energy, $j_{\text{conv}} = (\rho c_p V_{\text{fluid}})T$. Here, ρ is the *fluid density* and c_p is the *specific heat capacity*, representing the amount of energy required to raise the fluid's temperature.

The steady-state energy balance is $\frac{d(j_{\text{total}})}{dx} = f_{\text{vol}}(x)$, where f_{vol} is the volumetric heat source (that is, heat source per unit volume in W/m^3). Substituting the flux terms gives:

$$\frac{d}{dx}\left(-k\frac{dT}{dx} + (\rho c_p V_{\text{fluid}})T\right) = f_{\text{vol}}(x)$$

Assuming constant material properties (k, ρ, c_p) and velocity (V_{fluid}), this expands to:

$$-k\frac{d^2T}{dx^2} + (\rho c_p V_{\text{fluid}})\frac{dT}{dx} = f_{\text{vol}}(x)$$

This equation is commonly written in the more general form of Eq. (18), where $V = \rho c_p V_{\text{fluid}}$ and $f(x)$ represent the lumped parameter coefficients:

$$\underbrace{-k\frac{d^2T}{dx^2}}_{\text{Diffusion (self-adjoint)}} + \underbrace{V\frac{dT}{dx}}_{\text{Convection (non-self-adjoint)}} = \underbrace{f(x)}_{\text{Source}} \tag{18}$$

We can formally verify that the differential operator in this equation is non-self-adjoint using the criteria from Section 3. Comparing Eq. (18) to the general form $\mathcal{L}u = a(x)u'' + b(x)u' + c(x)u$ (Eq. (9)), we identify the coefficients as $a(x) = -k$ (a constant) and $b(x) = V$ (a constant). The condition for self-adjointness is $b(x) = a'(x)$ from Eq. (10). In our case, $a'(x) = \frac{d}{dx}(-k) = 0$. Since $b(x) = V \neq 0$, the condition is not met, confirming that the convection-diffusion operator is non-self-adjoint. We also see that if there is no convection, then $V = 0$ and the linear differential operator of the governing equation will be self-adjoint.

As noted above, the diffusion term arises from Fourier's Law, and the governing differential equation (18) is an expression of the First Law of Thermodynamics (energy conservation) for an open, flowing system with thermal sources. We apply the following boundary conditions:

- $T(0) = T_0$ (fixed temperature at the inlet)
- $\frac{dT}{dx}(L) = 0$ (insulated end at the outlet)

Physically, the boundary condition $\frac{dT}{dx}(L) = 0$ implies that the *conductive* heat flux at the outlet is zero, as per Fourier's Law ($j_{\text{cond}} = -k\frac{dT}{dx}$). This "thermally insulated" condition does not impede the *convective* heat flux, which is the heat carried out of the domain by the bulk fluid motion. This is a common "zero-gradient" outlet assumption, meaning we are modeling a system where heat is assumed to exit only by being carried away with the flow.

Heat from a source at any point x propagates both upstream and downstream via diffusion, but primarily downstream via convection. This directional preference is what breaks the physical reciprocity of the system.

4.2. Continuous Adjoint Operator ($\mathcal{L}^*$)

Let the forward differential operator be $\mathcal{L} = -k\frac{d^2}{dx^2} + V\frac{d}{dx}$. To find its formal adjoint $\mathcal{L}^*$, we employ Lagrange's identity (Eq. (8) in Section 3). We consider the inner product $\langle v, \mathcal{L}u \rangle$

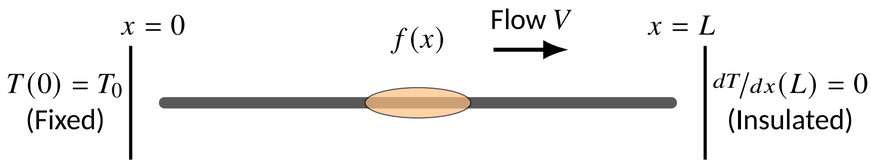

Fig. 1. The forward (physical) problem: one-dimensional convection-diffusion. A heat source $f(x)$ introduces heat into a pipe with forced convective flow V. Heat primarily flows downstream.

and integrate by parts twice for the second-order term, and once for the first-order term.

$$\begin{aligned}\langle v, \mathcal{L}T\rangle &= \int_0^L v\left(-k\frac{d^2T}{dx^2} + V\frac{dT}{dx}\right)dx \\ &= \left[-kv\frac{dT}{dx} + k\frac{dv}{dx}T\right]_0^L + \int_0^L T\left(-k\frac{d^2v}{dx^2}\right)dx \quad \text{(for diffusion term)} \\ &+ [VvT]_0^L - \int_0^L T\left(V\frac{dv}{dx}\right)dx \quad \text{(for convection term)}\end{aligned}$$

Rearranging terms, we identify the adjoint operator $\mathcal{L}^*$ and the boundary term $\mathcal{B}(T, v)$:

$$\mathcal{L}^* = -k\frac{d^2}{dx^2} - V\frac{d}{dx} \tag{19}$$

$$\mathcal{B}(T, v) = \left[kT\frac{dv}{dx} - kv\frac{dT}{dx} + VTv\right]_0^L \tag{20}$$

A key insight that can be gleaned from this equation is that the adjoint operator $\mathcal{L}^*$ is a new operator different from the forward operator $\mathcal{L}$ due to the *reversed convection term* $(-V\frac{d}{dx})$.

To complete the adjoint problem, we must define the adjoint source $c(x)$. This term is derived from the quantity of interest, Q. For this model problem, let us select a quantity of interest that is localized in space, such as the temperature at the outlet:

$$Q = T(L)$$

This objective can be written as an integral over the domain using a Dirac delta function: $Q = \int_0^L T(x)\delta(x-L)dx$. Comparing this to the general form $Q = \int g(u)dx$, we can identify $g(T) = T(x)\delta(x - L)$. The adjoint source $c(x)$, which is $\partial g/\partial T$, is therefore:

$$c(x) = \delta(x - L)$$

The full adjoint problem is thus to solve $\mathcal{L}^*v = \delta(x - L)$. This means the adjoint system is driven by a single, unit "virtual source" applied at the exact location (the outlet) of our

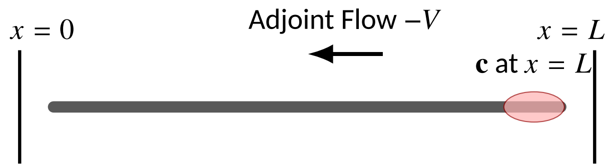

Fig. 2. The adjoint problem for the convection-diffusion model example.

quantity of interest. The equation describes a convection-diffusion problem where the *fluid is flowing backward* (velocity $-V$). This adjoint problem is depicted in Fig. 2.

To determine the appropriate boundary conditions for the adjoint variable $v(x)$, we examine the boundary term $\mathcal{B}(T, v)$ resulting from the integration by parts:

$$\mathcal{B}(T, v) = \left[-kv\frac{dT}{dx} + \left(k\frac{dv}{dx} + Vv\right)T\right]_0^L \tag{21}$$

We must choose adjoint boundary conditions such that this expression vanishes, utilizing the known boundary conditions of the forward problem.

- **At the outlet ($x = L$):** The physical boundary condition is $\frac{dT}{dx}(L) = 0$ (insulated). Substituting this into the expression eliminates the first term at L. To eliminate the remaining term involving the unknown temperature $T(L)$, we require its coefficient to be zero:
$$k\frac{dv}{dx}(L) + Vv(L) = 0 \tag{22}$$
- **At the inlet ($x = 0$):** The physical boundary condition is $T(0) = T_0$ (fixed). In the context of sensitivity analysis, variations in the fixed boundary value are zero. To eliminate the term involving the unknown heat flux $\frac{dT}{dx}(0)$, we require its coefficient to be zero:
$$v(0) = 0 \tag{23}$$

Thus, the mathematically consistent adjoint boundary conditions are a homogeneous Dirichlet condition at the inlet ($x = 0$) and a Robin condition at the outlet ($x = L$).

It is important to note that this new adjoint problem, $\mathcal{L}^* v = c(x)$, does not violate the laws of physics. It is a well-posed convection-diffusion equation that physically describes a system with a reversed fluid velocity ($-V$). Just as the physical flow in the forward problem transports mass downstream, this reversed flow in the adjoint problem can be viewed as transporting *information* upstream from the outlet to the inlet. The presence of the second-order diffusion term ensures that the adjoint system is stable.

Similar to the temporal case we will discuss later, we can reconcile the structure of the adjoint operator by introducing a reversed spatial coordinate, $\xi = L - x$. Since $d/dx = -d/d\xi$, the first derivative term changes sign while the second derivative remains unchanged. Substituting this into the adjoint operator yields:

$$-k\frac{d^2v}{d\xi^2} + V\frac{dv}{d\xi} = c(\xi) \tag{24}$$

In this reversed coordinate system, the effective velocity becomes positive ($+V$). This mathematically confirms that the adjoint problem can be viewed as the forward problem flowing in the reverse direction, from the outlet towards the inlet.

4.3. Discrete Adjoint Operator ($\mathbf{A}^T$)

When the forward problem (Eq. (18)) is discretized using numerical methods, a non-
symmetric matrix $\mathbf{A}$ results. To make this concret e, let us construct $\mathbf{A}$ for a 5-node discretization of the pipe.

Let the nodes be indexed $i = 1 \ldots 5$, with positions $x = 0, L/4, L/2, 3L/4, L$. The mesh width is $h = L/4$.

- The boundary condition at $i = 1$ is $T_1 = T_0$ (known value).
- The unknowns are the temperatures at the other four nodes, $\mathbf{u} = [T_2, T_3, T_4, T_5]^T$.
- We use a central difference for diffusion ($-k\frac{T_{i-1}-2T_i+T_{i+1}}{h^2}$) and a first-order upwind scheme for convection ($V\frac{T_i-T_{i-1}}{h}$), assuming $V > 0$.

The discretized equation for an internal node i is:

$$\left(-\frac{k}{h^2} - \frac{V}{h}\right) T_{i-1} + \left(\frac{2k}{h^2} + \frac{V}{h}\right) T_i + \left(-\frac{k}{h^2}\right) T_{i+1} = f_i \tag{25}$$

For the first unknown node ($i = 2$), the term involving the known boundary $T_1 = T_0$ is moved to the right-hand side. For the outlet node ($i = 5$), we approximate the Neumann condition $dT/dx = 0$ using a "ghost" node, which simplifies to $T_6 = T_4$.

Assembling these equations yields the linear system $\mathbf{Au} = \mathbf{f}'$. Letting $D = k/h^2$ (diffusion stiffness) and $C = V/h$ (convection stiffness), the matrix $\mathbf{A}$ is:

$$\mathbf{A} = \begin{bmatrix} (2D+C) & -D & 0 & 0 \\ -(D+C) & (2D+C) & -D & 0 \\ 0 & -(D+C) & (2D+C) & -D \\ 0 & 0 & -(2D+C) & (2D+C) \end{bmatrix} \tag{26}$$

The vector $\mathbf{f}'$ is the *modified source vector*, which includes the original physical sources f_i plus the boundary contribution $(D + C)T_0$ at node 2:

$$\mathbf{f}' = \begin{bmatrix} f_2 + (D+C)T_0 \\ f_3 \\ f_4 \\ f_5 \end{bmatrix} \tag{27}$$

We immediately observe that $\mathbf{A}$ is non-symmetric. For example, $A_{12} = -D$, while $A_{21} = -(D + C)$. While some local asymmetry arises from boundary discretizations (a numerical vagary: specifically, the diffusion contribution is $-2D$ instead of $-D$ in the last row of $\mathbf{A}$ unless the boundary equation is scaled by $1/2$ to account for the half-cell control volume), the asymmetry due to C is global and physical. It is the direct algebraic consequence of the underlying differential operator $\mathcal{L}$ being non-self-adjoint.

The discrete adjoint problem is defined as $\mathbf{A}^T\mathbf{v} = \mathbf{c}$. The transposed matrix $\mathbf{A}^T$ is:

$$\mathbf{A}^T = \begin{bmatrix} (2D+C) & -(D+C) & 0 & 0 \\ -D & (2D+C) & -(D+C) & 0 \\ 0 & -D & (2D+C) & -(2D+C) \\ 0 & 0 & -D & (2D+C) \end{bmatrix} \tag{28}$$

A keen observer might notice an apparent discrepancy here regarding the sign of the convection term. In the continuous derivation, the adjoint operator reverses the flow velocity ($+V \to -V$). However, in $\mathbf{A}^T$, the coefficient C appears to retain its positive sign.

This contradiction is resolved by examining the stencil geometry. In the forward matrix $\mathbf{A}$, stability requires an *upwind* difference (looking left at $i-1$), creating a lower-diagonal term $-(D+C)$. When transposed, this term moves to the upper diagonal of $\mathbf{A}^T$ (at $i, i+1$). The resulting discrete adjoint operator at a node i becomes:

$$\text{Adjoint}_i \propto Cv_i - Cv_{i+1} = C(v_i - v_{i+1}) \tag{29}$$

We can rewrite this to reveal the continuous limit:

$$\frac{V}{h}(v_i - v_{i+1}) = -V\left(\frac{v_{i+1} - v_i}{h}\right) \approx -V\frac{dv}{dx} \tag{30}$$

Thus, the algebraic transposition naturally produces a *forward difference* scheme. Since the adjoint velocity is negative ($-V$), a forward difference acts as a stable "upwind" scheme for the reverse flow. The negative sign required by the physics is therefore implicitly encoded in the transposition of the grid stencil. This confirms that the "discretize-then-differentiate" approach ($\mathbf{A}^T$) yields a system physically consistent with the continuous "differentiate-then-discretize" approach ($\mathcal{L}^*$).

4.4. Physical Interpretation of $\mathbf{v}$

We now have all the pieces to form a complete physical interpretation of the adjoint solution vector $\mathbf{v}$.

As established in Section 4.2, our quantity of interest is the outlet temperature, $Q = T(L)$. In the discrete system, this corresponds to $Q = T_5$. This defines the gradient vector $\mathbf{c} = \nabla_{\mathbf{u}} Q$ as a standard basis vector:

$$\mathbf{c} = [0, 0, 0, 1]^T \tag{31}$$

The adjoint system $\mathbf{A}^T\mathbf{v} = \mathbf{c}$ solves for the vector $\mathbf{v} = [v_2, v_3, v_4, v_5]^T$.

The solution $\mathbf{v}$ is not a physical temperature field. Instead, it is an *influence map* that quantifies the *receptivity* of the system. We can confirm this interpretation through dimensional analysis. The adjoint vector relates the source term $\mathbf{f}$ (units of Power Density, [W/m^3]) to the quantity of interest Q (units of Temperature, [K]) via the sensitivity relation $\delta Q = \mathbf{v}^T \delta \mathbf{f}$. To satisfy dimensional homogeneity, the unit of $\mathbf{v}$ must be:

$$[\mathbf{v}] = \frac{[Q]}{[\mathbf{f}]} = \frac{\mathrm{K}}{\mathrm{W/m^3}}$$

Physically, the magnitude of an entry v_j represents the rise in outlet temperature (in Kelvins) caused by introducing a unit volumetric heat source (1 W/m^3) at node j.

To illustrate the utility of this map, consider a thought experiment. Suppose we wish to control the outlet temperature Q by placing a small auxiliary heater (a perturbation δf) somewhere in the pipe. We ask: *Where is the most effective location to place this heater?*

- If v_4 (near the outlet) is large, the system is highly *receptive* there; a heater placed at node 4 efficiently changes Q.
- If v_2 (near the inlet) is small—perhaps because diffusion dissipates the heat before it travels downstream—the system has low receptivity there; a heater at node 2 is inefficient.

Therefore, $\mathbf{v}$ maps the "domain of dependence" for the target Q. Consistent with the reversed flow physics of $\mathbf{A}^T$, the adjoint solution originates at the target (the outlet) and propagates upstream against the physical velocity. The boundary condition implies that v decays to zero at the inlet, consistent with the fact that a fixed Dirichlet boundary at the inlet ($T = T_0$) overwrites any perturbations introduced there, rendering them incapable of influencing the outlet.

4.5. Connection to Reciprocity

This model problem allows us to revisit the concept of *reciprocity* (Maxwell's theorem), typically discussed in the context of self-adjoint systems. Through the lens of the adjoint method, we can rigorously define reciprocity as *symmetry in receptivity*.

In the general convection-diffusion case ($V \neq 0$), receptivity is highly directional. As shown in Fig. 2, the outlet is receptive to heat sources at the inlet, but the inlet has little receptivity to sources at the outlet. Consequently, the "influence map" $\mathbf{v}$ is distinct from the physical temperature field $\mathbf{u}$.

However, consider the limiting case where the convective velocity vanishes ($V = 0$). The system becomes a pure diffusion problem, which is physically isotropic and reciprocal. This implies that the *temperature rise at a point x_B due to a unit heat source applied at point x_A is exactly equal to the temperature rise at x_A if that same unit source were applied at x_B*.

Mathematically, this physical symmetry guarantees that the continuous operator is symmetric ($\mathcal{L} = \mathcal{L}^*$) and that the boundary conditions are identical (Dirichlet at the inlet, Neumann at the outlet). Similarly, the discrete matrix becomes symmetric ($\mathbf{A} = \mathbf{A}^T$), provided that the discretization consistently accounts for boundary control volumes (as noted in Section 4.3). This state of *isotropic receptivity* is directly analogous to static elasticity (e.g., trusses), where the stiffness matrix is symmetric and Maxwell's Reciprocal Theorem applies.

In this special self-adjoint scenario, the system' s receptivity structure becomes symmetric, causing the adjoint vect or $\mathbf{v}$ (the influence map) t o become mathema tically identical t o the f orward vect or $\mathbf{u}$ (the ph ysical response). Thus, the "ph ysical int erpret ation" of the adjoint vect or as a physical field — such as a displacement field in structur al mechanics — is essentially a degenerat e case. It occurs only when the syst em's receptivity structur e is perfect ly symmetric, rendering the "backward" adjoint problem indistinguishable from the "forward" physical problem.

5. Model Problem 2: Temporal Asymmetry (Damped Structure)

We now explore a second class of non-self-adjoint syst ems, where the asymmetr y or non-reciprocity is in the *time* domain. The classic example is a damped structur al syst em, which is dissipative (loses energy) over time.

5.1. Forward (Physical) Pɒblem

We consider a linear, time-dependent structur al syst em. The governing equation is a set of second-order ordinary differential equations (ODEs) derived from *Newton's Second Law* $\sum F = ma$), which states that the sum of the external, stiffness, and damping forces equals (the inertial force:

$$M\ddot{\mathbf{u}}(t) + C\dot{\mathbf{u}}(t) + K\mathbf{u}(t) = \mathbf{f}(t) \tag{32}$$

where M, C, and K are the mass, damping, and stiffness matrices, respectively. We assume M and K are symmetric. The problem is defined by a set of initial conditions: $\mathbf{u}(0) = \mathbf{u}_0$ and $\dot{\mathbf{u}}(0) = \dot{\mathbf{u}}_0$.

For our analysis, we will select a simple 1-DOF (Degree of Freedom) mass-spring-damper system: $m\ddot{u} + c\dot{u} + ku = f(t)$. Figure 3 illustrates this simple example. Our quantity of interest Q is the displacement at the final time, T_f:

$$Q = u(T_f) \tag{33}$$

5.2. Continuous Adjoint (Differentiate-then-Discretize)

As established in Section 3, we can derive the continuous adjoint operator, $\mathcal{L}^*$, using Lagrange's identity. The forward operator is $\mathcal{L} = m\frac{d^2}{dt^2} + c\frac{d}{dt} + k$. By applying integration by parts over the time domain $[0, T_f]$, the adjoint operator is found to be:

$$\mathcal{L}^* = m\frac{d^2}{dt^2} - c\frac{d}{dt} + k \tag{34}$$

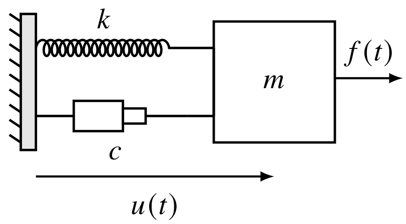

Fig. 3. The forward (physical) problem: a 1-DOF mass-spring-damper system. A time-dependent force $f(t)$ acts on the mass, and its response $u(t)$ evolves forward in time due to inertia, stiffness, and damping.

The continuous adjoint equation $\mathcal{L}^* v = 0$ is:

$$m\ddot{v} - c\dot{v} + kv = 0. \tag{35}$$

To determine the appropriate boundary conditions for the adjoint variable $v(t)$, we examine the boundary terms arising from the integration by parts over the time interval $[0, T_f]$. We require the variation of the Lagrangian (defined in Section 3) with respect to the state variables to vanish.

The boundary terms at the initial time $t = 0$ vanish automatically because the initial conditions $u(0)$ and $\dot{u}(0)$ are fixed (i.e., their variations are zero). At the final time $t = T_f$, the total variation includes terms from the governing equation and the sensitivity of the quantity of interest $Q = u(T_f)$:

$$\delta\mathcal{J}\Big|_{t=T_f} = \delta u(T_f) - [mv\delta\dot{u} - m\dot{v}\delta u + cv\delta u]_{t=T_f}$$

Grouping the terms by the variations $\delta u(T_f)$ and $\delta\dot{u}(T_f)$, we obtain:

$$\delta\mathcal{J}\Big|_{t=T_f} = -\Big(mv(T_f)\Big)\delta\dot{u}(T_f) + \Big(1 + m\dot{v}(T_f) - cv(T_f)\Big)\delta u(T_f)$$

For the Lagrangian to be stationary, the coefficients of these arbitrary variations must independently be zero.

1. The coefficient of $\delta\dot{u}(T_f)$ yields $mv(T_f) = 0$, which implies $v(T_f) = 0$.
2. Substituting this result into the coefficient of $\delta u(T_f)$ yields $1 + m\dot{v}(T_f) = 0$, which implies $m\dot{v}(T_f) = -1$.

This derivation reveals two critical insights:

- *Key Insight 1 (Reversed Operator):* The adjoint operator $\mathcal{L}^*$ is physically different from $\mathcal{L}$. The physical, dissipative damping term $+c\dot{u}$ has become a *negative damping term* ($-c\dot{v}$). This adjoint system is unstable and gains energy, precisely reversing the dissipative nature of the forward problem.

- *Key Insight 2 (Reversed Time)*: The integration by parts also generates boundary terms. To make them vanish, the physical *initial conditions* at $t = 0$ are replaced by *adjoint final conditions* at $t = T_f$. For our quantity of interest $Q = u(T_f)$, the derivation yields the conditions:

$$v(T_f) = 0 \quad \text{and} \quad m\dot{v}(T_f) = -1.$$

  The adjoint problem is thus solved *backward in time*, from $t = T_f$ to $t = 0$.

We can also explain how to deal with the apparent instability of the negative damping term by introducing a reversed time variable, $\tau = T_f - t$. Since $d/dt = -d/d\tau$, the first derivative changes sign while the second derivative remains unchanged. Substituting this into the adjoint equation yields:

$$m\frac{d^2v}{d\tau^2} + c\frac{dv}{d\tau} + kv = 0 \tag{36}$$

In this reversed time coordinate τ, the damping term becomes positive ($+c$). This transforms the problem into a standard, stable Initial Value Problem starting from $\tau = 0$ (which corresponds to the physical final time $t = T_f$). The solution $v(\tau)$ is stable and dissipative in τ, meaning the influence of the final condition decays as we look further back into the past (i.e., as τ increases).

5.3. Discrete Adjoint (Discretize-then-Differentiate)

We now implement the discrete algebraic methodology from Section 2 by discretizing the forward problem *first*. Consider a simple implicit (Backward Euler) time-stepping scheme with time step Δt, where the first and second derivatives are approximated using backward differences to respect causality. Specifically, $\dot{u}_n \approx (u_n - u_{n-1})/\Delta t$ and $\ddot{u}_n \approx (u_n - 2u_{n-1} + u_{n-2})/\Delta t^2$ (a first-order backward approximation at t_n). The discretized governing equation at time t_n is:

$$m\left(\frac{u_n - 2u_{n-1} + u_{n-2}}{\Delta t^2}\right) + c\left(\frac{u_n - u_{n-1}}{\Delta t}\right) + ku_n = f_n$$

Rearranging terms to isolate the unknown u_n, we obtain:

$$\left(\frac{m}{\Delta t^2} + \frac{c}{\Delta t} + k\right)u_n - \left(\frac{2m}{\Delta t^2} + \frac{c}{\Delta t}\right)u_{n-1} + \left(\frac{m}{\Delta t^2}\right)u_{n-2} = f_n$$

This transformation converts the ODE into a monolithic, block-structured algebraic system:

$$\mathbf{AU} = \mathbf{F} \tag{37}$$

where $\mathbf{U} = [u_1, u_2, \ldots, u_N]^T$ is the global vector containing the unknown displacements at all time steps. For an illustrative case with $N = 4$ (incorporating initial conditions u_0, u_{-1}

into the right-hand side), the system matrix $\mathbf{A}$ takes the form:

$$\mathbf{A} = \begin{bmatrix} k_1 & 0 & 0 & 0 \\ k_2 & k_1 & 0 & 0 \\ k_3 & k_2 & k_1 & 0 \\ 0 & k_3 & k_2 & k_1 \end{bmatrix}$$

where k_1, k_2, and k_3 represent the collected coefficients for the terms u_n, u_{n-1}, and u_{n-2}, respectively. This structure reveals several critical properties:

- *Key Insight (Matrix Structure):* The global matrix $\mathbf{A}$ is *banded lower-triangular* (specifically, lower tridiagonal). This is the discrete representation of *causality*: the state at time t_n depends solely on past events ($t \leq t_n$). Crucially, this lower-triangular structure persists even if damping is zero ($c = 0$); the inertial terms (mass) also link the current state strictly to its history. Thus, unlike the spatial problem where setting the flow velocity term $V = 0$ restores symmetry, in the time domain, the discrete system matrix $\mathbf{A}$ remains fundamentally non-symmetric due to the causal nature of time-stepping.
- The discrete adjoint problem is defined as $\mathbf{A}^T\mathbf{V} = \mathbf{C}$. Since the transpose of a lower tridiagonal matrix is an *upper tridiagonal* matrix, the adjoint operator physically inverts the flow of information about receptivity.
- Consequently, solving the upper-triangular system $\mathbf{A}^T\mathbf{V} = \mathbf{C}$ requires *back substitution*. In this block-structured form, the solution algorithm starts with the *last* block of equations (at time T_f) and marches backward to the *first* block (at time $t = 0$). The upper-triangular structure of $\mathbf{A}^T$ is the most striking discrete illustration of why the solution to the adjoint problem must evolve from the final time to the initial time.

This result confirms that the “discretize-then-differentiate” approach (using $\mathbf{A}^T$) perfectly recovers the “backward-in-time” solution property identified by the continuous “differentiate-then-discretize” approach (using $\mathcal{L}^*$).

5.4. Physical Interpretation of $v(t)$

The adjoint solution $v(t)$ (the components of the discrete vector $\mathbf{V}$) is *not a physical displacement*. We can confirm this by a simple unit analysis. The adjoint problem is initiated by the quantity of interest $Q = u(T_f)$, which results in a final condition $m\dot{v}(T_f) = -1$ (dimensionless). This implies that the units of $v(t)$ are [Displacement]/[Impulse] (or $L/(F \cdot T)$). It is therefore a *temporal influence map* that quantifies *receptivity*.

The adjoint’s negative damping term ($-c\dot{v}$) is the mathematical mechanism that governs this map. In the forward time coordinate t, this term appears anti-dissipative (gaining energy), which would violate the Second Law of Thermodynamics for a passive (that is, without any internal energy source in the damper) system. However, this apparent violation is resolved by the backward direction of integration mandated by the Final Value Problem in Section 5.2. When viewed in the reversed time coordinate $\tau = T_f - t$, the system recovers its positive damping ($+c\frac{dv}{d\tau}$) and behaves as a normal dissipative system obeying the laws of thermodynamics.

This mathematical behavior has a precise physical meaning. The fact that the adjoint solution acts as a dissipative system in reverse time means that the "receptivity" decays as one goes backward into the past. Consider the physics of the forward problem: if an impulsive force is applied early in the simulation (near $t = 0$), the system's physical damping mechanisms have a long duration to dissipate the resulting energy, leaving little residual displacement at the final time T_f. Consequently, the system's receptivity to early inputs is low, and the corresponding adjoint value $v(t)$ is small. Conversely, if an impulse is applied just before T_f, the damping has insufficient time to act, and the impulse significantly alters the final state. Thus, the influence map $v(t)$ is maximal near T_f and decays as we look further back into the past.

5.5. Connection to Time-Reversal Symmetry

This model problem allows us to interpret the breakdown of reciprocity in the time domain. In dynamic systems, reciprocity is often linked to *time-reversal symmetry*: the idea that if we run the "movie" of a physical process backward, the governing laws remain unchanged. However, physical processes with increasing entropy (such as those involving friction, viscosity, and heat dissipation) are macroscopically irreversible and therefore do not possess time-reversal symmetry.

Consider the limiting case where damping vanishes ($c = 0$). The system becomes a conservative mass-spring system, and the operator becomes formally self-adjoint ($\mathcal{L} = m\frac{d^2}{dt^2} + k = \mathcal{L}^*$). In this special case, the governing differential equation is invariant under time reversal ($t \to -t$).

However, even in this conservative limit, the full *adjoint system* remains distinct from the forward system due to causality. The forward problem is an *Initial Value Problem* (driven by initial conditions at $t = 0$), while the adjoint is strictly a *Final Value Problem* (driven by the quantity of interest at $t = T_f$). Even though the operators are identical for $c = 0$, the boundary conditions are not. The adjoint system is therefore non-self-adjoint in the sense that it requires a reversal of the temporal integration direction—a constraint imposed not by energy dissipation, but by the causal structure of time.

6. Synthesis: Origins and Interpretation of the Reversed System

Throughout this analysis, we have observed that the adjoint operators for convection and damping manifest as "reversed" physical systems — specifically, flows with reversed velocity ($-V$) or dynamics evolving in reversed time (τ). A fundamental question arises: Is this reversal merely a mathematical artifact of the constant-coefficient assumption, or does it reflect a deeper physical principle?

This distinction can be illuminated by a simple physical analogy. Consider a tracer dye injected into a fluid stream. The *forward problem* asks: "If dye is injected at the inlet, where will it go?" The physical intuition is clear: the dye transports downstream. Conversely, the *adjoint problem* asks the retrospective question: "If dye is detected at the outlet, where did it originate?"

To answer this, one must trace the signal *upstream* against the current. This requires a coordinate reversal: the flow physics must be reversed (the operator), and the tracking must begin at the destination and proceed backward (the boundary condition). Thus, the *Adjoint System* is defined not by the differential equation alone, but by the specific coupling of the adjoint operator with adjoint boundary conditions. We propose that this "reversed system" is not an accident of algebra, but a fundamental necessity arising from the interplay between mathematics and physics.

In the following subsections, we rigorously deconstruct this necessity. We demonstrate that the physical reversal is mandated by the convergence of four distinct factors: the algebraic properties of odd-order derivatives, the analytic requirements of the boundary value problem, the thermodynamic conditions for numerical stability, and finally, the nature of causality itself.

6.1. Mathematical Mechanism: Anti-Self-Adjointness

Consider the general second-order linear operator used in our model problems:

$$\mathcal{L}u(\xi) = a(\mathbf{p})u''(\xi) + b(\mathbf{p})u'(\xi) + c(\mathbf{p})u(\xi)$$

where ξ represents the independent variable (space x or time t). The coefficients are assumed to be independent of ξ. The corresponding adjoint operator is:

$$\mathcal{L}^*v(\xi) = a(\mathbf{p})v''(\xi) - b(\mathbf{p})v'(\xi) + c(\mathbf{p})v(\xi)$$

The mathematical reason for non-self-adjointness lies in the *first derivative term*, $b(\mathbf{p})u'(\xi)$. Self-adjoint operators, such as diffusion (u''), involve even-order derivatives. Integrating by parts twice produces two sign changes ($(-1)^2 = +1$), preserving the sign of the operator.

In contrast, transport phenomena — whether spatial convection (Vd/dx) or temporal evolution (Cd/dt) — are governed by first-order (odd) derivatives. Integration by parts is applied only once, introducing a single sign change ($(-1)^1 = -1$). This sign change transforms the operator into one that is mathematically identical to the forward operator but with a negated coefficient ($b \to -b$). Thus, the "reversed system" arises algebraically because odd-order derivatives, which characterize directional transport, are inherently anti-self-adjoint.

6.2. Analytic Necessity: The Adjoint System and Boundary Conditions

While the differential operator establishes the *potential* for a reversed interpretation, it is the *adjoint boundary conditions* that fully define the *Adjoint System* and mandate the direction of solution. This arises from the requirement to eliminate boundary terms generated by the variation of the Lagrangian.

In a forward problem (an Initial Value Problem, such as the structural dynamic problem illustrated in Section 5), the state $\mathbf{u}$ is anchored at the initial time $t = 0$, but the final state at $t = T_f$ is unknown. Consequently, the variation $\delta\mathbf{u}(T_f)$ is arbitrary. To ensure the boundary term vanishes at T_f, the adjoint variable must satisfy a strict condition, typically $\mathbf{v}(T_f) = 0$ (or a value derived from the gradient of Q).

This condition acts as a mathematical "anchor." Because the only known value for $\mathbf{v}$ is at the final time, the adjoint problem becomes a *FinalValueProblem*(FVP). We are analytically compelled to integrate the system from $t = T_f$ backward to $t = 0$. The "reversed" nature of the solution path is therefore not a choice, but a requirement imposed by the adjoint system's unique boundary constraints.

6.3. Physical Necessity: Thermodynamics and Stability

The most profound insight comes from examining the physical validity of this backward inte- gration. Consider the forward damped operator $(+c\dot{u})$, which describes energy dissipation. If one were to solve this *same* operator backward in time, the system would simulate "neg-ative damping" (spontaneous energy generation). This would constitute a direct violation of the Second Law of Thermodynamics. Mathematically, this physical violation manifests as exponential instability, rendering the mathematical problem ill-posed.

Here, the sign reversal of the adjoint operator ($+c \to -c$) becomes a physical necessity. In the forward time coordinate t, the term $-c\dot{v}$ appears as negative damping. However, when combined with the backward integration direction required by the Final Value Problem, the physics stabilizes. In the reversed time coordinate $\tau = T_f - t$, the term $-c(d/dt)$ becomes $+c(d/d\tau)$. The sign reversal of the operator perfectly cancels the sign reversal of the time coordinate. Thus, the "reversed physical system" is the only mathematically stable mechanism for tracing the path of influence back to its source while obeying the laws of physics.

6.4. Information Flow and Causality

This synthesis reveals that the adjoint system describes the *Information Dual* of the physical system.

- **The Forward System** is *Prospective*: It propagates mass and energy along the arrows of space and time (downstream/future), respecting the Second Law of Thermodynamics (dissipation).
- **The Adjoint System** is *Retrospective*: It propagates receptivity and information against the arrows of space and time (upstream/past).

It is useful here to distinguish between two uses of the term "causality". The first is *logical causality* (or the cause-and-effect principle), which defines the general structure of the forward problem: sources $\mathbf{f}$ produce effects $\mathbf{u}$. The second is *temporal causality*, a specific constraint in dynamic systems which mandates that an effect cannot precede its cause in time. It is this temporal causality that breaks the symmetry of receptivity in dynamical systems, even without damping. While the forward problem respects both, the adjoint problem exhibits a fascinating duality: it respects logical causality (the adjoint source $\mathbf{c}$ drives the adjoint response $\mathbf{v}$) but, to quantify influence correctly, it must reverse the direction of temporal causality.

This distinction allows us to classify engineering analysis into two complementary problems:

1. **The Forward Problem ($\mathbf{Au} = \mathbf{f}$):** A *logical causality problem* (constrained by *temporal causality* in dynamic systems) that calculates the *effects* ($\mathbf{u}$) propagating *forward* from *sources* ($\mathbf{f}$).

2. **The Adjoint Problem ($\mathbf{A}^T\mathbf{v} = \mathbf{c}$):** A distinct system defined by the adjoint operator and adjoint boundary conditions. It is an *importance problem* that calculates the *receptivity* ($\mathbf{v}$) propagating *backward* (against the flow of spatial or temporal causality) from the gradient ($\mathbf{c}$) of the quantity of interest Q.

The adjoint vector $\mathbf{v}$ (equivalently, v) is therefore a general *influence map*. It quantifies the sensitivity of the quantity of interest Q to a local perturbation anywhere in the spatio-temporal domain. Its physical units are not fixed, but depend on the specific quantity of interest.

Finally, this synthesis explains the special nature of some self-adjoint systems (e.g., the Warren truss in [2]). In this particular case, the “forward” flow of causality and the “backward” flow of importance become identical. Here *receptivity becomes symmetric* in the form of reciprocity, and the influence map $\mathbf{v}$ becomes indistinguishable from the physical response $\mathbf{u}$.

7. Summary and Concluding Remarks

This report has extended the physical interpretation of the adjoint method from ideal, simple, self-adjoint linear systems to a more general domain of non-self-adjoint linear systems. We have demonstrated that the loss of *reciprocity* — whether arising from spatial transport, energy dissipation, or the fundamental causal asymmetry of time — is the direct cause of the mathematical loss of *self-adjointness*.

By analyzing two model problems, we have demonstrated that the adjoint operator, whether in its continuous ($\mathcal{L}^*$) or discrete ($\mathbf{A}^T$) form, represents a *reversed* system. As we established, this reversal is physically necessary to maintain stability and thermodynamic consistency. For convection-diffusion, this reversal is in *space*; for dynamic systems, this reversal is in *time*.

Crucially, we have identified the *Adjoint System* as the necessary coupling of this reversed operator with specific *adjoint boundary conditions* (such as Final Value specifications). This distinction clarifies that while the adjoint equation describes a mathematically valid reversed process, the adjoint vector $\mathbf{v}$ (or adjoint function v) is not a physical state of the *forward* world. Rather, it is an *informational* entity: an *influence map* that quantifies *receptivity*. It is the solution to a reversed problem, and its value at any point in space or time quantifies precisely how much a local perturbation at that point will influence the final quantity of interest.

It is certainly possible to avoid the adjoint formulation by solving the forward sensitivity equation (2) for each parameter, though this incurs a high computational cost. However, such a brute-force approach sacrifices the deep physical insight provided by the adjoint formulation, which reveals precisely how information regarding the sensitivity of a quantity of interest flows through the system against the current of causality.

Although the analysis presented herein focused on systems governed by second-order linear differential equations, the conceptual understanding and physical insights derived — specifically the interpretation of the adjoint as a reversed system describing receptivity — extend to the broader class of all non-self-adjoint linear systems [7–9].

Finally, we can connect these results back to the uncertainty quantification methodology established in Part I [2]. The adjoint-based sensitivities derived here serve a critical dual purpose: they are not only gradients for optimization but also the essential weighting factors for error propagation. This confirms that even in non-self-adjoint linear systems, the adjoint performs an important and efficient role in computing the uncertainties.

This interpretive paradigm may extend to more general systems, pointing to several avenues for future work:

- **Nonlinear Systems:** In a nonlinear problem, the adjoint equation is a linear system based on the transpose of the *Jacobian* of the forward operator, evaluated at the forward solution.

- **Nonsquare Systems:** Over- and under-determined systems, which are fundamental to least-squares problems in data assimilation and inverse analysis.

- **Connection to Machine Learning:** This interpretation provides a formal link to modern artificial intelligence. The *backpropagation algorithm*, which is the cornerstone of training deep neural networks, is mathematically identical to the discrete adjoint method applied to a large, nonlinear, non-self-adjoint system.

- **Digital Twins and VVUQ:** In advanced manufacturing contexts, the physical interpretation of adjoints for transport and dissipative processes establishes a rigorous foundation for the Verification, Validation, and Uncertainty Quantification (VVUQ) of predictive digital twins, enabling efficient model calibration and process optimization.

By grounding the abstract mathematics of non-self-adjoint systems in the tangible physics of "reversed flow" and "receptivity," we transform the adjoint method from a mere computational recipe into a transparent analytical instrument. As scientific and engineering models grow in complexity—incorporating directional transport, dissipation, and irreversibility— the ability to trace the flow of information becomes as critical as tracing the flow of mass or energy. In a computational landscape increasingly dominated by automated optimiza- tion and learning algorithms, this deep conceptual clarity ensures that the human analyst remains the ultimate authority on the solution, not merely the operator of the software.

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