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Abstract: Inverse problems in science and engineering aim at estimating model parameters of a physical system using observations of the model's response. Variational least square type approaches are typically adopted, solving the forward model, and then comparing the resulting modeled data with the actual measured data. The data mismatch is minimized and the process is iterated until the best match is achieved. However, data measurements are associated with uncertainties, and deterministic inverse algorithms hardly provide the associated error estimates for the model parameters. In this work, an interval-based iterative solution is presented to predict bounds on such errors, using optimization and the containment-stopping criterion.

Keywords: Inverse, Interval, FEM

1. Introduction

Inverse problems in science and engineering aim at estimating model parameters of a physical system from available observations (data) of his response or output (see Tarantola 1987). A classical example is that of wave tomography in geophysics for a full seismic waveform inversion (see, for example, Fichtner 2010), or the optical tomography for the recognition of cancer in breast tissue via fluorescence (see, for example, Eppstein et al. 2003). In both cases, a forward model is given to predict the (seismic or light) wave propagation through a heterogeneous medium (soil subsurface or human tissue). The forward model is solved only if the (elastic or optical) properties of the medium are known in advance. These, however, are exactly what are not known and what one wants to predict. This leads to a formulation of an inverse problem if measurements of wave amplitudes and phases at given points on the accessible boundaries of medium are available. Using these data, an appropriate 'inverse' algorithm can be formulated to estimate maps of the properties of the medium, from which regions of high/low stiffness can be localized, or malign tissue detected. Variational least square type approaches are typically adopted by making an initial guess (either random or educated) for the unknown variables, solving the forward model, and then comparing the resulting modeled data with the actual measured data. The initial guess is then corrected by minimizing the data mismatch to yield a better match. The process is iterated until the best match is achieved.

A deep look into the mathematics used to model the wave propagation through a medium and the associated physical phenomena, such as scattering and absorption, will reveal an underlying mathematical structure, characterized by Helmholtz wave equations. These, as other partial differential equations encountered in engineering and sciences are typically solved by finite-element methods (FEM) on an unstructured mesh to adequately model the geometry of the medium, and to increase discretization density where appropriate. The inverse algorithm highly depends upon the forward model. If FEM is used the domain is discretized into elements and the number of unknowns depends on the mesh size and on the element type. Typically, the number of unknowns to be estimated exceeds the number of boundary

measurements available and that will result in an ill-posed problem. Ill-posedness is treated by regularization procedures (Tikhonov & Arsenin 1977), by adding appropriate additional constraints that yield well-posed inverse algorithms. Robustness is typically achieved by a course-to-fine regularization that exploits arc-length or surface-area minimizers.

Clearly, data measurements are affected by errors, whose nature depends upon both controllable and uncontrollable factors, such as, for example, the precision of the adopted instrumentation or the environmental conditions during the measurement campaign, respectively. Deterministic inverse algorithms hardly provide error bounds on the parameter estimates given uncertainties in the data. Indeed, this would require a combinatory approach that explores all the possible combinations of data within the given bounds, and this is computationally unfeasible even for small-to-medium scale problems. On the other hand, a probabilistic approach to solve the inverse problem, as in Kalman Filter estimation (Kalman 1960, see also Brown and Hwang 1992), allows identifying the propagation of uncertainties and it also provides errors on the parameter estimates. However, such approaches have their own limitations since they require a prior assumption on the nature of uncertainties, i.e. data errors are usually assumed as Gaussian. It is desirable to have inverse algorithms that do not rely on the type of uncertainties.

This work addresses this issue, by proposing an interval-based iterative solution for inverse problems that not only minimize the overestimation in the target quantities, but also exploits the same overestimation to track propagation of uncertainties of the target estimates. The paper is structured as follows. First, to illustrate the proposed theoretical approach, we present a one-dimensional (1-D) inverse problem that is estimating the Young's modulus of an elastic bar from known measurements of displacements due to traction/compression. The inverse algorithm is then introduced by combining an 'optimize-then-discretize' strategy with interval FEM in order to minimize the mismatch functional between modeled and actual data. Examples are finally presented and discussed.

2. Formulation of inverse problem in elastostatics

2.1. DETERMINISTIC FORMULATION

Consider an elastic bar of length L subject to distributed tensional forces f(x). The differential equation

$$\frac{\mathrm{d}}{\mathrm{d}x} \left(\alpha \frac{\mathrm{d}u}{\mathrm{d}x} \right) + f = 0, \qquad 0 < x < L, \tag{1a}$$

with prescribed boundary conditions

$$u(0) = u_0, \qquad \alpha \frac{\mathrm{d}u}{\mathrm{d}x} = Q_0, \tag{1b}$$

define the 'continuous' forward model that allows to predict the displacements u(x) given the parameter $\alpha(x) = E(x)A(x)$, where E(x) is the Young's Modulus and A(x) is the cross-sectional area, both assumed as spatially varying. When α is unknown, it can be estimated if measurements \tilde{u}_j of u are available at N points $x = x_j$, j = 1, ...N on the bar surface. To solve for α we consider the following functional

$$F(u,\alpha,\tilde{u},w) = \frac{1}{2} \sum_{j=1}^{N} (u(x_j) - \tilde{u}_j)^2 + \int_{0}^{L} w \left[\frac{\mathrm{d}}{\mathrm{d}x} \left(\alpha \frac{\mathrm{d}u}{\mathrm{d}x} \right) + f \right] \mathrm{d}x + \gamma \int_{0}^{L} \left(\frac{\mathrm{d}\alpha}{\mathrm{d}x} \right)^2 \mathrm{d}x, \tag{2}$$

here, the first term in the right-hand side is the square of the mismatch between data and the unknown theoretical displacements u (modelled data) at the locations x_j in accord to the forward model (1). The second term introduces the Lagrange multiplier w(x) to enforce the 'strong' constraint (1), and the third integral is a standard course-to-fine regularization term to control the smoothness/roughness of α , and to guarantee the well-posedness of the inverse problem (γ is the regularization parameter).

To find the optimal α that minimizes (2), we introduce an imaginary time that rules the evolution/convergence of an initial guess for α toward the minimal solution of (2). Thus, u, w and α also depend upon the fictitious t, and we wish to find the rate $\dot{\alpha} = d\alpha/dt$ at which α should change in time so that F always decreases, i.e. $\dot{F} < 0$. The time derivative of F follows after several integrations by parts and some algebra as (see appendix A)

$$\dot{F} = -\int_{0}^{L} \dot{\alpha} \frac{\mathrm{d}u}{\mathrm{d}x} \frac{\mathrm{d}w}{\mathrm{d}x} \mathrm{d}x - 2\gamma \int_{0}^{L} \dot{\alpha} \frac{\mathrm{d}^{2}\alpha}{\mathrm{d}x^{2}} \mathrm{d}x + w(0) \left(\dot{\alpha} \frac{\mathrm{d}u}{\mathrm{d}x} + \alpha \frac{\mathrm{d}\dot{u}}{\mathrm{d}x}\right)\Big|_{x=0} - \dot{u}(L) \left(\alpha \frac{\mathrm{d}w}{\mathrm{d}x}\right)\Big|_{x=L} + \int_{0}^{L} \dot{u} \left[\frac{\mathrm{d}}{\mathrm{d}x} \left(\alpha \frac{\mathrm{d}w}{\mathrm{d}x}\right) + \sum_{j=1}^{N} (u_{j} - \tilde{u}_{j})\delta(x - x_{j})\right] \mathrm{d}x,$$
(3)

where we have set $u_j = u(x_j)$. Since the multiplier w is arbitrary, it can be properly chosen to further simplify (3). Indeed, if we impose the following boundary value problem

$$\frac{\mathrm{d}}{\mathrm{d}x} \left(\alpha \frac{\mathrm{d}w}{\mathrm{d}x} \right) + \sum_{j=1}^{N} (u_j - \tilde{u}_j) \delta(x - x_j) = 0, \qquad 0 < x < L, \tag{4a}$$

with boundary conditions as

$$w(0) = 0, \qquad \alpha \left. \frac{\mathrm{d}w}{\mathrm{d}x} \right|_{x=L} = 0, \tag{4b}$$

then (3) reduces to the minimal form

$$\dot{F} = -\int_{0}^{L} \dot{\alpha} \left(\frac{\mathrm{d}u}{\mathrm{d}x} \frac{\mathrm{d}w}{\mathrm{d}x} + 2\gamma \frac{\mathrm{d}^{2}\alpha}{\mathrm{d}x^{2}} \right) \mathrm{d}x$$
(5)

We are still free to choose the time rate of α so that F is always decreasing. To do so, $\dot{F} < 0$ is always satisfied at any t if we choose

$$\dot{\alpha} = \frac{\mathrm{d}u}{\mathrm{d}x}\frac{\mathrm{d}w}{\mathrm{d}x} + 2\gamma \frac{\mathrm{d}^2 \alpha}{\mathrm{d}x^2} \tag{6}$$

This yields the evolution equation of the unknown parameter α so that at steady state, i.e. $t \to \infty$, *F* is minimized. Observe that (6) depends upon the field *u*, which satisfies (1), and the associated adjoint or multiplier *w*, given by the boundary value problem (4). If we approximate the time derivative of α as

$$\dot{\alpha} \cong \frac{\alpha_{i+1} - \alpha_i}{\Delta t}$$

and follow the FEM-based 'discrete' version of the 'continuous' equations (1-4-6), a deterministic inverse algorithm can be formulated as

$$\begin{cases} K(\alpha_i)u_i = P\\ K(\alpha_i)w_i = (u_i - \widetilde{u})\\ \alpha_{i+1} = \alpha_i + Du_i \circ Dw_i \Delta t + 2\gamma \Delta t D_2 \alpha_i. \end{cases}$$
(7)

here, a_i is the $(m \times 1)$ vector at iteration *i* that lists the individual values of α parameters within each of the *m* elements, u_i is a $(n \times 1)$ vector of the nodal displacements, and $K(a_i)$ is the assembled FEM stiffness matrix, which depends upon a_i . Further, $P(n \times 1)$ is the vector of nodal forces, $\tilde{u}(n \times 1)$ is the data vector of measured displacements interpolated at the nodes, $Du_i(m \times 1)$ and $Dw_i(m \times 1)$ are the vector of element strains, and the vector of first derivative of w_i , respectively. $D_2a_i(m \times 1)$ is an approximation of the second space derivative of $\alpha(x)$. The Hadamard product $a \circ b = (a_i b_i)$ is the element-by-element product. We point out that (7) can also be obtained via a 'discretize-then-optimize' strategy. To do so, one first discretizes the forward model (1) and then optimizes the 'discrete' version of the functional (2) with respect to the vector α .

The free parameter Δt can be chosen to control the smallness of the correction $\|\Delta \alpha\| = \|\alpha_{i+1} - \alpha_i\| \ll \|\alpha_i\|$ during the iterations, where $\|b\|$ is the norm of a vector *b*. Typically, one starts with an initial guess for α , say α_0 , and iterates Eq. (7) until convergence is achieved, viz. when the relative error $\|\Delta \alpha\| / \|\alpha_i\|$ is smaller than a prescribed threshold ε .

In the following, we present an interval formulation of Eq. (7) that will provide bounds on the uncertainties of the estimates for α .

3. Interval FEM Formulation

One of the main features of interval arithmetic is its capability of providing guaranteed results. However, it has the disadvantage of overestimation if variables have multiple occurrences in the same expression. For example, if x is an interval, the function f(x) = x - x is not equal to zero but to an interval that contains zero. Such dependencies lead to meaningless results, and have discouraged some researchers of pursuing further developments of FEM techniques using interval representations.

Only recently, Interval Finite Element Methods (IFEM) have been developed to handle the analysis of systems for uncertain parameters described as intervals. Since the early development of IFEM during the mid-1990s of the last century (Koyluoglu et al., 1995; Muhanna and Mullen, 1995; Nakagiri and Yoshikawa, 1996; Rao and Sawyer, 1995; Rao and Berke, 1997; Rao and Chen 1998) researchers have focused, among other issues, on two major problems: the first is how to obtain solutions with reasonable bounds on the system response that make sense from a practical point of view, or in other words, with the least possible overestimation of their bounding intervals; the second is how to obtain reasonable bounds on the derived quantities that are functions of the system response.

The most successful approaches for overestimation reduction are those that relate the dependency of interval quantities to the physics of the problem being considered (for details see Muhanna and Mullen, 1995; Muhanna and Mullen, 2001; Zhang, 2005). A brief description of IFEM formulation is presented below, but a detailed explanation of the method can be found in Rama Rao et al., 2011. The two major issues resolved by this formulation are:

- 1. Reducing of overestimation in the bounds on the system response due to the coupling and transformation in the conventional FEM formulation as well as due to the nature of used interval linear solvers (Muhanna and Mullen, 2001).
- 2. Obtaining the secondary variables (derived) such as forces, stresses, and strains of the conventional displacement FEM along with the primary variables (displacements) and with the same accuracy of the primary ones.

3.1. DISCRETE STRUCTURAL MODELS

The FEM variational formulation for a static discrete structural model is given by minimizing the total potential energy functional

$$\Pi = \frac{1}{2} U^T K_c U - U^T P, \qquad (8)$$

which yields

$$\frac{\partial \Pi}{\partial U} = K_c U - P = 0 ,$$

where Π , K_c , U, and P are total potential energy, stiffness matrix, displacement vector, and load vector respectively. For structural problems this formulation includes both direct and indirect approaches. For the direct approach, the strain ε is selected as a secondary variable of interest, where a constraint can be introduced as $C_2 U = \varepsilon$. For the indirect approach, constraints are introduced on displacements of the form $C_1U = V$ in such a way that Lagrange multipliers will be equal to the internal forces. C_1 and C_2 are matrices of orders $m \times n$ and $k \times n$, respectively, and m is the number of displacements' constraints, k is the number of strains, and n is the number of displacements' degrees of freedom. We note that V is a constant and ε is a function of U. We amend the right-hand side of Eq. (8) to obtain

$$\Pi^{*} = \frac{1}{2} U^{T} K_{c} U - U^{T} P + \lambda_{1}^{T} (C_{1} U - V) + \lambda_{2}^{T} (C_{2} U - \mathcal{E}),$$
(9)

where λ_1 and λ_2 are vectors of Lagrange multipliers with the dimensions *m* and *k*, respectively. Invoking the stationarity of Π^* , that is $\delta \Pi^* = 0$, we obtain

$$\begin{pmatrix} K_{c} & C_{1}^{T} & C_{2}^{T} & 0\\ C_{1} & 0 & 0 & 0\\ C_{2} & 0 & 0 & -I\\ 0 & 0 & -I & 0 \end{pmatrix} \begin{pmatrix} U\\ \lambda_{1}\\ \lambda_{2}\\ \mathcal{E} \end{pmatrix} = \begin{pmatrix} P\\ V\\ 0\\ 0 \end{pmatrix}$$
(10)

The solution of Eq. (10) will provide the values of dependent variable U and the derived ones λ_1 , λ_2 , and ε at the same time and with the same accuracy. The present interval formulation is an extension of the Element-By-Element (EBE) finite element technique developed by Muhanna and Mullen (2001).

The main sources of overestimation in IFEM are the multiple occurrences of the same interval variable (*dependency problem*), the width of interval quantities, the problem size, and the problem complexity, in addition to the nature of the used interval solver of the interval linear system of equations.

The current formulation is modifying the displacements' constraints used in the previous EBE formulation to yield the element forces as Lagrange Multipliers directly and the system strains. *All interval*

quantities will be introduced in non-italic boldface font. Following the procedures given in Rama Rao et al. (2011) we obtain the interval linear system $\mathbf{KU} = \mathbf{P}$, or explicitly,

$$\begin{pmatrix} \mathbf{K}_{c} & C_{1}^{T} & B^{T} & 0 \\ C_{1} & 0 & 0 & 0 \\ B & 0 & 0 & -I \\ 0 & 0 & -I & 0 \end{pmatrix} \begin{pmatrix} \mathbf{U}_{c} \\ \boldsymbol{\lambda}_{1} \\ \boldsymbol{\lambda}_{2} \\ \boldsymbol{\mathcal{E}} \end{pmatrix} = \begin{pmatrix} \mathbf{P}_{c} \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$
(11)

here, \mathbf{K}_c is a $(k \times k)$ interval matrix, which contains the individual elements' local stiffness and zeros corresponding to the free nodes' degrees of freedom, where k is the sum of number of elements and free nodes.

The accuracy of the system solution depends mainly on the structure of Eq. (11) and on the nature of the used solver. The associated solution provides the enclosures of the values of dependent variables which are the interval displacements U, interval element forces λ_1 , the multiplier λ_2 , and the elements' interval strains. An iterative solver is discussed in the next section.

3.2. INTERVAL SOLVERS AND ITERATIVE ENCLOSURE

Any solver for interval linear system of equations can be used to solve for u_i and w_i in Eq. (7), however, the best known method for obtaining very sharp enclosures of interval linear system of equations that have the structure introduced in Eq. (11) and with large uncertainty is the iterative method developed in the work of Neumaier and Pownuk (2007). The current formulation results in the interval linear system of equations given in (11) which can be transformed to have the general form:

$$(K + B \mathbf{D} A)\mathbf{u} = a + F \mathbf{b} \tag{12}$$

where **D** is diagonal. Furthermore, defining

$$C := (K + BD_0A)^{-1} \tag{13}$$

where D_0 is chosen to ensure invertability (often D_0 is selected as the midpoint of **D**), the solution **u** can be written as:

$$\mathbf{u} = (Ca) + (CF)\mathbf{b} + (CB)\mathbf{d}$$
(14)

To obtain a solution with tight interval enclosure we define two auxiliary interval quantities,

$$\mathbf{v} = A\mathbf{u} \tag{15}$$
$$\mathbf{d} = (D_0 - \mathbf{D})\mathbf{v}$$

which, given an initial estimate for **u**, we iterate as follows:

$$\mathbf{v}^{k+1} = \{ACa\} + (ACF)\mathbf{b} + (ACB)\mathbf{d}^k\} \cap \mathbf{v}^k, \quad \mathbf{d}^{k+1} = \{(D_{c0} - \mathbf{D}_c)\mathbf{v}^{k+1} \cap \mathbf{d}^k$$
(16)

until the enclosures converge, from which the desired solution **u** can be straightforwardly obtained.

Observe that not only are the interval displacements U obtained but also the derived quantities λ_1 , λ_2 , and ε with the same accuracy. The next section will discuss the use of this formulation in the solution of the inverse problem Eq. (2) under interval uncertainties.

4. Interval Inverse Problem

The interval solution of the inverse problem of Eq. (2) is based on the notion that the measurements (data) are given as intervals. In this work we are introducing an initial attempt to provide such a solution using interval finite element. From a closer look at the deterministic solution presented in Eq. (7), it can be seen that the iterative update of the sought parameters is given by: $\alpha_{i+1} = \alpha_i + Du_i \circ Dw_i \Delta t + 2\gamma \Delta t D_2 \alpha_i$, where the terms Du_i and Dw_i are the first derivative of u_i and w_i respectively. A naive interval FEM formulation will result in an enormous overestimation of the solution enclosure and with additional excessive overestimations in derived quantities such as stresses and strains. In our case, the solution is the displacement and the derived quantity is the strain. The IFEM formulation described in the previous section provides an exact solution for the interval loads and the tightest possible enclosure when both load and stiffness being intervals. Moreover, the formulation provides the stresses (λ_1) and strains (ϵ) as part of Eq. (11) solution and of course with the same accuracy as that of the displacements. Furthermore, we speculate that the course-to-fine regularizer can be neglected, viz. set $\gamma_1 = 0$, because one can exploit the natural relaxation induced by intervals, which allows to seek for a 'thick vector' a = EA, a vector with thickened (relaxed) values that can span the range naturally imposed by the uncertainty of the data. This is similar to the Tikhonov regularization that imposes vector solutions with small norm.

In summary, the solution of the inverse problem of Eq. (2) as interval is accomplished by implementing the following steps:

- 1. Solve for \mathbf{u}_i and $D\mathbf{u}_i$ using Eq. (11) as $\mathbf{U}_i = \mathbf{K}^{-1}\mathbf{P}_i$, where the interval vector \mathbf{U}_i contains \mathbf{u}_i and $D\mathbf{u}_i$.
- Solve for Dw_i using Eq. (11) in the form W_i = K_i⁻¹(u_i − ũ), where the interval vector W_i contains w_i and Dw_i. Instead of computing (u_i − ũ) as a conventional interval operation, the subtraction is done on bounds due to inherited dependency of u_i upon ũ, since u_i → ũ when convergence is attained (see Eq. 7). In particular, u_i − ũ = [u_i − ũ, ū_i − ū], where u and ū are the lower and upper bounds of u, respectively.
- 3. Compute the updated interval value of $\boldsymbol{\alpha}_{i+1}$ as

$$\boldsymbol{a}_{i+1} = \boldsymbol{a}_i + D \boldsymbol{u}_i \circ D \boldsymbol{w}_i \varDelta t \tag{17}$$

with $\Delta t = c \times \min(\underline{a}_i / D\mathbf{u}_i \circ D\mathbf{w}_i)$, and $\gamma = 0$. The optimal choice of the constant *c* is problem dependent, and in our case we set c = 0.005.

4. The iterations are stopped when the estimated displacements \mathbf{u}_i contain the data $\mathbf{\tilde{u}}$ (containment-stopping criterion), or in other words when $\mathbf{u}_i \supseteq \mathbf{\tilde{u}}$.

4.1. EXAMPLE

For an illustrative example, we are using a 5 m long bar, pinned at one end and simply supported at the other as shown in Fig. (1). The bar has a constant cross sectional area $A = 0.005 \text{ m}^2$ and is subjected to an axial force of 1000 kN applied at C. The bar is modelled using 25 finite elements each has a different modulus of elasticity. The values: 100, 105,110,115,120, 120, 115, 110, 105, 100, 105,110, 115, 120, 130, 140, 150, 140, 130, 125, 120, 115, 100, and 90 GPa are the assumed moduli of elasticity of elements 1 through 25, respectively.



Figure 1. Truss bar.

The problem to be solved is that to predict the values of elasticity moduli for each element given that the displacements at the 26 nodes are known intervals (measurements with interval uncertainty). As an initial guess for the Young's modulus we set E(x) = 60 GPa.

4.2. DETERMINISTIC SOLUTION

First, the algorithm in Eq. (7) has been tested for the case where the measured data are assumed to be deterministic. The solution converged to the measured data and the moduli were predicted correctly (results are not reported). Hereafter, we will apply the interval-based formulation of the algorithm.



Figure 2. Premature solution of the Interval Inverse Problem. (top) Exact Young's modulus *E* (dash) and upper and lower bounds (solid) of the interval estimate $\mathbf{E} = \boldsymbol{\alpha}/A$, where *A* is the cross-sectional area; (bottom) Given interval data $\tilde{\mathbf{u}}$ (dash) and associated \mathbf{u} displacements. Note that estimates contain data.

4.3. SOLUTION FOR UNCERTAIN MEASUREMENTS

For the uncertain case, a 5% interval uncertainty is considered in the measurements. Fig. 2 shows the obtained interval solution and the associated containment of the measurements, i.e. the estimated \mathbf{u}

displacements contain the measured $\tilde{\mathbf{u}}$ data. However, a pre-mature prediction of the elasticity moduli occurred. This phenomenon is due to the overestimation in the solution (the measurements are contained before the final solution is attained). Work is in progress to improve overestimation reduction of Eq. (17) by simultaneously solving for \mathbf{u} and \mathbf{w} (see Eq. 7) in an interval block-matrix form similar to that of Eq. (11).

A simpler alternative strategy has been adopted to avoid a significant overestimation and to obtain the correct solution. We first proceed with the solution in a deterministic form until the $\Delta \alpha = \alpha_{i+1} - \alpha_i$ update becomes insignificant after several iterations (usually of the order of hundreds). At this stage the update for α is switched to a full interval form using the interval algorithm based on Eq. (17). Fig. 3 shows the resulting mature solution, where both the measurements and the estimated unknown Young's moduli are contained.



Figure. 3. Mature solution of the Interval Inverse Problem. (top) Exact Young's modulus *E* (dash) and upper and lower bounds (solid) of the interval estimate $\mathbf{E} = \mathbf{a}/A$, where *A* is the cross-sectional area; (bottom) Given interval data $\tilde{\mathbf{u}}$ (dash) and associated \mathbf{u} displacements. Note that estimates contain data.

5. Conclusion

An initial formulation for interval inverse problems is introduced. Uncertainty in the measurements is considered in an interval form. The containment stopping criterion is used which is intrinsic for interval arithmetic. Overestimation control and reduction play crucial role in achieving correct solutions. Results show a great potential for further developments.

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Appendix A

In Eq. (2), we set $u_i = u(x_i)$ and integrate by parts once to obtain

$$F(u,\alpha,\tilde{u},w) = \frac{1}{2} \sum_{j=1}^{N} (u_j - \tilde{u}_j)^2 - \int_0^L \alpha \frac{\mathrm{d}u}{\mathrm{d}x} \frac{\mathrm{d}w}{\mathrm{d}x} \mathrm{d}x + w\alpha \frac{\mathrm{d}u}{\mathrm{d}x} \Big|_0^L + \int_0^L wf \mathrm{d}x + \gamma \int_0^L \left(\frac{\mathrm{d}\alpha}{\mathrm{d}x}\right)^2 \mathrm{d}x \tag{A1}$$

Since u, w and α are assumed time dependent, the time derivative of F follows from (A1) as

$$\dot{F} = \sum_{j=1}^{N} (u_j - \tilde{u}_j) \dot{u}_j + \dot{w} \alpha \frac{\mathrm{d}u}{\mathrm{d}x} \Big|_0^L + \left(w \dot{\alpha} \frac{\mathrm{d}u}{\mathrm{d}x} + w \alpha \frac{\mathrm{d}\dot{u}}{\mathrm{d}x} \right) \Big|_0^L - \int_0^L \dot{\alpha} \frac{\mathrm{d}u}{\mathrm{d}x} \frac{\mathrm{d}w}{\mathrm{d}x} \mathrm{d}x - \int_0^L \alpha \frac{\mathrm{d}\dot{u}}{\mathrm{d}x} \frac{\mathrm{d}w}{\mathrm{d}x} \mathrm{d}x - \int_0^L \alpha \frac{\mathrm{d}\dot{u}}{\mathrm{d}x} \frac{\mathrm{d}w}{\mathrm{d}x} \mathrm{d}x + \int_0^L \alpha \frac{\mathrm{d}\dot{u}}{\mathrm{d}x} \frac{\mathrm{d}\dot{w}}{\mathrm{d}x} \mathrm{d}x + \int_0^L \alpha \frac{\mathrm{d}\dot{u}}{\mathrm{d}x} \frac{\mathrm{d}\dot{u}}{\mathrm{d}x} \frac{\mathrm{d}\dot{u}}{\mathrm{d}x} \mathrm{d}x + \int_0^L \alpha \frac{\mathrm{d}\dot{u}}{\mathrm{d}x} + \int_0^L \alpha \frac{\mathrm{d}\dot{u}}{\mathrm{d}x} \mathrm{d}x + \int_0^L \alpha \frac{\mathrm{d}\dot{u}}$$

$$\int_{0}^{L} \dot{w}f \, dx + 2\gamma \int_{0}^{L} \frac{d\alpha}{dx} \frac{d\dot{\alpha}}{dx} dx$$

Here, applying integration by parts once to terms A, B and C yield (for simplicity, we set $\gamma = 0$ at the boundaries)

$$\dot{F} = \sum_{j=1}^{N} (u_j - \tilde{u}_j) \dot{u}_j + w \left(\dot{\alpha} \frac{\mathrm{d}u}{\mathrm{d}x} + \alpha \frac{\mathrm{d}\dot{u}}{\mathrm{d}x} \right) \Big|_0^L - \int_0^L \dot{\alpha} \frac{\mathrm{d}u}{\mathrm{d}x} \frac{\mathrm{d}w}{\mathrm{d}x} \mathrm{d}x - \dot{u}\alpha \frac{\mathrm{d}w}{\mathrm{d}x} \Big|_0^L - 2\gamma \int_0^L \dot{\alpha} \frac{\mathrm{d}^2 \alpha}{\mathrm{d}x^2} \mathrm{d}x$$
(A3)
$$\int_0^L \dot{u} \frac{\mathrm{d}}{\mathrm{d}x} \left(\alpha \frac{\mathrm{d}w}{\mathrm{d}x} \right) \mathrm{d}x + \int_0^L \dot{w} \left[\frac{\mathrm{d}}{\mathrm{d}x} \left(\alpha \frac{\mathrm{d}u}{\mathrm{d}x} \right) + f \right] \mathrm{d}x$$

Note that the underlined term vanishes because of (1a). Further, taking the time derivative of the boundary conditions (1b) for u yields

$$\dot{u}\Big|_{x=0} = 0, \qquad \left(\dot{\alpha}\frac{\mathrm{d}u}{\mathrm{d}x} + \alpha\frac{\mathrm{d}\dot{u}}{\mathrm{d}x}\right)\Big|_{x=L} = 0$$
 (A4)

and (A3) simplifies to

$$\dot{F} = \sum_{j=1}^{N} (u_j - \tilde{u}_j) \dot{u}_j + w(0) \left(\dot{\alpha} \frac{\mathrm{d}u}{\mathrm{d}x} + \alpha \frac{\mathrm{d}\dot{u}}{\mathrm{d}x} \right) \bigg|_{x=0} - \int_0^L \dot{\alpha} \frac{\mathrm{d}u}{\mathrm{d}x} \frac{\mathrm{d}w}{\mathrm{d}x} \mathrm{d}x - \dot{u}(L) \left(\alpha \frac{\mathrm{d}w}{\mathrm{d}x} \right) \bigg|_{x=L} + \int_0^L \dot{u} \frac{\mathrm{d}}{\mathrm{d}x} \left(\alpha \frac{\mathrm{d}w}{\mathrm{d}x} \right) \mathrm{d}x$$
(A5)

$$-2\gamma\int_{0}^{L}\dot{\alpha}\,\frac{\mathrm{d}^{2}\alpha}{\mathrm{d}x^{2}}\,dx.$$

Eq. (3) follows from (A5) after re-writing the mismatch term as

$$\sum_{j=1}^{N} (u_j - \tilde{u}_j) \dot{u}_j = \sum_{j=1}^{N} \int_{0}^{L} (u_j - \tilde{u}_j) \dot{u}(x) \delta(x - x_j) dx$$
(A6)

where $\delta(x - x_j)$ is the Dirac function centered at x_j .