Goal-oriented reduced basis approximation for linear elastodynamic problems

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Abstract

In this paper, we study numerically the linear damped second-order hyperbolic partial differential equation (PDE) with affine parameter dependence using a goal-oriented approach by finite element (FE) and reduced basis (RB) methods. The main contribution of this paper is the “goal-oriented” proper orthogonal decomposition (POD)-Greedy sampling procedure within the RB approximation context. This proposed procedure makes use of the information of the solution of the associated dual (or adjoint) problem and the primal residual similarly to the well-known dual-weighted residual (DWR) technique developed earlier. First, we introduce the RB recipe: Galerkin projection onto a space \( Y_N \) spanned by solutions of the governing PDE at \( N \) selected points in parameter space. This set of \( N \) parameter points is constructed very optimally by the proposed goal-oriented POD–Greedy sampling procedure. Second, based on the affine parameter dependence, we make use of the offline-online computational procedures: in the offline stage, we generate the RB space; in the online stage, given a new parameter value, we calculate rapidly the RB output of interest. We then, in turn, test this new goal-oriented and the standard POD–Greedy sampling procedures on a three-dimensional dental implant model problem. Numerical results show that the new goal-oriented POD–Greedy sampling procedure improves significantly the accuracy of the output computation in comparison with the standard POD–Greedy one; and the method is thus ideally suited for repeated, rapid, reliable evaluation of input-output relationships in the many-query or real-time contexts.

Keywords: second-order hyperbolic partial differential equation; reduced basis method; goal-oriented POD–Greedy algorithm; dual problem; sensitivity problem; dental implant problem

1 Introduction

The design, optimization and control procedures of engineering problems often require several forms of performance measures or outputs — such as displacements, heat fluxes or flowrates [1]. Generally, these outputs are functions of field variables such as displacements, temperature or velocities which are usually governed by a PDE. The parameter or input will frequently define a particular configuration of the model problem. Therefore, the relevant system behavior will be described by an implicit input-output relationship; where its computation requires the solution of the underlying parameter-PDE (or \( \mu \text{PDE} \)). We pursue the RB method [2, 3, 4, 5] which permits the efficient and reliable evaluation of this PDE-induced input-output relationship in many query and real-time contexts.

The RB method was first introduced in the late 1970s for nonlinear analysis of structures and has been further investigated and developed more broadly [6]. Recently, the RB method was well developed for various kinds and classes of parametrized PDEs such as: the eigenvalue problems, the coercive/non-coercive affine/non-affine linear/nonlinear elliptic PDEs, the coercive/non-coercive...
affine/non-affine linear/nonlinear parabolic PDEs, the coercive affine linear hyperbolic PDEs, and several highly nonlinear problems such as Burger’s equation and Boussinesq equation. All of these works, which were proposed and performed by Patera and co-workers, can be found under an abstract list form in the website [6]. (The interested readers are encouraged to visit the site [6] for all related references therein.) For the linear wave equation, the RB method and associated a posteriori error estimation was developed successfully with some levels [7, 8, 9]; however, none of these works have focused on goal-oriented RB approximation or the dual problem of the wave equation.

Adaptive finite element (FE) methods and goal-oriented error estimates for the wave equation have been investigated widely in many applications [9]. Among these methods, the most well-known one is the dual-weighted residual (DWR) method which was proposed by Rannacher and co-workers [10, 11, 12, 13]. In those works, the authors have used the DWR method to quantify the a posteriori error in the output of interest in order to control adaptively the discretized finite element mesh. The final goal is to minimize computational efforts and maximize the accuracy in the output of interest in an adaptive and controllable manner. In particular, the DWR method makes use of an auxiliary dual (or sensitivity) equation to derive an a posteriori error expression for the interest output from the primal residual and the dual solution of that dual equation (and some other given data) [9]. The name “dual-weighted residual” is thus derived from this fact.

In this work, we will apply the essential idea of the DWR method in the RB context, namely, the goal-oriented POD–Greedy sampling procedure. In essence, in the standard POD–Greedy sampling procedure currently used [14, 15, 16, 5], after the POD method is implemented over the time space, the Greedy algorithm is then performed over the parameter space to “pick up” optimally all parameter points such that the error (or error indicator) of the field variable is minimized. On the contrary, in our proposed goal-oriented POD–Greedy algorithm, the Greedy algorithm will pick up the parameter points such that the error (or error indicator) of the output functional is minimized. By this way, we expect to improve significantly the accuracy of the RB output functional computations; but consequently, we might lose the rapid convergent rate of the field variable as in the standard POD–Greedy algorithm. In fact, as we can see later in Section 5 the convergent rate of the field variable by the two algorithms are quite similar; while the convergent rate of the output by the goal-oriented POD–Greedy algorithm is significantly faster than that of the standard POD–Greedy one.

The paper is organized as follows. In Section 2 we derive an error representation by using the space-time approach in general context. The essential idea found here is that we can approximate the error of the interest output by the primal residual of the dual solution in the space-time domain. In Section 3 we introduce the necessary definitions, concepts and notations and then state the problem using a semidiscrete approach: fully discretize in space using Galerkin FEM and discretize in time using Newmark’s trapezoidal rule. The RB approximation and the proposed goal-oriented POD–Greedy sampling algorithm will be presented in Section 4. In Section 5 a three-dimensional dental implant model problem [5] is investigated by using both POD–Greedy algorithms (i.e., standard vs. goal-oriented); numerical results are also demonstrated in this section. Finally, we provide some concluding remarks in Section 6.

## 2 Preliminary

### 2.1 Primal problem

In this paper, we will consider the following strong form of a linear damped second-order hyperbolic PDE system [13]

\[
\rho(x) \frac{\partial^2 u(x, t)}{\partial t^2} + \frac{\partial}{\partial t} \left( \alpha \rho(x) u(x, t) + \beta A u(x, t) \right) + A u(x, t) = f(x, t) \quad \text{for} \quad (x, t) \in \Omega \times I, \tag{1a}
\]

\[
u(x, t) = 0 \quad \text{for} \quad (x, t) \in \partial \Omega_D \times I, \tag{1b}
\]
\[ \partial^A_d u(x, t) = \tilde{t} \quad \text{for} \quad (x, t) \in \partial \Omega_N \times I, \]  
\[ u(x, 0) = u^0_0(x) \quad \text{for} \quad x \in \Omega, \]  
\[ \frac{\partial u(x, 0)}{\partial t} = u^1_0(x) \quad \text{for} \quad x \in \Omega, \]

with a positive density function \( \rho \). Here, \( u(x, t) \) is the field variable which depends on both space and time; \( f(x, t) \) is the source function; \( I = (0, T) \) denotes a finite time interval; \( \Omega \) is a bounded convex domain in \( \mathbb{R}^d \) \( (d \in \{1, 2, 3\}) \). We also denote \( Q_T = \Omega \times I \) as the considered space-time domain. In addition, \( \alpha \) and \( \beta \) are the mass-proportional and stiffness-proportional damping coefficients, respectively. Furthermore, \( \partial \Omega_D \) and \( \partial \Omega_N \) are disjoint, time-independent parts of the boundary where we impose (homogeneous) Dirichlet and (nonhomogeneous) Neumann boundary conditions, respectively. The operator \( \partial^A_d \) is the directional normal derivative associated to the operator \( \mathcal{A} \).

The operator \( \mathcal{A} \) is assumed to be a second-order, elliptic spatial differential operator with sufficiently regular coefficients. In this work, we consider particularly the Lamé-Navier operator

\[ \mathcal{A} \mathbf{v} = -\mu \Delta \mathbf{v} + (\lambda + \mu) \nabla \cdot \mathbf{v}, \]

which governs the linear elastic wave equation. (And thus \( \tilde{t} \) in \( (1c) \) denotes the surface traction acting on the Neumann boundary \( \partial \Omega_N \).)

We first recall the usual spaces: the Hilbert space \( H^1(\Omega)^d \) and the space of square-integrable functions \( L^2(\Omega)^d \) with appropriate inner products and norms. For the initial data, we assume \( u^0_0 \in H^1_0(\Omega)^d \) and \( u^0_1 \in L^2(\Omega)^d \), where \( H^1_0(\Omega)^d \) is the space of all \( H^1 \)-functions vanishing on \( \partial \Omega_D \) with the dual space denoted by \( H^{-1}_0(\Omega)^d \). The function \( f \) is assumed to be in \( L^2(I; H^{-1}_0(\Omega)^d) \).

We then define the necessary space-time spaces (i.e., the trial and test spaces) for the variational formulations which will be presented afterward. From now on, for the sake of clarity we will use the abbreviations \( X = L^2(\Omega)^d \) and \( Y = H^1_0(\Omega)^d \) with the dual space \( Y^* \). Let us define the following trial spaces

\[ Y^0 = \left\{ v \in L^2(I; Y) \mid v \in C(\bar{I}; Y), \frac{\partial v}{\partial t} \in C(\bar{I}; Y), \frac{\partial^2 v}{\partial t^2} \in L^2(I; Y^*) \right\}, \]

\[ Y^1 = \left\{ v \in L^2(I; Y) \mid v \in C(\bar{I}; Y), \frac{\partial v}{\partial t} \in L^2(I; Y^*) \right\}, \]

and the test space

\[ \mathcal{W} = \left\{ v \in L^2(I; Y) \right\}. \]

We approximate the problem \( (1) \) by a “velocity-displacement” formulation \([13, 12]\) which is obtained by introducing a new velocity variable \( u^1 = \frac{\partial u}{\partial t} \) and denote \( u^0 = u \):

\[ \frac{\partial u^0(x, t)}{\partial t} - u^1(x, t) = 0, \]

\[ \rho(x) \frac{\partial u^1(x, t)}{\partial t} + (\alpha \rho(x) u^1(x, t) + \beta \frac{\partial}{\partial t} \mathcal{A} u^0(x, t)) + \mathcal{A} u^0(x, t) = f(x, t), \]

where the boundary and initial conditions are defined as in \( (1b), (1c) \). We note that the solution of the system \( (5) \) is \( \hat{u} = \{ u^0, u^1 \} \in Y^0 \times Y^1 \). Multiplying each equation of \( (5) \) in turn with an appropriate test function \( (\varphi^1 \text{ and } \varphi^0) \), then integrating the two resulting equations over the space-time domain \( Q_T \) and finally adding up these equations, we obtain the following exact primal variational formulation

\[ A(\hat{u}, \varphi) = F(\varphi), \quad \text{for all test functions} \quad \varphi = \{ \varphi^1, \varphi^0 \} \in \mathcal{W} \times \mathcal{W}. \]

In the equation \( (6) \) above, the bilinear and linear functional forms are defined as
\[ A(\hat{u}, \varphi) = \left( \frac{\partial u_0}{\partial t}, \varphi^1 \right)_{Q_T} - (u^1, \varphi^1)_{Q_T} + (u^0(0), \varphi^0(0))_{Q_T} + \left( \rho \frac{\partial u^1}{\partial t}, \varphi^0 \right)_{Q_T} \\
+ (Au^0, \varphi^0)_{Q_T} + \alpha \rho (u^1, \varphi^0)_{Q_T} + \beta \frac{\partial}{\partial t} (Au^0, \varphi^0)_{Q_T} + (u^1(0), \varphi^0(0))_{Q_T}, \] (7)

and

\[ F(\varphi) = (u_0^0, \varphi^1)_{Q_T} + (u_1^1, \varphi_0^0)_{Q_T} + (f, \varphi^0)_{Q_T}, \] (8)

respectively. We point out that the variational form (6) is completely equivalent to the problem (5) [13].

We next introduce our linear output functional which is given in the form

\[ J(\hat{u}) = j^0(u^0) + j^1(u^1), \quad \forall \hat{u} = \{u^0, u^1\}, \quad u^0 \in \mathcal{Y}^0, \quad u^1 \in \mathcal{Y}^1, \] (9)

with certain linear functionals \( j^0 \) and \( j^1 \). For simplicity, we will consider the case \( j^1(\varphi^1) = 0 \). Typical output functionals have the following forms

\[ j^0(\varphi^0) = \int_0^T \int_{\Omega_0} \varphi^0(x, t) \Sigma(x, t) dx \, dt, \] (10a)

\[ j^0(\varphi^0) = \int_0^T \int_{\Gamma_0} \varphi^0(x, t) \Sigma(x, t) dx \, dt, \] (10b)

where \( \Sigma(x, t) \) is an extractor which depends on the view position of an “observer” in the space-time domain \( Q_T; \Omega_0 \) and \( \Gamma_0 \) are some output spatial regions of interest.

All the above statements and equations are for the exact problem (11), now assume that we will solve approximately (11) (or equivalently (12)) by the Galerkin finite element method. Therefore, let \( P_r(I; Y) \) denote the space of all polynomial functions of maximum degree \( r \) on \( I \) with values in \( Y \). We then introduce the following two finite dimensional subspaces, for \( r \in \mathbb{N} \)

\[ S_h^{r,c}(I; Y) = \{ p \in C(\overline{I}; Y)^d \mid p|_I \in P_r(I; Y)^d \}, \] (11)

which will be the space of continuous trial functions, and

\[ S_h^{r-1,d}(I; Y) = \{ p \in L^2(I; Y)^d \mid p|_I \in P_{r-1}(I; Y)^d \}, \] (12)

which will be the space of discontinuous test functions. Here, the superscripts “c” and “d” refer to the continuity or discontinuity of trial and test functions over the whole time interval \( I \), respectively. We will use the abbreviated notation \( \mathcal{Y}_h = S_h^{r,c}(I; Y) \) and \( \mathcal{W}_h = S_h^{r-1,d}(I; Y) \). Clearly, there holds \( \mathcal{Y}_h \subset \mathcal{Y}^0 \) and \( \mathcal{W}_h \subset \mathcal{W} \). Having defined all these finite element spaces, we can now state the FE primal variational formulation of (13) as follows: we look for the solution \( \hat{u}_h = \{u^0_h, u^1_h\} \in \mathcal{Y}_h \times \mathcal{Y}_h \) which satisfies

\[ A(\hat{u}_h, \varphi_h) = F(\varphi_h), \quad \text{for all test functions} \quad \varphi_h = \{\varphi^1_h, \varphi^0_h\} \in \mathcal{W}_h \times \mathcal{W}_h. \] (13)

### 2.2 Dual problem

Consider the exact primal problem (11), the strong form of the associated dual (or sensitivity) problem is derived as follows [13, 12]

\[ \rho(x) \frac{\partial^2 z(x, t)}{\partial t^2} - \frac{\partial}{\partial t} \left( \alpha \rho(x) z(x, t) + \beta \frac{\partial}{\partial t} Az(x, t) \right) + Az(x, t) = j^0 \quad \text{for} \quad (x, t) \in \Omega \times I, \] (14a)
\[ z(x,t) = 0 \quad \text{for} \quad (x,t) \in \partial \Omega_D \times I, \quad (14b) \]
\[ \partial_n z(x,t) = 0 \quad \text{for} \quad (x,t) \in \partial \Omega_N \times I, \quad (14c) \]
\[ z(x,T) = 0 \quad \text{for} \quad x \in \Omega, \quad (14d) \]
\[ -\frac{\partial z(x,T)}{\partial t} = 0 \quad \text{for} \quad x \in \Omega, \quad (14e) \]

where \( z(x,t) \) is the dual solution of the system and (14d), (14e) are now “final” conditions. Note that (14) is the wave equation which evolves backward in time. Thus, if we let \( \tilde{t} = T - t \) then (14) will have the form exactly similar to (1).

Similarly to Section 2.1 above, the strong solution \( \hat{z} = \left\{ \frac{\partial z}{\partial t}, z \right\} \in Y^1 \times Y^0 \) shall satisfy the exact dual variational formulation
\[
A(\psi, \hat{z}) = J(\psi), \quad \text{for all test functions} \quad \psi = \{\psi^0, \psi^1\} \in Y^0 \times Y^1.
\]

Finally, the \( FE \) dual variational formulation is also defined as follows: we look for the solution \( \hat{z}_h = \left\{ \frac{\partial z_h}{\partial t}, z_h \right\} \in Y_h \times Y_h \) that satisfies
\[
A(\psi_h, \hat{z}_h) = J(\psi_h), \quad \text{for all test functions} \quad \psi_h = \{\psi^0_h, \psi^1_h\} \in Y_h \times Y_h.
\]

### 2.3 Error representation

**Proposition 2.1.** Let \( \hat{e} = \hat{u} - \hat{u}_h \) be the error in the solution of the primal form (6), \( R(\varphi) = F(\varphi) - A(\hat{u}, \varphi) \) be the residual of (6); then the error in the interest output \( J(\hat{e}) \) can be evaluated a posteriori as follows:

\[
J(\hat{e}) = R(\hat{z}) \approx R(\hat{z}_h),
\]

where \( \hat{z} \) and \( \hat{z}_h \) are the dual solutions of the dual variational forms (15) and (16), respectively.

**Proof.** From the primal formulation (6), we have:
\[
A(\hat{u} - \hat{u}_h, \varphi) = F(\varphi) - A(\hat{u}_h, \varphi), \quad \forall \varphi \in W \times W.
\]

Or, equivalently:
\[
A(\hat{e}, \varphi) = R(\varphi), \quad \forall \varphi \in W \times W.
\]

Take \( \psi = \hat{e} \) from the dual formulation (15), we have:
\[
A(\hat{e}, \hat{z}) = J(\hat{e}), \quad \text{with} \quad \hat{z} \in Y^1 \times Y^0 (\subset W \times W). \quad (19)
\]

Lastly, take \( \varphi = \hat{z} \) in (18) and then from (19) we obtain \( J(\hat{e}) = R(\hat{z}) \). Since \( \hat{z} \approx \hat{z}_h \), we finally obtain (17).

\[ \square \]

**Remark:**

- From the Galerkin orthogonal property \[11, 13\]: \( A(\hat{e}, \varphi_h) = 0, \quad \forall \varphi_h \in W_h \times W_h, \) we can predict that the terms \( R(\hat{z}) \) and \( R(\hat{z}_h) \) will be quite small or close to 0 since \( R(\hat{z}_h) \approx R(\hat{z}) = A(\hat{e}, \hat{z}), \quad \hat{z} \in W_h \times W_h. \)

- Let \( e^0 = u^0 - u^0_h \) and with the assumption \( j^1(\varphi^1) = 0 \), we can also obtain the \textit{a posteriori} error representation for the output functional of the variable \( u^0 \) as
\[
J(\hat{e}) = j^0(\hat{e}^0) = R(\hat{z}) \approx R(\hat{z}_h) \quad \text{or} \quad j^0(\hat{e}^0) \approx R(\hat{z}_h).
\]
3 Problem statement

The purpose of Section 2 is to derive the error representation (17) by using the space-time approach. The essential idea here is that we can approximate the error of the interest output by the primal residual of the dual solution. We will apply this idea to the FE and RB approximation contexts, namely, the goal-oriented POD–Greedy sampling procedure. From now on, we will solve the system (1) by the FE and RB approximations; and the departure point of our approach shall be the weak formulation of (1). The approach now is to fully discretize in space by Galerkin FEM and discretize in time by the Newmark’s trapezoidal rule. Therefore, all definitions, concepts and notations will be restated appropriately in the remaining sections.

3.1 Abstract statement

We still consider a spatial domain \( Ω \in \mathbb{R}^d \) with Lipschitz continuous boundary \( ∂Ω \). We denote the Dirichlet portion of the boundary by \( Γ^D_i, 1 ≤ i ≤ d \). We then introduce the Hilbert spaces

\[
Y^e = \{ v \equiv (v_1, \ldots, v_d) \in (H^1(Ω))^d \mid v_i = 0 \text{ on } Γ^D_i, i = 1, \ldots, d \},
\]

\[
X^e = (L^2(Ω))^d.
\]

Here, \( H^1(Ω) = \{ v \in L^2(Ω) \mid ∇v \in (L^2(Ω))^d \} \) where \( L^2(Ω) \) is the space of square-integrable functions over \( Ω \). We equip our spaces with inner products and associated norms \((.,.)_{Y^e}, (.,.)_{X^e}\) respectively; a typical choice is

\[
(w, v)_{Y^e} = \int_{Ω} \frac{∂w_i}{∂x_j} \frac{∂v_i}{∂x_j} + w_i v_i,
\]

\[
(w, v)_{X^e} = \int_{Ω} w_i v_i,
\]

where the summation over repeated indices is assumed.

We next define our parameters set \( D \in \mathbb{R}^p \), a typical point in which shall be denoted \( μ \equiv (μ_1, \ldots, μ_p) \). We then define the parametrized bilinear forms \( a \) in \( Y^e, a : Y^e \times Y^e \times D \to \mathbb{R} ; m, c, f, ℓ \) are continuous bilinear and linear forms in \( X^e, m : X^e \times X^e \times D \to \mathbb{R}, c : X^e \times X^e \times D \to \mathbb{R}, f : X^e \times D \to \mathbb{R} \) and \( ℓ : X^e \to \mathbb{R} \).

The exact (primal) linear elasticity problem is stated follows: given a parameter \( μ \in D \subset \mathbb{R}^p \), we evaluate the output of interest

\[
s^e(μ, t) = ℓ(u^e(μ, t)), \quad t \in [0, T],
\]

where the field variable \( u^e(μ, t) \in Y^e \) satisfies the weak form of the \( μ \)-parametrized hyperbolic PDE

\[
m \left( \frac{∂^2 u^e(μ, t)}{∂t^2}, v; μ \right) + c \left( \frac{∂u^e(μ, t)}{∂t}, v; μ \right) + a(u^e(μ, t), v; μ) = g(t)f(v; μ),
\]

\[
∀v \in Y^e, t \in [0, T], \quad (24)
\]

with initial conditions \( u^e(μ, 0) = 0, \frac{∂u^e(μ, 0)}{∂t} = 0 \).

We next introduce a reference finite element approximation space \( Y \subset Y^e(⊂ X^e) \) of dimension \( N \); we further define \( X ≡ X^e \). Note that \( Y \) and \( X \) shall inherit the inner product and norm from \( Y^e \) and \( X^e \), respectively. Our “true” finite element approximation \( u(μ, t) \in Y \) to the “exact” primal problem is stated as
on in Section 5. The assumption is the dental implant problem [5, 17]. We shall provide the details of this model problem is thus linear time-invariant (LTI) [1]. We shall point out that one application which satisfies this assumption is computationally efficient and stable as \( N \to \infty \).

Finally, we also require that all linear and bilinear forms be independent of time – the system will thus be evaluated with respect to \( u(\mu, t) \in Y \). Clearly, our methods must remain stable as \( N \to \infty \).

We shall make the following assumptions. First, we assume that the bilinear forms \( a(\cdot , ; \mu) \) and \( m(\cdot , ; \mu) \) are continuous,

\[
a(w, v; \mu) \leq \gamma \|w\|_Y \|v\|_Y \leq \gamma_0 \|w\|_Y \|v\|_Y, \quad \forall w, v \in Y, \forall \mu \in D, \\
m(w, v; \mu) \leq \rho \|w\|_X \|v\|_X \leq \rho_0 \|w\|_X \|v\|_X, \quad \forall w, v \in Y, \forall \mu \in D,
\]

coercive,

\[
0 \leq \alpha_0 \leq \alpha(\mu) \equiv \inf_{v \in Y} \frac{a(v, v; \mu)}{\|v\|_Y^2}, \quad \forall \mu \in D, \\
0 \leq \sigma_0 \leq \sigma(\mu) \equiv \inf_{v \in Y} \frac{m(v, v; \mu)}{\|v\|_X^2}, \quad \forall \mu \in D;
\]

and symmetric \( a(v, w; \mu) = a(w, v; \mu), \forall w, v \in Y, \forall \mu \in D, \) and \( m(v, w; \mu) = m(w, v; \mu), \forall w, v \in X, \forall \mu \in D, \) (We (plausibly) suppose that \( \gamma_0, \rho_0, \alpha_0 \) and \( \sigma_0 \) may be chosen independent of \( N \) [1]). We also require that the linear forms \( f(\cdot ; \mu) : Y \to \mathbb{R} \) and \( \ell(\cdot) : Y \to \mathbb{R} \) be bounded with respect to \( \| \cdot \|_Y \) and \( \| \cdot \|_X \), respectively.

Second, we shall assume that \( a, m, c \) and \( f \) depend affinely on the parameter \( \mu \) and thus can be expressed as

\[
m(w, v; \mu) = \sum_{q=1}^{Q_m} \Theta_m^{q}(\mu) m^q(w, v), \quad \forall w, v \in Y, \mu \in D, \\
c(w, v; \mu) = \sum_{q=1}^{Q_c} \Theta_c^{q}(\mu) c^q(w, v), \quad \forall w, v \in Y, \mu \in D, \\
a(w, v; \mu) = \sum_{q=1}^{Q_a} \Theta_a^{q}(\mu) a^q(w, v), \quad \forall w, v \in Y, \mu \in D, \\
f(v; \mu) = \sum_{q=1}^{Q_f} \Theta_f^{q}(\mu) f^q(v), \quad \forall v \in Y, \mu \in D;
\]

for some (preferably) small integers \( Q_{m,c,a,f} \). Here, the smooth functions \( \Theta_m^{q}, \Theta_c^{q}, \Theta_a^{q} \) and \( \Theta_f^{q} \) depend on \( \mu \), but the bilinear and linear forms \( m^q, c^q, a^q \) and \( f^q \) do not depend on \( \mu \).

Finally, we also require that all linear and bilinear forms be independent of time – the system is thus linear time-invariant (LTI) [1]. We shall point out that one application which satisfies this assumption is the dental implant problem [5, 17]. We shall provide the details of this model problem in Section 5.
In order to improve the quality of the interest output, we introduce the dual (or adjoint) problem which shall evolve backward in time. The associated FE dual problem is defined as follows \[13, 18\] where \( z(\mu, t) \) is the FE dual solution

\[
m \left( \frac{\partial^2 z(\mu, t)}{\partial t^2}, v; \mu \right) - c \left( \frac{\partial z(\mu, t)}{\partial t}, v; \mu \right) + a (z(\mu, t), v; \mu) = \ell(v),
\]

\( \forall v \in Y, t \in [0, T] \), \( (30) \)

with “final” conditions \( z(\mu, T) = 0, \frac{\partial z(\mu, T)}{\partial t} = 0 \). Let \( \tilde{t} = T - t \), then \( (30) \) will have the form which is exactly similar to \( (25) \)

\[
m \left( \frac{\partial^2 z(\mu, \tilde{t})}{\partial \tilde{t}^2}, v; \mu \right) + c \left( \frac{\partial z(\mu, \tilde{t})}{\partial \tilde{t}}, v; \mu \right) + a (z(\mu, \tilde{t}), v; \mu) = \ell(v),
\]

\( \forall v \in Y, \tilde{t} \in [0, T] \), \( (31) \)

with corresponding “initial” conditions \( z(\mu, \tilde{t} = 0) = 0, \frac{\partial z(\mu, \tilde{t} = 0)}{\partial \tilde{t}} = 0 \).

### 3.2 Time discretization by Newmark’s scheme

We shall use the Newmark’s trapezoidal scheme with coefficients \( \left( \varphi = \frac{1}{2}, \psi = \frac{1}{4} \right) \) \[19\] to approximate the time derivative terms of the “true” statements \( (25) \) and \( (31) \). For time integration: we divide \( [0, T] \) into \( K \) subintervals of equal lengths \( \Delta t = \frac{T}{K} \); and define \( t^k \) \( = k \Delta t, 0 \leq k \leq K \), for the primal problem; and \( \tilde{t}^k = t^K - t^k = (K - k) \Delta t, 0 \leq k \leq K \), for the dual problem, respectively. Our time discretization FE approximation is then given by

\[
m(u(\mu, t^{k+1}), v; \mu) + \frac{1}{2} \Delta t c(u(\mu, t^{k+1}), v; \mu) + \frac{1}{4} \Delta t^2 a(u(\mu, t^{k+1}), v; \mu)
\]

\[
= -m(u(\mu, t^{k-1}), v; \mu) + \frac{1}{2} \Delta t c(u(\mu, t^{k-1}), v; \mu) - \frac{1}{4} \Delta t^2 a(u(\mu, t^{k-1}), v; \mu)
\]

\[
+ 2m(u(\mu, t^k), v; \mu) - \frac{1}{2} \Delta t^2 a(u(\mu, t^k), v; \mu) + \Delta t g^e(t^k) f(v; \mu), \quad \forall v \in Y, 1 \leq k \leq K - 1,
\]

\( (32) \)

with

\[
g^e(t^k) = \frac{1}{4} g(t^{k-1}) + \frac{1}{2} g(t^k) + \frac{1}{4} g(t^{k+1}), \quad 1 \leq k \leq K - 1,
\]

\( (33) \)

and initial conditions: \( u(\mu, t^0) = 0, \frac{\partial u(\mu, t^0)}{\partial t} = 0 \). In order to start the procedure \[32\], \( u(\mu, t^1) \) is computed as on page 491 of \[20\]. The output is then evaluated from

\[
s(\mu, t^k) = \ell(u(\mu, t^k)), \quad 1 \leq k \leq K.
\]

\( (34) \)

For the dual problem, the time discretized version of \( (31) \) is similar to \( (32) \) as
m(z(μ, \hat{t}^{k+1}), v; μ) + \frac{1}{2} \Delta t c(z(μ, \hat{t}^{k+1}), v; μ) + \frac{1}{4} \Delta t^2 a(z(μ, \hat{t}^{k+1}), v; μ) \\
= -m(z(μ, \hat{t}^{k-1}), v; μ) + \frac{1}{2} \Delta t c(z(μ, \hat{t}^{k-1}), v; μ) - \frac{1}{4} \Delta t^2 a(z(μ, \hat{t}^{k-1}), v; μ) \\
+ 2m(z(μ, \hat{t}^k), v; μ) - \frac{1}{2} \Delta t^2 a(z(μ, \hat{t}^k), v; μ) + \Delta t^2 \ell(v), \quad \forall v \in Y, 1 \leq k \leq K - 1, \quad (35)

with “final” conditions: \( z(μ, \hat{t}^0) = 0 \), \( \frac{∂z(μ, \hat{t}^0)}{∂t} = 0 \). We point out here that the treatment of (35) is exactly similar to that of (32), the only difference is the applied force term: dual force \( \ell(v) \) versus primal force \( g(t^k)f(v; μ) \).

3.3 Impulse response

In many dynamical systems, generally, the applied force to excite the system (i.e., \( g(t^k) \) and \( g^{eq}(t^k) \)) in (32) is not known in advance (or a priori) and thus we cannot solve (32) for \( u(μ, t^k) \). In such situations, fortunately, we may appeal to the LTI hypothesis to justify an impulse approach as described now[1]. We note from the Duhamel’s principle that the solution of any LTI system can be written as the convolution of the impulse response with the control input: for any control input \( g_{any}(t^k) \) (and hence \( g_{any}^{eq}(t^k) \), \( 1 \leq k \leq K - 1 \)), we can obtain \( u_{any}(μ, t^k) \), \( 1 \leq k \leq K \) from

\[
u_{any}(μ, t^k) = \sum_{j=1}^{k} u_{unit}(μ, t^{k-j+1})g_{any}^{eq}(t^j), \quad 1 \leq k \leq K,
\]

where \( u_{unit}(μ, t^k) \) is the solution of (32) for a unit impulse control input \( g_{unit}(t^k) = δ_{1k}, 1 \leq k \leq K \) (δ is the Kronecker delta symbol). Therefore, it is sufficient to perform all computations related to FE and RB approximations based on this impulse response[1].

4 Reduced basis approximation

4.1 Approximation

We first introduce the nested sample sets \( S^\text{pr}_{N_{pr}} = \{ μ^\text{pr}_1 \in D, μ^\text{pr}_2 \in D, \ldots, μ^\text{pr}_{N_{pr}} \in D \} \), \( 1 \leq N_{pr} \leq N_{pr,max} \), and \( S^\text{du}_{N_{du}} = \{ μ^\text{du}_1 \in D, μ^\text{du}_2 \in D, \ldots, μ^\text{du}_{N_{du}} \in D \}, 1 \leq N_{du} \leq N_{du,max} \). Here, \( N_{pr} \) and \( N_{du} \) are the dimensions of the RB spaces for the primal and dual variables, respectively; in general, \( S^\text{pr}_{N_{pr}} \neq S^\text{du}_{N_{du}} \) and in fact \( N_{pr} \neq N_{du} \). We then define the associated nested Lagrangian RB spaces

\[
Y^\text{pr}_{N_{pr}} = \text{span} \{ ϵ^\text{pr}_n, 1 \leq n \leq N_{pr,max} \}, \quad 1 \leq N_{pr} \leq N_{pr,max}, \quad (37a)
\]

\[
Y^\text{du}_{N_{du}} = \text{span} \{ ϵ^\text{du}_n, 1 \leq n \leq N_{du,max} \}, \quad 1 \leq N_{du} \leq N_{du,max}, \quad (37b)
\]

where \( ϵ^\text{pr}_n \in Y^\text{pr}_{N_{pr}}, 1 \leq n \leq N_{pr,max} \) (\( ϵ^\text{du}_n \in Y^\text{du}_{N_{du}}, 1 \leq n \leq N_{du,max} \)) are mutually \( (\cdot, \cdot)_Y \) – orthonormal RB basis functions. We note that \( Y^\text{pr}_{N_{pr}} \) shall be constructed by our proposed goal-oriented POD–Greedy sampling procedure, while \( Y^\text{du}_{N_{du}} \) shall be constructed by the standard POD–Greedy sampling one[5][14].

Our reduced basis approximation \( u_N(μ, t) \) to \( u(μ, t) \) is then obtained by a standard Galerkin projection: given \( μ \in D \), we now look for \( u_N(μ, t) \in Y^\text{pr}_{N_{pr}} \) satisfies
\[
m\left( \frac{\partial^2 u_N(\mu, t)}{\partial t^2}, v; \mu \right) + c \left( \frac{\partial u_N(\mu, t)}{\partial t}, v; \mu \right) + a(u_N(\mu, t), v; \mu) = g(t)f(v; \mu),
\]
\[
\forall v \in Y_{N, pr}^{pr}, t \in [0, T],
\]
with initial conditions \( u_N(\mu, 0) = 0, \ \frac{\partial u_N(\mu, 0)}{\partial t} = 0 \). For the dual problem, similarly, we also obtain the RB approximation \( z_N(\mu, \tilde{t}) \in Y_{N, du}^{du} \) to \( z(\mu, \tilde{t}) \) as the solution of
\[
m\left( \frac{\partial^2 z_N(\mu, \tilde{t})}{\partial t^2}, v; \mu \right) + c \left( \frac{\partial z_N(\mu, \tilde{t})}{\partial t}, v; \mu \right) + a(z_N(\mu, \tilde{t}), v; \mu) = \ell(v),
\]
\[
\forall v \in Y_{N, du}^{du}, \tilde{t} \in [0, T],
\]
with “final” conditions \( z_N(\mu, \tilde{t} = 0) = 0, \ \frac{\partial z_N(\mu, \tilde{t} = 0)}{\partial t} = 0 \). Finally, we evaluate the interest output, \( s_N(\mu, t) \), from
\[
s_N(\mu, t) = \ell(u(\mu, t)), \quad t \in [0, T].
\]
In a completely similar manner, the discrete primal RB approximation \( u_N(\mu, t^k) \) to \( u(\mu, t^k) \) is then obtained by a standard Galerkin projection: given \( \mu \in D \), \( u_N(\mu, t^k) \in Y_{N, pr}^{pr} \) will satisfy
\[
m(u_N(\mu, t^{k+1}), v; \mu) + \frac{1}{2} \Delta t c(u_N(\mu, t^{k+1}), v; \mu) + \frac{1}{4} \Delta t^2 a(u_N(\mu, t^{k+1}), v; \mu)
\]
\[
= -m(u_N(\mu, t^{k-1}), v; \mu) + \frac{1}{2} \Delta t c(u_N(\mu, t^{k-1}), v; \mu) - \frac{1}{4} \Delta t^2 a(u_N(\mu, t^{k-1}), v; \mu)
\]
\[
+ 2m(u_N(\mu, t^k), v; \mu) - \frac{1}{2} \Delta t^2 a(u_N(\mu, t^k), v; \mu) + \Delta t^2 g^{eq}(t^k)f(v; \mu),
\]
\[
\forall v \in Y_{N, pr}^{pr}, 1 \leq k \leq K - 1,
\]
where the zero initial conditions are defined and treated as mentioned in Section 3.2. For the discrete dual RB equation, we also obtain the RB approximation \( z_N(\mu, \tilde{t}^k) \in Y_{N, du}^{du} \) to \( z(\mu, \tilde{t}^k) \) as the solution of
\[
m(z_N(\mu, \tilde{t}^{k+1}), v; \mu) + \frac{1}{2} \Delta t c(z_N(\mu, \tilde{t}^{k+1}), v; \mu) + \frac{1}{4} \Delta t^2 a(z_N(\mu, \tilde{t}^{k+1}), v; \mu)
\]
\[
= -m(z_N(\mu, \tilde{t}^{k-1}), v; \mu) + \frac{1}{2} \Delta t c(z_N(\mu, \tilde{t}^{k-1}), v; \mu) - \frac{1}{4} \Delta t^2 a(z_N(\mu, \tilde{t}^{k-1}), v; \mu)
\]
\[
+ 2m(z_N(\mu, \tilde{t}^k), v; \mu) - \frac{1}{2} \Delta t^2 a(z_N(\mu, \tilde{t}^k), v; \mu) + \Delta t^2 \ell(v),
\]
\[
\forall v \in Y_{N, du}^{du}, 1 \leq k \leq K - 1,
\]
with zero “final” conditions as above. Finally, we evaluate the output estimate, \( s_N(\mu, t^k) \), from
\[
s_N(\mu, t^k) = \ell(u_N(\mu, t^k)), \quad 1 \leq k \leq K.
\]
\[ R(z_N(\mu, t_k); \mu, t_k) = \Delta t \sum_{k'=1}^{k} R^p(z_N(\mu, t_{k+1-k'}); \mu, t_k), \quad 1 \leq k \leq K. \] (44)

Note that the terms \( R^p(v; \mu, t_k) \) and \( R^{du}(v; \mu, t_k) \) are the primal and dual residuals associated with the RB equations (41) and (42), respectively.

\[
\begin{align*}
R^p(v; \mu, t_k) &= g^q(t_k) f(v; \mu) \\
&- \frac{1}{\Delta t^2} \left( m(u_N(\mu, t_{k+1}), v; \mu) - 2m(u_N(\mu, t_k), v; \mu) + m(u_N(\mu, t_{k-1}), v; \mu) \right) \\
&- \frac{1}{\Delta t} \left( \frac{1}{2} c(u_N(\mu, t_{k+1}), v; \mu) - \frac{1}{2} c(u_N(\mu, t_{k-1}), v; \mu) \right) \\
&- \left( \frac{1}{4} a(u_N(\mu, t_{k+1}), v; \mu) + \frac{1}{2} a(u_N(\mu, t_k), v; \mu) + \frac{1}{4} a(u_N(\mu, t_{k-1}), v; \mu) \right), \quad (45a)
\end{align*}
\[
\begin{align*}
R^{du}(v; \mu, t_k) &= \ell(v) \\
&- \frac{1}{\Delta t^2} \left( m(z_N(\mu, t_{k+1}), v; \mu) - 2m(z_N(\mu, t_k), v; \mu) + m(z_N(\mu, t_{k-1}), v; \mu) \right) \\
&- \frac{1}{\Delta t} \left( \frac{1}{2} c(z_N(\mu, t_{k+1}), v; \mu) - \frac{1}{2} c(z_N(\mu, t_{k-1}), v; \mu) \right) \\
&- \left( \frac{1}{4} a(z_N(\mu, t_{k+1}), v; \mu) + \frac{1}{2} a(z_N(\mu, t_k), v; \mu) + \frac{1}{4} a(z_N(\mu, t_{k-1}), v; \mu) \right), \quad (45b)
\end{align*}
\]

\( \forall v \in Y, 1 \leq k \leq K \). Note that here \( N \equiv (N_{pr}, N_{du}) \).

### 4.2 Goal-oriented POD–Greedy sampling procedure

#### 4.2.1 The proper orthogonal decomposition

We aim to generate an optimal (in the mean square error sense) basis set \( \{ \xi_m \}_{m=1}^M \) from any given set of \( M_{\text{max}} \geq M \) snapshots \( \{ \xi_k \}_{k=1}^{M_{\text{max}}} \). To do this, let \( V_M = \text{span} \{ v_1, \ldots, v_M \} \subset \text{span} \{ \xi_1, \ldots, \xi_{M_{\text{max}}} \} \) be an arbitrary space of dimension \( M \). We assume that the space \( V_M \) is orthonormal such that \( (v_n, v_m) = \delta_{nm}, 1 \leq n, m \leq M \) (\( (\cdot, \cdot) \) denotes an appropriate inner product and \( \delta_{nm} \) is the Kronecker delta symbol). The POD space, \( W_M = \text{span} \{ \xi_1, \ldots, \xi_M \} \) is defined as

\[ W_M = \arg \min_{V_M \subset \text{span} \{ \xi_1, \ldots, \xi_{M_{\text{max}}} \}} \left( \frac{1}{M_{\text{max}}} \sum_{k=1}^{M_{\text{max}}} \inf_{\alpha^k \in \mathcal{R}^M} \left\| \xi_k - \sum_{m=1}^{M} \alpha_{m}^{k} v_m \right\|^2 \right). \] (46)

In essence, the POD space \( W_M \) which is extracted from the given set of snapshots \( \{ \xi_k \}_{k=1}^{M_{\text{max}}} \) is the space that best approximate this given set of snapshots and can be written as \( W_M = \text{POD} \left( \{ \xi_1, \ldots, \xi_{M_{\text{max}}} \}, M \right) \). We can construct this POD space by using the method of snapshots which is presented concisely in the Appendix of [21].

#### 4.2.2 Goal-oriented POD–Greedy algorithm

We now discuss the POD–Greedy algorithms [3, 5] to construct the nested sets \( S_N^{pr} \) and \( Y_N^{pr} \) of interest. Let \( \Xi_{\text{train}} \) be a finite set of the parameters in \( D (\Xi_{\text{train}} \subset D) \); and \( S_N^{pr} \) denote the set of greedily selected parameters in \( \Xi_{\text{train}} \). Initialize \( S_N^{pr} = \{ \mu_{0}^{pr} \} \), where \( \mu_{0}^{pr} \) is an arbitrarily chosen
parameter. Let \(e_{\text{proj}}(\mu, t^k) = u(\mu, t^k) - \text{proj}_{ Y^{\text{pr}}_{N_{pr}}}(u(\mu, t^k))\), where \(\text{proj}_{ Y^{\text{pr}}_{N_{pr}}}(u(\mu, t^k))\) is the \(Y^{\text{pr}}_{N_{pr}}\)-orthogonal projection of \(u(\mu, t^k)\) into the \(Y^{\text{pr}}_{N_{pr}}\) space.

The standard POD–Greedy and our proposed goal-oriented POD–Greedy algorithms are presented simultaneously in Table 1.

| Set \(Y^{\text{pr}}_{N_{pr}} = 0\) | Set \(Y^{\text{pr}}_{N_{pr}} = 0\) |
| Set \(\mu^{\text{pr}}_* = \mu^{\text{pr}}_0\) | Set \(\mu^{\text{pr}}_* = \mu^{\text{pr}}_0\) |
| While \(N_{pr} \leq N_{pr,\text{max}}\) | While \(N_{pr} \leq N_{pr,\text{max}}\) |
| \(\mathcal{V} = \{e_{\text{proj}}(\mu^{\text{pr}}_*, t^k), 0 \leq k \leq K\};\) | \(\mathcal{V} = \{e_{\text{proj}}(\mu^{\text{pr}}_*, t^k), 0 \leq k \leq K\};\) |
| \(Y^{\text{pr}}_{N_{pr}+M} \leftarrow Y^{\text{pr}}_{N_{pr}} \bigoplus \text{POD}(\mathcal{V}, M);\) | \(Y^{\text{pr}}_{N_{pr}+M} \leftarrow Y^{\text{pr}}_{N_{pr}} \bigoplus \text{POD}(\mathcal{V}, M);\) |
| \(N_{pr} \leftarrow N_{pr} + M;\) | \(N_{pr} \leftarrow N_{pr} + M;\) |
| \(\mu^{\text{pr}}_* = \arg \max_{\mu \in \Xi_{\text{train}}} \{\square(\mu)\};\) | \(\mu^{\text{pr}}_* = \arg \max_{\mu \in \Xi_{\text{train}}} \{\bigcirc(\mu)\};\) |
| \(S^{\text{pr}}_{N_{pr}} \leftarrow S^{\text{pr}}_{N_{pr}} \bigcup \{\mu^{\text{pr}}_*\};\) | \(S^{\text{pr}}_{N_{pr}} \leftarrow S^{\text{pr}}_{N_{pr}} \bigcup \{\mu^{\text{pr}}_*\};\) |
| end. | end. |

\[\square(\mu) = \frac{\sqrt{\sum_{k=1}^{K} \| R^{\text{pr}}(v; \mu, t^k) \|^2}}{\sqrt{\sum_{k=1}^{K} \| u_N(\mu, t^k) \|^2}}\]

\[\bigcirc(\mu) = \frac{\sqrt{\sum_{k=1}^{K} \| R^2(z_N(\mu, \tilde{t}^k); \mu, t^k) \|^2}}{\sqrt{\sum_{k=1}^{K} s_N^2(\mu, t^k)}}\]

Table 1: (Left) Standard POD–Greedy sampling algorithm and (Right) our proposed goal-oriented POD–Greedy sampling algorithm.

There are several main points that we will discuss here:

- First, regarding the term \(\square(\mu)\): in essence, this term is the ratio of the dual norm of the primal residual to the RB solution. Thus, this term was considered as an error indicator for the error in the field variable; and has been used widely in the current standard POD–Greedy algorithm [14, 15, 16, 5].

- Second, regarding the auxiliary term \(R(z_N(\mu, \tilde{t}^k); \mu, t^k)\) in [14]: in essence, this term is actually the primal residual of the dual solution (similar to \(R(\tilde{\mu})\) or \(R(\tilde{\eta})\) in (17)) as derived in Section 2.3. Apply (17) to our current RB context, the FE statements (in Section 2) now play the role of the exact statements (in Section 2); while the RB statements (in Section 3) now play the role of the FE statements (in Section 2), respectively. From then, we can conclude that this auxiliary term is a kind of error indicator (or an error surrogate, although not accurate) for the true output error (i.e., \(s(\mu, t^k) - s_N(\mu, t^k)\)). (Of course (17) is derived in the space-time space and our approach here is semidiscrete in space-time, however, the ideas are equivalent.)

- Third, in the work [1], the authors did improve the output computation by adding this auxiliary term to the output (i.e., adding (14) to the right-hand side of (13)). However, the effect of this term on the output is very small (or nearly 0) because of the Galerkin orthogonal property mentioned in the remark of Section 2.3. Therefore, we emphasize here that we only compute this auxiliary term for the estimation of \(\bigcirc(\mu)\) in the goal-oriented POD–Greedy algorithm (offline stage). We will not add this term to the output as in [1] to save significant cost in the online computations.
• Fourth, regarding the POD–Greedy algorithms: as observed from Table [1] the main difference between these two algorithms is that we somehow try to minimize the error indicator of the output functional (the term $\bigcirc(\mu)$ in the goal-oriented POD–Greedy) rather than minimize an error indicator of the field variable (the term $\Box(\mu)$ in the standard POD–Greedy) through Greedy iterations. By this way, we expect to improve the accuracy (or convergent rate) of the RB output computation; but consequently, we might lose the rapid convergent rate of the field variable as in the standard POD–Greedy algorithm. In fact, however, as we can see later in Section 5 the convergent rate of the field variable by the two algorithms are quite similar; while the convergent rate of the output by the goal-oriented POD–Greedy algorithm is significantly faster than that of the standard POD–Greedy one.

• Fifth, in order to implement the goal-oriented POD–Greedy algorithm, we need to compute the auxiliary term $\mathcal{R}(z_N(\mu^k, t^k); \mu, t^k)$ which requires the dual solution $z_N(\mu, t^k)$ as defined in (44). Therefore, we proposed using the standard POD–Greedy algorithm to approximate the RB dual equation (42) to obtain the RB dual solution $z_N(\mu, t^k)$. In short, the standard POD–Greedy algorithm will be implemented for the RB dual equation first, and then the goal-oriented POD–Greedy algorithm will be performed for the RB primal equation subsequently.

• Lastly, the most important point of this work is that we found that the behavior of the auxiliary term $\mathcal{R}(z_N(\mu^k, t^k); \mu, t^k)$ with respect to the RB space dimension $N_{pr}$ is very similar to the behavior of the true error term $s(\mu, t^k) - s_N(\mu, t^k)$ with respect to $N_{pr}$. Therefore, in fact, the term $\bigcirc(\mu)$ will guide the Greedy procedure to select parameter points such that it minimizes the true output error. We will clearly see this point in Section 5 later.

4.3 Error evaluation

There are two kinds of error evaluation in our work: the first kind is to evaluate the quality of RB approximation with respect to the benchmark FE approximation; and the second kind serves as choosing the “worst” parameter point within the Greedy iterations as in Table [1]. We will mention in details these kinds of errors in the following.

4.3.1 RB error

In order to evaluate the efficiency of the two POD–Greedy algorithms presented as well as the quality of RB approximations, the RB errors will be used in this work. The RB error for the solution $u_N(\mu, t^k)$ and output $s_N(\mu, t^k)$ are defined as

\[ e_u(\mu, t^k) = u(\mu, t^k) - u_N(\mu, t^k), \quad \text{and} \quad e_s(\mu, t^k) = s(\mu, t^k) - s_N(\mu, t^k), \quad 1 \leq k \leq K, \quad (47) \]

where $u(\mu, t^k)$, $s(\mu, t^k)$ and $u_N(\mu, t^k)$, $s_N(\mu, t^k)$, $1 \leq k \leq K$ are the solution and output by FE and RB approximations, respectively. The relative RB error of solution and relative RB error of output are also defined as:

\[ \varepsilon_u(\mu) = \sqrt{\frac{\sum_{k=1}^{K} ||e_u(\mu, t^k)||_Y^2}{\sum_{k=1}^{K} ||u_N(\mu, t^k)||_Y^2}} \quad \text{and} \quad \varepsilon_s(\mu) = \sqrt{\frac{\sum_{k=1}^{K} e_s^2(\mu, t^k)}{\sum_{k=1}^{K} s_N^2(\mu, t^k)}}, \quad 1 \leq k \leq K, \quad (48) \]

respectively.

4.3.2 Error indicator

Consider the POD–Greedy algorithms in Table [1] the terms $\Box(\mu)$ and $\bigcirc(\mu)$ are the error indicators serve as selecting the right parameter points within algorithms’ iterations. Alternatively, we can use
the RB error \( \varphi \) as the error indicators rather than \( \square(\mu) \) or \( \bigcirc(\mu) \). However, in that situation, the computational time, computational effort and required storage will be huge because we need to solve and store all the FEM solutions of all \( \mu \in \Xi_{\text{train}} \); hence, the use of RB error is not feasible. Another choice for the error indicator (and also for the error evaluation) is the rigorous \( a \text{ posteriori} \) error bounds \([1, 15, 5]\). Tan derived the \( a \text{ posteriori} \) error bound for linear hyperbolic PDEs \([7]\); however, this bound is for the Newmark’s scheme \( \left( \varphi = \frac{1}{2}, \psi = \frac{1}{2} \right) \) and is thus not applicable for our work.

Recently, Huynh et al. \([8]\) used the Laplace transform technique to derive a new \( a \text{ posteriori} \) error bound for linear hyperbolic PDEs. The technique improves the situation but also introduces much additional complication.

As analyzed above, we need to have another error indicator since both the error bound and RB error are not available for our particular problem. Therefore, in order to implement the POD–Greedy strategies we use either \( \square(\mu) \) or \( \bigcirc(\mu) \) as error surrogates. These error indicators are actually not rigorous because they do not include stability information, i.e., some temporal terms as present in the full error bound of \([7]\). However, there are three advantages in using these terms. Firstly, they are nearly the only remaining choice; secondly, they can evaluate relatively the accuracy of the RB solution/output errors for various choices of \( \mu \); and thirdly – most important, their calculation are very convenient: fast and efficient offline-online decomposition for many \( \mu \) computations as required in the Greedy strategies. Furthermore, the operation counts to compute these terms only depend on \( N_{\text{pr}} \) (the RB space dimension) and thus are totally independent from \( N \) – the underlying FE space dimension.

### 4.4 Offline-online computational procedure

In this section, we develop offline-online computational procedures in order to fully exploit the dimension reduction of the problem \([1, 15, 5]\). We first express \( u_N(\mu, t^k) \) and \( z_N(\mu, t^k) \) as

\[
\begin{align*}
    u_N(\mu, t^k) &= \sum_{n=1}^{N_{\text{pr}}} u_{N,n}(\mu, t^k) \zeta_{n,\text{pr}}, \\
    z_N(\mu, t^k) &= \sum_{n=1}^{N_{\text{du}}} z_{N,n}(\mu, t^k) \zeta_{n,\text{du}},
\end{align*}
\]

respectively.

We then choose a test function \( v = \zeta_{n,\text{pr}}^c, 1 \leq n \leq N_{\text{pr}} \), for the RB primal equation \([41]\) and \( v = \zeta_{n,\text{du}}^c, 1 \leq n \leq N_{\text{du}} \), for the dual problem \([42]\). It then follows from \([41]\) that \( u_N(\mu, t^k) = [u_N(\mu, t^k) \quad u_{N,2}(\mu, t^k) \ldots u_{N,N}(\mu, t^k)]^T \in \mathbb{R}^{N_{\text{pr}}} \) satisfies

\[
\begin{align*}
    \left( M_N^p(\mu) + \frac{1}{2} \Delta t C_N^p(\mu) + \frac{1}{4} \Delta t^2 A_N^p(\mu) \right) u_N(\mu, t^{k+1}) &= \left( -M_N^p(\mu) + \frac{1}{2} \Delta t C_N^p(\mu) - \frac{1}{4} \Delta t^2 A_N^p(\mu) \right) u_N(\mu, t^{k-1}) \\
    &+ \left( 2M_N^p(\mu) - \frac{1}{2} \Delta t^2 A_N^p(\mu) \right) u_N(\mu, t^k) + \Delta t^2 g^\mu(t^k) F_N^p(\mu), \quad 1 \leq k \leq K - 1.
\end{align*}
\]

The initial condition is treated similar to that in \([32]\) of Section \([3.2]\). Here, \( C_N^p(\mu), A_N^p(\mu), M_N^p(\mu) \in \mathbb{R}^{N_{\text{pr}} \times N_{\text{pr}}} \) are symmetric positive definite matrices with entries \( C_N^p_{i,j}(\mu) = c(\zeta_i^c, \zeta_j^c; \mu), \)

\footnote{In this work, note that we use the Newmark’s trapezoidal scheme \( \left( \varphi = \frac{1}{2}, \psi = \frac{1}{4} \right) \) as described in Section \([3.2]\).}
\( A_{N,i,j}^{pr}(\mu) = a(c_i^{pr}, c_j^{pr}; \mu), M_{N,i,j}^{pr}(\mu) = m(c_i^{pr}, c_j^{pr}; \mu), 1 \leq i, j \leq N_{pr} \) and \( F_N^{pr} \in \mathbb{R}^{N_{pr}} \) is the RB load vector with entries \( F_{N,i}^{pr} = f(c_i^{pr}; \mu), 1 \leq i \leq N_{pr} \), respectively.

The RB output is then computed from

\[
s_N(\mu, t^k) = L_N^T u_N(\mu, t^k), \quad 1 \leq k \leq K.
\]

Invoking the affine parameter dependence (29), we obtain

\[
M_{N,i,j}^{pr}(\mu) = m(c_i^{pr}, c_j^{pr}; \mu) = \sum_{q=1}^{Q_m} \Theta_m^q(\mu) m^q(c_i^{pr}, c_j^{pr}),
\]

\[
C_{N,i,j}^{pr}(\mu) = c(c_i^{pr}, c_j^{pr}; \mu) = \sum_{q=1}^{Q_c} \Theta_c^q(\mu) c^q(c_i^{pr}, c_j^{pr}),
\]

\[
A_{N,i,j}^{pr}(\mu) = a(c_i^{pr}, c_j^{pr}; \mu) = \sum_{q=1}^{Q_a} \Theta_a^q(\mu) a^q(c_i^{pr}, c_j^{pr}),
\]

\[
F_{N,i}^{pr}(\mu) = f(c_i^{pr}; \mu) = \sum_{q=1}^{Q_f} \Theta_f^q(\mu) f^q(c_i^{pr}),
\]

which can be written as

\[
M_N^{pr} = \sum_{q=1}^{Q_m} \Theta_m^q(\mu) M_N^{pr,q}, \quad C_N^{pr} = \sum_{q=1}^{Q_c} \Theta_c^q(\mu) C_N^{pr,q},
\]

\[
A_N^{pr} = \sum_{q=1}^{Q_a} \Theta_a^q(\mu) A_N^{pr,q}, \quad F_N^{pr} = \sum_{q=1}^{Q_f} \Theta_f^q(\mu) F_N^{pr,q},
\]

where the parameter independent quantities \( M_N^{pr,q}, C_N^{pr,q}, A_N^{pr,q}, F_N^{pr,q} \in \mathbb{R}^{N_{pr} \times N_{pr}} \) are given by

\[
M_N^{pr,q} = m^q(c_i^{pr}, c_j^{pr}), \quad 1 \leq i, j \leq N_{pr,\text{max}}, \quad 1 \leq q \leq Q_m,
\]

\[
C_N^{pr,q} = c^q(c_i^{pr}, c_j^{pr}), \quad 1 \leq i, j \leq N_{pr,\text{max}}, \quad 1 \leq q \leq Q_c,
\]

\[
A_N^{pr,q} = a^q(c_i^{pr}, c_j^{pr}), \quad 1 \leq i, j \leq N_{pr,\text{max}}, \quad 1 \leq q \leq Q_a,
\]

\[
F_N^{pr,q} = f^q(c_i^{pr}), \quad 1 \leq i \leq N_{pr,\text{max}}, \quad 1 \leq q \leq Q_f,
\]

respectively.

A similar computational procedure for the dual problem (42) and the auxiliary term in (44) can also be developed. The details of those calculations are summarized in Appendix A.

The offline-online decomposition is now clear. In the offline stage – performed only once, we first implement the standard POD–Greedy algorithm: we solve for the \( c_{\text{ed}}^{n}, 1 \leq n \leq N_{\text{du,\text{max}}} \); then compute and store the \( \mu \)-independent quantities in (60) for the estimation of the RB dual solution. Once the RB dual solution is available, we now implement the goal-oriented POD–Greedy algorithm. Consider each goal-oriented POD–Greedy iteration in more details. We first need to solve (41) for the ‘true’ FE solutions; then do the error projection and solve for the POD/eigenvalue problem as in the right column of Table 1. In addition, we have to compute \( O(N_{pr,\text{max}}^2(Q_m + Q_c + Q_a)) \) \( N \)-inner products \((\cdot, \cdot)_V \) in (55); and \( O(N_{\text{du,\text{max}}}, N_{pr,\text{max}}(Q_m + Q_c + Q_a)) \) \( N \)-inner products \((\cdot, \cdot)_V \) in (45) for the estimation of the auxiliary terms. Since there are totally \( \frac{N_{pr,\text{max}}}{M} \) POD–Greedy iterations, the
above calculations are thus multiplied by \( \frac{N_{pr, max}}{M} \) times. In summary, for the offline stage, the operation counts depend on \( N \) and hence, its computational cost is very expensive.

In the online stage – performed many times, for each new parameter \( \mu \) – we first assemble the RB primal matrices in (53), this requires \( O \left( N_{pr}^2 (Q_m + Q_c + Q_a) \right) \) operations. We then solve the RB primal equation (54), the operation counts are \( O \left( N_{pr}^3 + K N_{pr}^2 \right) \) as the RB matrices are generally full. Finally, we evaluate the output displacement \( s_N(\mu, t^k) \) from (52) at the cost of \( O(K N_{pr}) \). Therefore, as required in real-time context, the online complexity is independent of \( N \), and since \( N_{pr} \ll N \) we can expect significant computational saving in the online stage relative to the classical FE approach.

5 Numerical example

In this section, we will verify both POD–Greedy algorithms by investigating an numerical example which is a three-dimensional dental implant model problem in the time domain. This model problem is similar to that in the work of Hoang et al. [5]. The details are described in the following.

5.1 A 3D dental implant model problem

![Figure 1: (a) The 3d simplified FEM model with sectional view, and (b) meshing in ABAQUS.](image-url)

We consider a simplified 3D dental implant-bone model in Fig.1(a). The geometry of the simplified dental implant-bone model is constructed by using SolidWorks 2010. The physical domain \( \Omega \) consists of five regions: the outermost cortical bone \( \Omega_1 \), the cancellous bone \( \Omega_2 \), the interfacial tissue \( \Omega_3 \), the dental implant \( \Omega_4 \) and the stainless steel screw \( \Omega_5 \). The 3D simplified model is then meshed and analyzed in the software ABAQUS/CAE version 6.10-1 (Fig.1(b)). A dynamic force opposite to the \( x \)-direction is then applied to a prescribed area on the body of the screw as shown in Fig.2(a). As mentioned in Section 3.3, all computations and simulations will be performed for the unit input loading case, since other input loading cases can be easily inferred from the Duhamel’s convolution. We show on Fig.2(b) the time history of an arbitrary loading case which we will show its Duhamel’s convolution later. The output of interest is defined as the average displacement responses of a prescribed area on the head of the screw (Fig.2(a)). The Dirichlet boundary condition (\( \partial \Omega^D \)) is specified in the bottom-half of the simplified model as illustrated in Fig.2(a). The finite element mesh consists of 9479 nodes and 50388 four-node tetrahedral solid elements. The coinciding nodes of the contact surfaces between
Figure 2: (a) Output area, applied load $F$ and boundary condition, and (b) time history of a particular load.

different regions (the regions $\Omega_1, \Omega_2, \Omega_3, \Omega_4, \Omega_5$) are assumed to be rigidly fixed, i.e. the displacements in the $x-$, $y-$ and $z-$directions are all set to be the same for the same coinciding nodes.

We assume that the regions $\Omega_i, 1 \leq i \leq 5,$ of the simplified model are homogeneous and isotropic.

The material properties: the Young’s moduli, Poisson’s ratios and densities of these regions are presented in Table 2 [22]. As similar to [5], we still use Rayleigh damping with stiffness-proportional damping coefficient $\beta_i, 1 \leq i \leq 5$ (Table 1) such that $C_i = \beta_i A_i$, $1 \leq i \leq 5$, where $C_i$ and $A_i$ are the FEM damping and stiffness matrices of each region, respectively. We also note in Table 2 that $(E, \beta)$ – the Young’s modulus and Rayleigh damping coefficient associated with the interfacial tissue are our sole parameters.

| Domain | Layers          | $E$ (Pa)          | $\nu$    | $\rho$ (g/mm$^3$) | $\beta$          |
|--------|-----------------|-------------------|----------|-------------------|-------------------|
| $\Omega_1$ | Cortical bone  | $2.3162 \times 10^{10}$ | 0.371    | $1.8601 \times 10^{-3}$ | $3.38 \times 10^{-6}$ |
| $\Omega_2$ | Cancellous bone | $8.2345 \times 10^8$  | 0.3136   | $7.195 \times 10^{-4}$  | $6.76 \times 10^{-6}$  |
| $\Omega_3$ | Tissue         | $E$                | 0.3155   | $1.055 \times 10^{-3}$  | $\beta$           |
| $\Omega_4$ | Titan implant  | $1.05 \times 10^{11}$ | 0.32     | $4.52 \times 10^{-3}$  | $5.1791 \times 10^{-10}$ |
| $\Omega_5$ | Stainless steel screw | $1.93 \times 10^{11}$ | 0.305    | $8.027 \times 10^{-3}$ | $2.5685 \times 10^{-8}$ |

Table 2: Material properties of the dental implant-bone structure.

Finally, with respect to our particular dental implant problem, the actual integral forms of the linear and bilinear forms are defined as:

$$m(w,v) = \sum_{r=1}^{5} \int_{\Omega_r} \rho_r w_i v_i,$$  \hfill (56a)

$$a(w,v;\mu) = \sum_{r=1, r \neq 3}^{5} \int_{\Omega_r} \frac{\partial v_i}{\partial x_j} C_{ijkl}^r \frac{\partial w_k}{\partial x_l} + \mu_1 \int_{\Omega_3} \frac{\partial v_i}{\partial x_j} C_{ijkl}^3 \frac{\partial w_k}{\partial x_l},$$  \hfill (56b)

$$c(w,v;\mu) = \sum_{r=1, r \neq 3}^{5} \beta_r \int_{\Omega_r} \frac{\partial v_i}{\partial x_j} C_{ijkl}^r \frac{\partial w_k}{\partial x_l} + \mu_2 \mu_1 \int_{\Omega_3} \frac{\partial v_i}{\partial x_j} C_{ijkl}^3 \frac{\partial w_k}{\partial x_l},$$  \hfill (56c)
for all \( w, v \in Y, \mu \in D \). Here, the parameter \( \mu = (\mu_1, \mu_2) \equiv (E, \beta) \) belongs to the region \( \Omega_3 \). \( C_{ijkl}^r \) is the constitutive elasticity tensor for isotropic materials and it is expressed in terms of the Young’s modulus \( E \) and Poisson’s ratio \( \nu \) of each region \( \Omega_r, 1 \leq r \leq 5 \), respectively. \( \Gamma^N_1 \) is the prescribed loading area (surface traction) and \( \Gamma_o \) is the prescribed output area as shown in Fig. 2(a), respectively.

5.2 Numerical results

![Comparison of the “unit” FEM output displacements computed by our code versus by ABAQUS software with respect time in the x− (a), y− (b), and z− direction (c) with \( \mu_{\text{test}} = (10 \times 10^6 \text{Pa}, 1 \times 10^{-5}) \).](image)

The FE space to approximate the 3d dental implant-bone problem is of dimension \( \mathcal{N} = 26343 \). For time integration, \( T = 1 \times 10^{-3} \text{s}, \Delta t = 2 \times 10^{-6} \text{s}, K = \frac{T}{\Delta t} = 500 \). The input parameter \( \mu \equiv (E, \beta) \in D \), where the parameter domain \( D \equiv [1 \times 10^6, 25 \times 10^6] \text{Pa} \times [5 \times 10^{-6}, 5 \times 10^{-5}] \subset \mathbb{R}^{P=2} \). (Note that this parameter domain is nearly two times larger than that of [5].) The \( \| \cdot \|_Y \) norm used
Figure 4: Comparison of “arbitrary” FEM output displacements (with the applied load in Fig 2(b)) computed by Duhamel’s convolution and direct computation with respect time in the $x$– (a), $y$– (b), and $z$–direction (c) with $\mu_{\text{test}} = (10 \times 10^6 \text{Pa}, 1 \times 10^{-5})$.

Figure 5: The $\Xi_{\text{train}}$ samples set.
in this work is defined as \( \|u\|_2^2 = a(w; w; \bar{\mu}) + m(w; w; \bar{\mu}) \), where \( \bar{\mu} = (13 \times 10^6 \text{Pa}, 2.75 \times 10^{-5}) \) is the arithmetic average of \( \mu \) in \( \mathcal{D} \); \( Q_a = 2, Q_x = 2 \). To verify our computational code (performed in Matlab R2012b), we first compare the FEM outputs computed by ABAQUS and by our code with the test parameter \( \mu_{\text{test}} = (10 \times 10^6 \text{Pa}, 1 \times 10^{-5}) \). Fig. 2 shows the “unit” output displacements (i.e., under the unit loading case) in the \( x \), \( y \), and \( z \) directions versus time at \( \mu_{\text{test}} \) via ABAQUS and our code, respectively. Fig. 3 demonstrates that the FEM results by our code match very well with the results computed by ABAQUS. Next, we show in Fig. 4 the FEM output displacements versus time under the loading history in Fig. 2(b) by direct computation and by Duhamel’s convolution. It is observed that these two results match perfectly well with each other.

We now discuss the POD–Greedy algorithms of interest. As shown in Fig. 5, a sample set \( \Xi_{\text{train}} \) is created by a uniform distribution over \( [\bar{\mu} \pm \delta] \). Again, we show the sample set \( \Xi_{\text{train}} \) illustrated in Fig. 8 (i.e., the plots of the set \( \Xi_{\text{train}} \)). By implementing the goal-oriented POD–Greedy algorithm, we obtain the similar results as shown on Fig. 10.

Finally, regarding computational time, all computations were performed on a desktop Intel(R) Core(TM) i7-3930K CPU @3.20GHz 3.20GHz, RAM 32GB, 64-bit Operating System. The computation time for the RB solver \( t_{\text{RB(online)}} \), the CPU-time for the FEM solver by our code \( t_{\text{FEM}} \) and the total computational time is approximately 2 weeks (including all FEM solutions/outputs and RB errors of the primal and dual problems) on this computer.
the CPU-time saving factor \( \kappa = t_{\text{FEM}} / t_{\text{RB(online)}} \) are listed on Table 3 respectively. We see that the RB solver is approximately 1000 times faster than the FEM solver; and thus it is clear that the RB is very efficient and reliable for solving time-dependent dynamic problems.

Table 3: Comparison of the CPU-time for a FEM and RB analysis.

| \( N \) | \( t_{\text{RB(online)}} \) (sec) | \( t_{\text{FEM}} \) (sec) | \( \kappa = t_{\text{FEM}} / t_{\text{RB(online)}} \) |
|---|---|---|---|
| 10 | 0.0172 | 29 | 1686 |
| 20 | 0.0187 | 29 | 1550 |
| 30 | 0.0202 | 29 | 1435 |
| 40 | 0.0222 | 29 | 1306 |
| 50 | 0.0271 | 29 | 1070 |
| 60 | 0.0295 | 29 | 983 |
| 70 | 0.0348 | 29 | 833 |

Figure 6: (a) Distribution of sampling points by the standard POD–Greedy algorithm, and (b) the maximum relative RB error of the solution and the output as functions of \( N_{\text{pr}} \) (primal problem).

6 Conclusion

A new goal-oriented POD–Greedy sampling algorithm was proposed. The proposed algorithm makes use of the primal residual of the dual solution rather than the dual norm of primal residual as error indicator in the standard POD–Greedy algorithm. It is demonstrated that this type of error indicator will guide the Greedy iterations to select the parameter points to optimize the true output error. The proposed algorithm is then verified by investigating a 3D dental implant problem in the time domain. In comparison with the standard algorithm, we conclude that our proposed algorithm performs better – in terms of output’s accuracy, and quite similar – in terms of solution’s accuracy. The proposed algorithm is applicable to any (regular) output functional and is thus very suitable within the goal-oriented RB approximation context.
Figure 7: (a) Distribution of sampling points by the standard POD–Greedy algorithm, and (b) the maximum relative RB error of the solution as a function of $N_{du}$ (dual problem).

Figure 8: (a) Distribution of sampling points by the goal-oriented POD–Greedy algorithm, and (b) the maximum relative RB error of the solution and the output as functions of $N_{pr}$.

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Figure 9: Comparison of maximum relative RB errors by standard and goal-oriented POD–Greedy algorithms: (a) solution and (b) output.

Figure 10: Comparison of the auxiliary term $R_{a}^{\text{max}}$ and the true output error $e_{s,a}^{\text{max}}$ over $\Xi_{\text{train}}$.

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A Computation of the auxiliary term

In order to compute the auxiliary term (44), we need to calculate the dual solution \( \bar{z}_N(\mu, \tilde{t}^k) \) of the dual equation (42). The offline-online decomposition of (42) is very similar to that of the primal equation (44) as described in Section 4.4. We will present briefly that procedure in this section.

For the dual problem we define \( \bar{z}_N(\mu, \tilde{t}^k) = [\bar{z}_N 1(\mu, \tilde{t}^k), \bar{z}_N 2(\mu, \tilde{t}^k), \ldots, \bar{z}_N N(\mu, \tilde{t}^k)]^T \in \mathbb{R}^{N \times 1} \) and obtain from (42) that

\[
\left( M^d N(\mu) + \frac{1}{2} \Delta t C^d N(\mu) + \frac{1}{4} \Delta t^2 A^d N(\mu) \right) \bar{z}_N(\mu, \tilde{t}^{k+1}) \\
= \left( -M^d N(\mu) + \frac{1}{2} \Delta t C^d N(\mu) - \frac{1}{4} \Delta t^2 A^d N(\mu) \right) \bar{z}_N(\mu, \tilde{t}^{k-1}) \\
+ \left( 2M^d N(\mu) - \frac{1}{2} \Delta t^2 A^d N(\mu) \right) \bar{z}_N(\mu, \tilde{t}^k) + \Delta t L^d N(\mu), \quad 1 \leq k \leq K - 1, \quad (58)
\]

where

\[
M^d N(\mu) = \sum_{q=1}^{Q_m} \Theta^q_m(\mu) M^d N(\mu) q, \quad C^d N(\mu) = \sum_{q=1}^{Q_a} \Theta^q_c(\mu) C^d N(\mu) q, \quad A^d N(\mu) = \sum_{q=1}^{Q_a} \Theta^q_a(\mu) A^d N(\mu) q, \quad (59)
\]

with entries

\[
M^d N_{i,j} = m^q(c^{du}_{i}, c^{du}_{j}), \quad 1 \leq i, j \leq N_{du,max}, \quad 1 \leq q \leq Q_m, \quad (60a)
\]

\[
C^d N_{i,j} = c^q(c^{du}_{i}, c^{du}_{j}), \quad 1 \leq i, j \leq N_{du,max}, \quad 1 \leq q \leq Q_c, \quad (60b)
\]

\[
A^d N_{i,j} = a^q(c^{du}_{i}, c^{du}_{j}), \quad 1 \leq i, j \leq N_{du,max}, \quad 1 \leq q \leq Q_a, \quad (60c)
\]

\[
L^d N_{i} = l(c^{du}_{i}), \quad 1 \leq i \leq N_{du,max}. \quad (60d)
\]

Note that the initial condition is treated as described in (52) of Section 3.2.

Finally, from the primal residual (53) and the auxiliary term (55a) the auxiliary term is evaluated as

\[
\mathcal{R}(z_N(\mu, \tilde{t}^k); \mu, t^k) = \Delta t \sum_{k'=1}^{k} \mathcal{R}^{pr}(z_N(\mu, \tilde{t}^{k+1-k'}); \mu, t^k) \\
= \Delta t \sum_{k'=1}^{k} \bar{z}_N(\mu, \tilde{t}^{k+k'} - 1) \times \\
\left\{ g^{eq}(t^k) F^d N(\mu) + M^d N^{pr}(\mu) \lambda_m(\mu, t^k) + C^d N^{pr}(\mu) \lambda_c(\mu, t^k) + A^d N^{pr}(\mu) \lambda_a(\mu, t^k) \right\}, \quad (61)
\]

for \( 1 \leq k \leq K \),

where

\[
\lambda_m(\mu, t^k) = \frac{-u_N(\mu, t^{k+1}) + 2u_N(\mu, t^k) - u_N(\mu, t^{k-1})}{\Delta t^2},
\]

\[
\lambda_c(\mu, t^k) = \frac{-u_N(\mu, t^{k+1}) + 2u_N(\mu, t^k) - u_N(\mu, t^{k-1})}{2 \Delta t}, \quad (62)
\]

\[
\lambda_a(\mu, t^k) = \frac{-u_N(\mu, t^{k+1}) + 2u_N(\mu, t^k) - u_N(\mu, t^{k-1})}{4}.
\]
and

\begin{align*}
M_N^{pr,du}(\mu) &= \sum_{q=1}^{Q_m} \Theta_m^q(\mu) M_N^{pr,du q}, \\
C_N^{pr,du}(\mu) &= \sum_{q=1}^{Q_c} \Theta_c^q(\mu) C_N^{pr,du q}, \\
A_N^{pr,du}(\mu) &= \sum_{q=1}^{Q_a} \Theta_a^q(\mu) A_N^{pr,du q}, \\
F_N^{du q}(\mu) &= \sum_{q=1}^{Q_f} \Theta_f^q(\mu) F_N^{du q}, \\
\end{align*}

(63)

with entries

\begin{align*}
M_N^{pr,du}_{i,j} &= m^q(\zeta_{i}^{du}, \zeta_{j}^{pr}), \quad 1 \leq i \leq N_{du,\text{max}}, \quad 1 \leq j \leq N_{pr,\text{max}}, \quad 1 \leq q \leq Q_m, \\
C_N^{pr,du}_{i,j} &= c^q(\zeta_{i}^{du}, \zeta_{j}^{pr}), \quad 1 \leq i \leq N_{du,\text{max}}, \quad 1 \leq j \leq N_{pr,\text{max}}, \quad 1 \leq q \leq Q_c, \\
A_N^{pr,du}_{i,j} &= a^q(\zeta_{i}^{du}, \zeta_{j}^{pr}), \quad 1 \leq i \leq N_{du,\text{max}}, \quad 1 \leq j \leq N_{pr,\text{max}}, \quad 1 \leq q \leq Q_a, \\
F_N^{du q}_{i} &= f^q(\zeta_{i}^{du}), \quad 1 \leq i \leq N_{du,\text{max}}, \quad 1 \leq q \leq Q_f.
\end{align*}

(64a-d)