Coupling Modified Constitutive Relation Error, Model Reduction and Kalman Filtering Algorithms for Real-Time Parameters Identification

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Abstract. In this work we propose a new identification strategy based on the coupling between a probabilistic data assimilation method and a deterministic inverse problem approach using the modified Constitutive Relation Error energy functional. The idea is thus to offer efficient identification despite of highly corrupted data for time-dependent systems. In order to perform real-time identification, the modified Constitutive Relation Error is here associated to a model reduction method based on Proper Generalized Decomposition. The proposed strategy is applied to two thermal problems with identification of time-dependent boundary conditions, or material parameters.

1. Introduction
The Dynamic Data-Driven Application Systems (DDDAS) concept has received an increasing interest during the last decade, in particular in the Computational Mechanics community [6]. The main idea is to create a feedback loop between a real system and its numerical model, in order to: (i) control the evolution of the system using model predictions; (ii) update model parameters using data measured on the physical system. A potential application, which is the final target of this work, is structural health monitoring with real-time identification and control of damage evolution in composite materials [13].

In this work, we focus on the identification step and model updating procedure; this requires solving an inverse problem which is usually ill-posed. In order to investigate inverse problems many approaches are possible: (i) deterministic approaches based on the definition of a cost function associated to a regularization method; (ii) stochastic approaches using Bayesian inference. The approach we propose here is based on a coupling between stochastic and deterministic approaches. More specifically, we introduce the modified Constitutive Relation Error (mCRE) which is an energy based method [11] and the Kalman filtering which is a bayesian data assimilation method [10]. On the one hand, Kalman filtering enables effective data assimilation and prediction of a dynamic system evolution from incomplete information; it can be extended to non-linear systems. On the other hand, mCRE is a robust and powerful tool for complex model identification; leaning on energy functionals as well as duality and convexity properties, it has the ability to identify model parameters from highly corrupted data [2]. In order to reach the real-time feature of the inverse method, mCRE is here associated with...
reduced order modelling based on Proper Generalized Decomposition [5, 4]. The proposed data assimilation strategy is applied to two thermal problems with real-time identification/updating of evolving boundary conditions, or material parameters.

2. Problem setting
We consider a thermal evolution of a body $\Omega \subset \mathbb{R}^d$ over the time interval $I_t = [0, T]$. The boundary of $\Omega$, denoted $\partial \Omega$, is split in $\partial \Omega_u$ (where Dirichlet boundary conditions $u = u^d$ are applied) and $\partial \Omega_q$ (where Neumann boundary conditions $q \cdot n = q^d$ are applied). We suppose that $\partial \Omega_u$ and $\partial \Omega_q$ are non-overlapping boundaries. In a direct approach, the thermal problem we consider can be written under the following weak form:

$$\mathcal{B}(u, v) = \mathcal{L}(v) \quad \forall v \in \mathcal{V} \otimes \mathcal{T}$$

with admissibility spaces $\mathcal{V} = \{u \in H^1(\Omega) \setminus u = u^d \forall x \in \partial \Omega_u\}$ and $\mathcal{T} = \{u \in L^2(I_t) \setminus u = u^0 \text{ for } t = 0\}$. The operators are defined by $\mathcal{B}(u, v) = \int_I \int_{\Omega} c(x) v(x) \Delta u(x) dx \, dt$ and $\mathcal{L}(v) = \int_I \int_{\Omega} f(x) v(x) dx \, dt + \int_I \int_{\partial \Omega} q(x) v(x) dx \, dt$ with $u$ the temperature field, $c$ the thermal capacity, $K$ the thermal conductivity and $f$ a source term.

In the context of inverse problems, we search to identify a set $\mathbf{p} \in \mathbb{R}^{n_p}$ of model parameters related for instance to material behavior. The problem we search to solve is then to find $\mathbf{p}$ such that:

$$\mathcal{G}(s, v; \mathbf{p}) = 0 \quad \forall v \in \mathcal{V} \otimes \mathcal{T}$$

(1)

where $s$ denotes observations data realized on the physical system and operator $\mathcal{G}$ is defined from the direct problem and introducing a measurement error term. Classically the problem (1) corresponds to a constrained minimization problem. However, according to DDDAS paradigm where observations are not known for the whole time interval but sequentially assimilated, we reformulate the problem under the form of a dynamical system. The dynamical system is given under space and time discrete form in (2) where we use a mesh of $n$ nodes for space discretization and a time discretization composed to $n_t$ steps; moreover we consider $m$ measurement nodes.

$$\begin{cases}
  u^{(k+1)}_t = \mathcal{M}^{(k)} u^{(k)} + e^{(k)}_M \\
  s^{(k)} = \mathcal{H}^{(k)} u^{(k)} + e^{(k)}_S
\end{cases}$$

(2)

$u^{(k)} \in \mathbb{R}^n$ is the nodal temperature field at time $t^{(k)}$, $e^{(k)}_M \in \mathbb{R}^n$ is a modeling error term, $s^{(k)} \in \mathbb{R}^m$ is the nodal values of observed data, and $e^{(k)}_S \in \mathbb{R}^m$ is an observation error reflecting sensor sensitivity. Operators $\mathcal{M}^{(k)} : \mathbb{R}^n \rightarrow \mathbb{R}^n$ and $\mathcal{H}^{(k)} : \mathbb{R}^n \rightarrow \mathbb{R}^m$ are respectively model (or transition) and observation operators.

3. Proposed model updating strategy
3.1. Classical way based on Kalman filtering
The Kalman filtering is a well-known data assimilation method [10], applicable for the resolution of inverse problems and widely used in mechanical identification problems (see for example [3]). It can be seen as a Bayesian filter in the Gaussian particular case. The Bayesian filter principle is to introduce the two following hypotheses in the Bayes theorem: (i) the state vector $u$ is a Markov process: $\pi(u^{(k)}|u^{(0:k-1)}) = \pi(u^{(k)}|u^{(k-1)})$; (ii) observations $s^{(k)}$ are independent of state history $u^{(0:k-1)}$: $\pi(s^{(k)}|u^{(0:k)}) = \pi(s^{(k)}|u^{(k)})$. The Bayes theorem can then be reformulated, for a time-dependent system, in the following form:

$$\pi(u^{(k)}|s^{(0:k)}) = \frac{\pi(u^{(k)}|s^{(0:k-1)}) \pi(s^{(k)}|u^{(k)})}{\pi(s^{(k)}|s^{(0:k-1)})}$$

(3)
In order to build the Kalman filter, we consider a linear dynamical system and it is necessary to add the three following hypotheses: (i) observation and model errors are statistically independent of the state; (ii) observation and model errors are statistically independent of each other; (iii) all probability density functions introduced in the Kalman filter are assumed to be Gaussian pdf. Moreover, pdf related to measurement and model errors are Gaussian white noise. Finally, introducing these hypotheses in the dynamical system (2) and using Bayes theorem (3) we can show that the Kalman filtering can be decomposed in two steps:

(i) a prediction step, wherein an a priori estimation $\bar{u}^{(k+\frac{1}{2})}$ of the state vector $u^{(k+1)}$ is realized
(ii) a correction or assimilation step, wherein the a priori estimation is corrected by observed data $s$ in order to obtain the a posteriori state vector $u^{(k+1)}$ which is the Kalman filter estimation of the real state.

To solve inverse problems using Kalman filtering, it is necessary to explicitly introduce the parameters vector, which contains parameters we search to identify, in the dynamical system. We thus define an expanded state vector, noted $\bar{u}$, and the associated dynamical system (4).

\[
\begin{align*}
\bar{u}^{(k+1)} &= \mathcal{N} \bar{u}^{(k)} + \bar{e}_M^{(k)} \\
\bar{s}^{(k)} &= \mathcal{H} \bar{u}^{(k)} + e_S^{(k)}
\end{align*}
\]

with $\bar{u}^{(k)} = \begin{bmatrix} u^{(k)} \\ p^{(k)} \end{bmatrix}$ (4)

The idea is then to apply a non-linear Kalman filter to the dynamical system (4), we consider here the Unscented Kalman Filter [8]. The main drawback of this approach, besides its low robustness with highly corrupted data, is the computational cost which is in $O(n + np)^2$. The idea is then to use a similar approach as in [1] in order to circumvent these two drawbacks. More specifically, we introduce the modified Constitutive Relation Error in the dynamical system definition.

### 3.2. The modified Constitutive Relation Error

The modified Constitutive Relation Error (mCRE) is a deterministic method used to solve identification problems based on energy functional minimization [11, 7, 2]. In the context of thermal transient problems, the mCRE functional is defined as follows:

\[
\mathcal{E}_m^2(u, q; p, s) = \frac{1}{2} \int_{I_t} \int_{\Omega} (q - K\nabla u) K^{-1} (q - K\nabla u) \, dx \, dt + \frac{1}{21 - r} \int_{I_t} ||\Pi u - s||^2 \, dt
\]

where $u \in U$ is the temperature field, $q \in S$ the thermal flux and $K$ the thermal conductivity operator. $r \in [0, 1]$ is a scalar penalty coefficient used to weight more or less the measurement error term, classically it is used $r = 0.5$ even though an optimal value can be obtained related to the measurement noise (Morozov principle). We define the two admissibility spaces $\mathcal{U}(I_t) = \{ u \in H^1(\Omega) \otimes L^2(I_t) \mid u = u^d \psi(x, t) \in \partial \Omega_u \times I_t, u = u^0 \psi(x, t) \in \Omega \times \{I_t(0)\} \}$ and $\mathcal{S}(I_t) = \{ q \in L^2(\Omega) \otimes L^2(I_t) \mid q = q^d \psi(x, t) \in \partial \Omega_q \times I_t, c\bar{u} + \nabla \cdot q = f \psi(x, t) \in \Omega \times I_t \}$ where $I_t(0)$ denotes the first value of time interval $I_t$.

The classical way to solve inverse problems using mCRE is then to define $p \in \mathcal{P}$, where $\mathcal{P}$ is the parameters admissibility space, as the solution of (5).

\[
p = \arg\min_{\xi \in \mathcal{P}} \min_{(u, q) \in \mathcal{U} \times \mathcal{S}} \mathcal{E}_m^2(u, q; \xi, s) \quad (5)
\]

In practice problem (5) is solved using an alternate minimization associated to a fixed point algorithm:

**M1** minimization over $\mathcal{U} \times \mathcal{S}$: $(u_{ad}, q_{ad}) = \arg\min_{(u, q) \in \mathcal{U} \times \mathcal{S}} \mathcal{E}_m^2(u, q; p, s)$
Minimization over $\mathcal{P}$:

$$p = \arg\min_{\xi \in \mathcal{P}} E_m^2(u_{ad}, q_{ad}; \xi, s)$$

Numerically, the most expensive step is the first minimization since it is necessary to solve a coupled forward-backward problem in time. Therefore, if we use a monolithic scheme like linear interpolation in time, it is necessary to solve a $2 \times n \times n_t$ linear system.

3.3. Coupling between the Kalman filter and the mCRE

The approach we propose here is to introduce the modified Constitutive Relation Error, and precisely the associated admissible fields computation, in the dynamical system (2). We can then write a new dynamical system as:

$$\begin{align*}
  p^{(k+1)} &= p^{(k)} + e_p^{(k)} \\
  s^{(k)} &= H_m(p^{(k)}, s^{(k-1:k)}) + e_s^{(k)}
\end{align*}$$

(6)

where the first equation translates the fact that without a priori knowledge about parameters time dependence we add a stationarity hypothesis and we perturb it by a Gaussian white noise. The new observation operator is then defined as follows:

$$H_m(p^{(k)}, s^{(k-1:k)}) := \mathcal{H} \circ \text{mCRE}_1 \left(p^{(k)}, s^{(k-1:k)}\right)$$

with $s^{(k-1:k)}$ used to denote $(s^{(k-1)}, s^{(k)})$. The application $\text{mCRE}_1(p^{(k)}, s^{(k-1:k)})$ returns the field $u^{(k)}_{ad}$ resulting from minimization M1. A small difference comes from the fact that in a classical way minimization M1 is over $\mathcal{U}(I_1) \times \mathcal{S}(I_1)$ however here we define admissible fields for each subinterval $I_i^{(k)} = [t^{(k-1)}, t^{(k)})$ so that we realize minimization according to $\mathcal{U}(I_i^{(k)}) \times \mathcal{S}(I_i^{(k)})$. In order to solve the identification problem we apply the Unscented Kalman Filter to dynamical system (6), we denote this approach Modified Kalman Filter (MFK). Advantages to reformulate the dynamical system under form (6) are of three kinds:

(i) The fact to introduce the modified Constitutive Relation Error in the Kalman filter increases its robustness compared to the classical formulation;

(ii) With this new formulation, the Kalman filter computation cost is considerably reduced as we pass from $O((n + n_p)^5)$ to $O(n_p^5)$. However we introduce a new computation cost source with the resolution of the first mCRE minimization;

(iii) The state system computation being based on mCRE admissible fields computation, it is possible to introduce reduced order modelling based on Proper Generalized Decomposition.

3.4. Reduced order modelling

In order to reduce the computation cost and speed-up identification process, we introduce reduced order modelling based on Proper Generalized Decomposition (PGD) [5]. The PGD basic idea is to compute in an offline step the solution under a separated variable representation and evaluate this solution in an online step. Another advantage to use PGD comes from the fact that is possible to include several parameters as extra-coordinates. The identification strategy we propose being an incremental method, the system state over each time increment depends on parameters $p^{(k)}$, observations data $(s^{(k-1)}, s^{(k)})$ and initial condition $u_0^{(k)} = u^{(k-1)}$. The main difficulty is associated to the initial condition which is non-homogeneous. To circumvent this problem we choose to project it on a reduced basis from a first PGD decomposition, we then write $u_0^{(k)} = \sum_{i=1}^{n_m} \gamma_i \psi_i(x)$ and we introduce only the $\gamma_i$ coefficients as extra-coordinates. Consequently, we construct a PGD approximation on the following form:

$$u \simeq \sum_{i=1}^{M} \prod_{j=1}^{n_{m_i}} \Gamma_{i}^{(j)}(\gamma_i) \cdot \prod_{l=1}^{m} \phi_l^{(i)}(s^{(k-1)}) \cdot \prod_{q=1}^{m} \beta_q^{(i)}(s^{(k)}) \cdot \phi_i(p) \cdot \lambda_i(t) \cdot w_i(x)$$
4. Numerical results

The strategy we propose here is applied on two parabolic problems (transient thermal problems) and results are compared to those obtained using the classical approach based on Unscented Kalman Filter (UKF). In order to simulate observations data the strategy used is the following:

(i) Solve the direct problem with true parameters values using the same space mesh than the one used for inverse problem but considering fine time discretization;

(ii) Extract temperature nodal values according to sensor placement and acquisition time (coarser than for direct resolution);

(iii) Add a Gaussian white noise: $s_i^{(k)} = u_i^{(k)} (1 + \mathcal{N}(0, \Sigma)) \ \forall i = 1, ..., m \ ; \ \forall k$

The first example we consider is the identification of time-dependent Neumann boundary condition. The problem setting is given in Figure 1(a) and we consider highly corrupted data with $\Sigma = 0.2$, that is to say 20% measurement noise. The identification results are presented in Figures (1(b),1(c)).

![Problem setting](image1)

**Figure 1.** Thermal-flow identification using UKF and MKF approaches with 20% measurement noise

In order to study tuning parameters influence on results obtained by the Modified Kalman Filter algorithm we realize a parametric study. We show in Figure 2(a) the influence of variance associated to parameters error $C_P$ and observation error variance $C_S$ in term of global error $\epsilon_{MKF} = \frac{\Vert \mathbf{p}_{true} - \mathbf{E}[\mathbf{p}_{MKF}] \Vert_{L^2(I)}}{\Vert \mathbf{p}_{true} \Vert_{L^2(I)}}$. And in Figure 2(b) we show the influence of mCRE penalty coefficient $r$ and measure noise level $\Sigma$. 

![Parametric study](image2)

**Figure 2.** Modified Kalman filter parametric study
The second problem treated with the MKF approach is the identification of time-independent material parameters in a multi-layers structure. The problem setting is given in Figure 3(a) and we consider a measurement noise of 10%, $\Sigma = 0.1$. The results are shown in Figures (3(b),3(c)) only for $\kappa_1$ identification but the identification of other parameters performs the same way.

Figure 3. Thermal conductivity identification using UKF and MKF approaches with 10% measurement noise

To conclude, using the MKF approach we observe: (i) a significant computation time gain; (ii) a better response of the identification process to abrupt changes of parameters to be identified; (iii) global better results on parameters identification.

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