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ORIGINAL PAPER

Detection of parametric changes in the Peyrard-Bishop-Dauxois model of DNA using nonlinear Kalman filtering

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Abstract The derivative-free nonlinear Kalman filter is proposed for state estimation and fault diagnosis in distributed parameter systems of the wave-type and particularly in the Peyrard-Bishop-Dauxois model of DNA dynamics. At a first stage, a nonlinear filtering approach is introduced for estimating the dynamics of the Peyrard-Bishop-Dauxois 1D nonlinear wave equation, through the processing of a small number of measurements. It is shown that the numerical solution of the associated partial differential equation results in a set of nonlinear ordinary differential equations. With the application of a diffeomorphism that is based on differential flatness theory it is shown that an equivalent description of the system is obtained in the linear canonical (Brunovsky) form. This transformation enables to obtain local estimates about the state vector of the DNA model through the application us of the standard Kalman filter recursion. At a second stage, the local statistical approach to fault diagnosis is used to perform fault diagnosis for this distributed parameter system by processing with statistical tools the differences (residuals) between the output of the Kalman filter and the measurements obtained from the distributed parameter system. Optimal selection of the fault threshold is succeeded by using the local statistical approach to fault diagnosis. The efficiency of the proposed filtering approach in the problem of fault diagnosis for parametric change detection, in nonlinear wave-type models of DNA dynamics, is confirmed through simulation experiments.

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1 Introduction

Parametric change detection in distributed parameter systems is a complicated problem that has been little explored up to now. A reason for this is that state estimation methods used for residual generation in distributed parameter systems and in infinite dimensional systems described by partial differential equations are much more complicated than state estimation methods for lumped parameter systems [1–6]. Of particular interest is state estimation of wave-type nonlinear phenomena, appearing in several engineering and biophysical systems [7–10]. The present paper proposes a solution to the problem of state estimation and parametric change detection in distributed parameter systems of the wave-type and particularly in the Peyrard-Bishop-Dauxois model of DNA dynamics [11].

It is known that the Peyrard-Bishop-Dauxois model of DNA dynamics takes the form of a wave partial differential equation. At a first stage the dynamics of this PDE model is computed through a state estimator that processes a small number of measurements. To this end, the following steps are followed. Using the method for numerical solution of the PDE through discretization, the initial partial differential equation is decomposed into a set of nonlinear ordinary differential equations with respect to time [13]. Next, each one of the local models associated with the ordinary differential equations is transformed into a model of the linear canonical (Brunovsky) form through a change of coordinates (diffeomorphism) which is based on differential flatness theory. This transformation provides an extended model of the nonlinear PDE for which state estimation is possible by application of the standard Kalman filter recursion [14–19]. Unlike other nonlinear estimation methods (e.g. extended Kalman filter) the application of the standard Kalman filter recursion to the linearized equivalent of the nonlinear PDE system does need the computation of Jacobian matrices and partial derivatives [20–22].

At a second stage, the paper proposes the *local statistical approach to fault diagnosis* for detecting parametric changes (which could stand for faults) in the distributed parameter system [23–28]. Residuals are generated by comparing the outputs measured from the distributed parameter system against the outputs obtained from the derivative-free nonlinear Kalman filter. The processing of these differences through the local statistical approach to fault diagnosis provides clear indications about the existence of incipient changes in the model of the monitored PDE. Fault diagnosis with the local statistical approach has two significant advantages: i) it provides a credible criterion (χ^2 test) to detect if faults have taken place in the distributed parameter system. This criterion is more efficient than the normalized square error and mean error tests since it employs the modeling error derivative and records the tendency for change. Thus, detection of incipient changes in the filter's parameters becomes possible, and ii) it recognizes the parameters of the PDE model which are responsible for the deviation of the filter's estimates from the real output of the monitored dynamical system (e.g., DNA molecule).

The contribution of the proposed method for parametric change detection in DNA dynamics is summarized in the following. Parametric changes in the dynamics of the DNA molecule imply also changes in the exhibited wave-dynamics predicted by the Peyrard-Bishop-Dauxois model. Thus by measuring specific oscillatory characteristics of the DNA molecule and by processing them with the local statistical approach to fault diagnosis it is

possible to detect changes in the DNA structure. Such changes can be the result of a disease or of pharmaceutical treatment. For example, one can obtain information about the effects that specific chemotherapy drugs have on the DNA structure.

The structure of the paper is as follows: In Section 2 nonlinear filtering using differential flatness theory and transformation of the system's dynamics (DNA molecule) into canonical forms is analyzed. A new filtering method, which we call derivative-free nonlinear Kalman filtering, is proposed for state estimation. In Section 3 it is shown how the derivative-free nonlinear Kalman filtering can be used for estimating the dynamics of systems described by 1D nonlinear PDEs of the wave type (Peyrard-Bishop-Dauxois DNA model). In Section 4 the equivalence between Kalman filtering and regressor models is analyzed. In Section 5 the local statistical approach is introduced as a systematic method for performing fault detection and isolation in dynamical systems. The method is proposed also for diagnosing parametric changes in distributed parameter systems described by PDEs. In Section 6 simulation tests are presented about the performance of the derivative-free nonlinear Kalman filter in the problem of state estimation of the wave-type type PDE and about detecting and isolating parametric changes in such systems. Finally, in Section 7 concluding remarks are stated.

2 Filtering using differential flatness theory and canonical forms

2.1 Conditions for applying differential flatness theory

A new filter will be developed, in accordance with differential flatness theory, aiming at performing state estimation in distributed parameter systems and particularly in the Peyrard-Bishop-Dauxois model of DNA dynamics. It will be shown that the filter can be efficiently used in the problem of state estimation in nonlinear PDE models. It will be proven that such models can be decomposed into an equivalent set of nonlinear ODEs of the form $\dot{x} = f(x, u)$. The latter can be transformed to the form of an affine in-the-input system by adding an integrator to each input [16, 18]:

$$\dot{x} = f(x) + \sum_{i=1}^{m} g_i(x) u_i \tag{1}$$

The following definitions are now used [22]:

(i) Lie derivative: $L_f h(x)$ stands for the Lie derivative $L_f h(x) = (\nabla h) f$ and the repeated Lie derivatives are recursively defined as $L_f^0 h = h$ for $i = 0$, $L_f^i h = L_f L_f^{i-1} h = \nabla L_f^{i-1} h f$ for $i = 1, 2, \cdots$.

(ii) Lie Bracket: $ad_f^i g$ stands for a Lie Bracket which is defined recursively as $ad_f^i g = [f, ad_f^{i-1} g]$ with $ad_f^0 g = g$ and $ad_f g = [f, g] = \nabla g f - \nabla f g$.

If the system (1) can be linearized by a diffeomorphism $z = \phi(x)$ and a static state feedback $u = \alpha(x) + \beta(x) v$ into the following form

$$\begin{aligned} \dot{z}_{i,j} &= z_{i+1,j} \text{ for } 1 \leq j \leq m \text{ and } 1 \leq i \leq v_j - 1 \\ \dot{z}_{v_{i,j}} &= v_j \end{aligned} \tag{2}$$

with $\sum_{j=1}^{m} v_j = n$, then $y_j = z_{1,j}$ for $1 \leq j \leq m$ are the 0-flat outputs which can be written as functions of only the elements of the state vector x. To define conditions for transforming

the system of (1) into the canonical form described in (2) the following theorem holds [18]:

Theorem 1 *For nonlinear systems described by (1) the following variables are defined: (i)* $G_0 = span[g_1, \cdots, g_m]$, *(ii)* $G_1 = span[g_1, \cdots, g_m, ad_f g_1, \cdots, ad_f g_m]$, $\cdots$ *(k)* $G_k = span\{ad_f^j g_i \text{ for } 0 \leq j \leq k,\ 1 \leq i \leq m\}$. *Then, the linearization problem for the system of (1) can be solved if and only if: (1). The dimension of* $G_i,\ i = 1, \cdots, k$ *is constant for* $x \in X \subseteq R^n$ *and for* $1 \leq i \leq n-1$, *(2). The dimension of* G_{n-1} *if of order n, (3). The distribution* G_k *is involutive for each* $1 \leq k \leq n-2$.

2.2 Transformation of the equivalent model into the canonical form

It is assumed now that after defining the flat outputs of the equivalent nonlinear system of (1), and after expressing the system state variables and control inputs as functions of the flat output and of the associated derivatives, the system can be transformed in the Brunovsky canonical form:

$$\begin{array}{ll} \dot{x}_1 = x_2 & \\ \cdots & \\ \dot{x}_{r_1 - 1} = x_{r_1} & y_1 = x_1 \\ \dot{x}_{r_1} = f_1(x) + \sum_{j=1}^{p} g_{1_j}(x) u_j + d_1 & y_2 = x_2 \\ & \cdots \\ \dot{x}_{r_1 + 1} = x_{r_1 + 2} & y_p = x_{n - r_p + 1} \\ \cdots & \\ \dot{x}_{p-1} = x_p & \\ \dot{x}_p = f_p(x) + \sum_{j=1}^{p} g_{p_j}(x) u_j + d_p & \end{array} \tag{3}$$

where $x = [x_1, \cdots, x_n]^T$ is the state vector of the transformed system (according to the differential flatness formulation), $u = [u_1, \cdots, u_p]^T$ is the set of control inputs, $y = [y_1, \cdots, y_p]^T$ is the output vector, f_i are the drift functions and $g_{i,j},\ i, j = 1, 2, \cdots, p$ are smooth functions corresponding to the control input gains, while d_j is a variable associated to external disturbances. It holds that $r_1 + r_2 + \cdots + r_p = n$. Having written the initial nonlinear system into the canonical (Brunovsky) form, we have

$$y_i^{(r_i)} = f_i(x) + \sum_{j=1}^{p} g_{ij}(x) u_j + d_j \tag{4}$$

Next the following vectors and matrices can be defined: $f(x) = [f_1(x), \cdots, f_n(x)]^T$, $g(x) = [g_1(x), \cdots, g_n(x)]^T$, with $g_i(x) = [g_{1i}(x), \cdots, g_{pi}(x)]^T$, $A = diag[A_1, \cdots, A_p]$, $B = diag[B_1, \cdots, B_p]$, $C^T = diag[C_1, \cdots, C_p]$, $d = [d_1, \cdots, d_p]^T$, where matrix A has the MIMO canonical form, i.e., with block-diagonal elements

$$\begin{aligned} A_i &= \begin{pmatrix} 0 & 1 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ldots & \vdots \\ 0 & 0 & \cdots & 1 \\ 0 & 0 & \cdots & 0 \end{pmatrix}_{r_i \times r_i} \\ B_i^T &= (\,0\ 0\ \cdots 0\ 1\,)_{1 \times r_i} \\ C_i &= (\,1\ 0\ \cdots 0\ 0\,)_{1 \times r_i} \end{aligned} \tag{5}$$

Thus, (4) can be written in state-space form

$$\begin{aligned} \dot{x} &= Ax + Bv + B\tilde{d} \\ y &= Cx \end{aligned} \tag{6}$$

where the control input is written as $v = f(x) + g(x)u$. The system of (5) and (6) is in observer canonical form.

3 Estimation of nonlinear wave dynamics

3.1 Peyrard-Bishop-Dauxois PDE model of DNA Dynamics

The Peyrard-Bishop-Dauxois model of DNA dynamics describes displacement from the equilibrium of nodal points of DNA strand. In this model it is assumed that the local opening of base pairs (or local melting of the double helix) is the result of the stretching of the hydrogen bonds. The variables that describe the nodal points' motion in this model are the displacements $y_{1,n}$ and $y_{2,n}$ of the bases from their equilibrium positions along the directions of the hydrogen bonds that connect the two bases into a pair (see Fig. 1). The potential V for the hydrogen bonds is modeled by a Morse potential and an harmonic coupling.

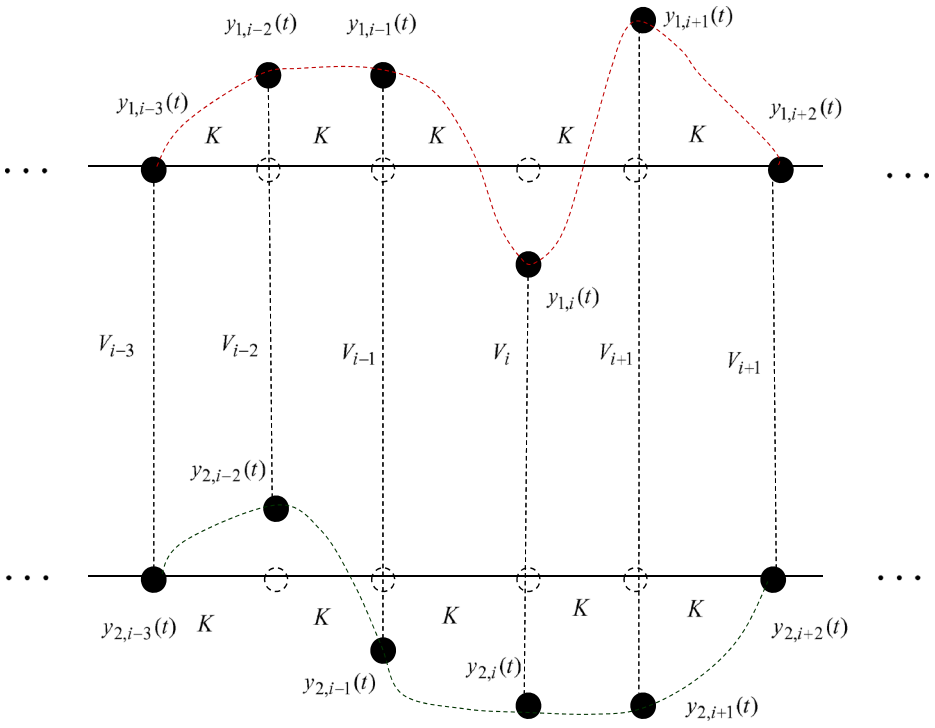

Fig. 1 Local opening of base pairs (stretching of the hydrogen bonds) results in the wave-type dynamics of the DNA strand

The Hamiltonian of this model (sum of the potential and kinetic energy) is [11, 12]:

$$H = \sum_n \{m(\dot{y}_{1,n}^2 + \dot{y}_{2,n}^2) + K[(y_{1,n} - y_{1,n-1})^2 + (\gamma_{2,n} - \gamma_{2,n-1})^2]/2 + V(y_{1,n} - y_{2,n})\} \tag{7}$$

with

$$V(y_{1,n} - y_{2,n}) = D\{e^{[-A(y_{1,n} - y_{2,n})]} - 1\}^2. \tag{8}$$

In the previous description the inhomogeneities of the model due to base sequence and asymmetry of strands are neglected. Under this assumption a common mass m is used for the bases and the same coupling constant k along each strand is considered. The Morse potential $V(y_{1,n} - y_{2,n})$ is an average potential representing the bonds which connect the two bases in a pair.

By introducing the new variables

$$x_{1,n} = (y_{1,n} + y_{2,n})/2^{1/2}$$
$$x_{2,n} = (y_{1,n} - y_{2,n})/2^{1/2} \tag{9}$$

one can represent the in-phase and the out-of-phase motion. Actually, the out-of-phase displacement $x_{2,n}$ denotes the stretching of the hydrogen bonds. Under these new state variables, the system's Hamiltonian is written as

$$H = H(x_1) + H(x_2) \tag{10}$$

where

$$H(x_1) = \sum_{i=1}^{n} \{m\dot{x}_{1,n}^2/2 + K(x_{1,n} - x_{1,n-1})^2/2\} \tag{11}$$

$$H(x_2) = \sum_{i=1}^{n} \left\{m\dot{x}_{2,n}^2/2 + K(x_{2,n} - x_{2,n-1})^2/2 + D[e^{-A2^{1/2}x_{2,n}} - 1]^2\right\} \tag{12}$$

The equations of the dynamic model which are obtained from the modified Hamiltonian of the system are

$$m\frac{\partial^2 x_{1,n}}{\partial t^2} - K(x_{1,n+1} - 2x_{1,n} + x_{1,n-1}) = 0 \tag{13}$$

$$m\frac{\partial^2 x_{2,n}}{\partial t^2} - K(x_{2,n+1} - 2x_{2,n} + x_{2,n-1}) - 2^{3/2}DA(e^{-2^{1/2}Ax_{2,n}})[e^{-2^{1/2}Ax_{2,n}} - 1] = 0 \tag{14}$$

Equation (13) describes usual linear waves (phonons), while (14) describes nonlinear waves (breathers). Equation (14) can be expanded in the continuous limit for small values of x as

$$m\frac{\partial^2 x_2}{\partial t^2} = K\Delta x^2 \frac{\partial^2 x_2}{\partial x^2} + f(x_2) \tag{15}$$

where Δx is the distance between two base pairs and $f(x_2)$ is a nonlinear function. Obviously, (15) is a nonlinear wave equation.

3.2 State estimation for a nonlinear wave-type PDE

As mentioned, the Peyrard-Bishop-Dauxois model of DNA dynamics takes the form of a wave partial differential equation. The following generic form of the nonlinear wave equation is considered next:

$$\frac{\partial^2 \phi}{\partial t^2} = K \frac{\partial^2 \phi}{\partial x^2} + f(\phi). \tag{16}$$

Using the approximation for the partial derivative

$$\frac{\partial^2 \phi}{\partial x^2} \simeq \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2}. \tag{17}$$

and considering spatial measurements of variable ϕ along axis x at points $x_0 + i\Delta x,\ i = 1, 2, \cdots, N$ one has

$$\frac{\partial^2 \phi_i}{\partial t^2} = \frac{K}{\Delta x^2}\phi_{i+1} - \frac{2K}{\Delta x^2}\phi_i + \frac{K}{\Delta x^2}\phi_{i-1} + f(\phi_i) \tag{18}$$

By considering the associated samples of ϕ given by $\phi_0, \phi_1, \cdots, \phi_N, \phi_{N+1}$ one has

$$\begin{aligned}
\frac{\partial^2 \phi_1}{\partial t^2} &= \frac{K}{\Delta x^2}\phi_2 - \frac{2K}{\Delta x^2}\phi_1 + \frac{K}{\Delta x^2}\phi_0 + f(\phi_1) \\
\frac{\partial^2 \phi_2}{\partial t^2} &= \frac{K}{\Delta x^2}\phi_3 - \frac{2K}{\Delta x^2}\phi_2 + \frac{K}{\Delta x^2}\phi_1 + f(\phi_2) \\
\frac{\partial^2 \phi_3}{\partial t^2} &= \frac{K}{\Delta x^2}\phi_4 - \frac{2K}{\Delta x^2}\phi_3 + \frac{K}{\Delta x^2}\phi_2 + f(\phi_3) \\
&\cdots \\
\frac{\partial^2 \phi_{N-1}}{\partial t^2} &= \frac{K}{\Delta x^2}\phi_N - \frac{2K}{\Delta x^2}\phi_{N-1} + \frac{K}{\Delta x^2}\phi_{N-2} + f(\phi_{N-1}) \\
\frac{\partial^2 \phi_N}{\partial t^2} &= \frac{K}{\Delta x^2}\phi_{N+1} - \frac{2K}{\Delta x^2}\phi_N + \frac{K}{\Delta x^2}\phi_{N-1} + f(\phi_N)
\end{aligned} \tag{19}$$

By defining the following state vector

$$x^T = (\phi_1, \phi_2, \cdots, \phi_N) \tag{20}$$

one obtains the state-space description

$$\begin{aligned}
\ddot{x}_1 &= \frac{K}{\Delta x^2}x_2 - \frac{2K}{\Delta x^2}x_1 + \frac{K}{\Delta x^2}\phi_0 + f(x_1) \\
\ddot{x}_2 &= \frac{K}{\Delta x^2}x_3 - \frac{2K}{\Delta x^2}x_2 + \frac{K}{\Delta x^2}x_1 + f(x_2) \\
\ddot{x}_3 &= \frac{K}{\Delta x^2}x_4 - \frac{2K}{\Delta x^2}x_3 + \frac{K}{\Delta x^2}x_2 + f(x_3) \\
&\cdots \\
\ddot{x}_{N-1} &= \frac{K}{\Delta x^2}x_N - \frac{2K}{\Delta x^2}x_{N-1} + \frac{K}{\Delta x^2}x_{N-2} + f(x_{N-1}) \\
\ddot{x}_N &= \frac{K}{\Delta x^2}\phi_{N+1} - \frac{2K}{\Delta x^2}x_N + \frac{K}{\Delta x^2}x_{N-1} + f(x_N)
\end{aligned} \tag{21}$$

Next, the following state variables are defined

$$\begin{aligned}
y_{1,i} &= x_i \\
y_{2,i} &= \dot{x}_i
\end{aligned} \tag{22}$$

and the state-space description of the system becomes as follows

$$
\begin{aligned}
\dot{y}_{1,1} &= y_{2,1} \\
\dot{y}_{2,1} &= \frac{K}{\Delta x^2} y_{1,2} - \frac{2K}{\Delta x^2} y_{1,1} + \frac{K}{\Delta x^2}\phi_0 + f(y_{1,1}) \\
\dot{y}_{1,2} &= y_{2,2} \\
\dot{y}_{2,2} &= \frac{K}{\Delta x^2} y_{1,3} - \frac{2K}{\Delta x^2} y_{1,2} + \frac{K}{\Delta x^2} y_{1,1} + f(y_{1,2}) \\
\dot{y}_{1,3} &= y_{2,3} \\
\dot{y}_{2,3} &= \frac{K}{\Delta x^2} y_{1,4} - \frac{2K}{\Delta x^2} y_{1,3} + \frac{K}{\Delta x^2} y_{1,2} + f(y_{1,3}) \\
&\cdots \\
&\cdots \\
\dot{y}_{1,N-1} &= y_{2,N-1} \\
\dot{y}_{2,N-1} &= \frac{K}{\Delta x^2} y_{1,N} - \frac{2K}{\Delta x^2} y_{1,N-1} + \frac{K}{\Delta x^2} y_{1,N-2} + f(y_{1,N-1}) \\
\dot{y}_{1,N} &= y_{2,N} \\
\dot{y}_{2,N} &= \frac{K}{\Delta x^2}\phi_{N+1} - \frac{2K}{\Delta x^2} y_{1,N} + \frac{K}{\Delta x} y_{1,N-1} + f(y_{1,N})
\end{aligned} \tag{23}
$$

The dynamical system described in (23) is a differentially flat one with flat output defined as the vector $\tilde{y} = [y_{1,1}, y_{1,2}, \cdots, y_{1,N}]$. Indeed all state variables can be written as functions of the flat output and its derivatives.

Moreover, by defining the new control inputs

$$
\begin{aligned}
v_1 &= \frac{K}{\Delta x^2} y_{1,2} - \frac{2K}{\Delta x^2} y_{1,1} + \frac{K}{\Delta x^2}\phi_0 + f(y_{1,1}) \\
v_2 &= \frac{K}{\Delta x^2} y_{1,3} - \frac{2K}{\Delta x^2} y_{1,2} + \frac{K}{\Delta x^2} y_{1,1} + f(y_{1,2}) \\
v_3 &= \frac{K}{\Delta x^2} y_{1,4} - \frac{2K}{\Delta x^2} y_{1,3} + \frac{K}{\Delta x^2} y_{1,2} + f(y_{1,3}) \\
&\cdots \\
v_{N-1} &= \frac{K}{\Delta x^2} y_{1,N} - \frac{2K}{\Delta x^2} y_{1,N-1} + \frac{K}{\Delta x^2} y_{1,N-2} + f(y_{1,N-1}) \\
v_N &= \frac{K}{\Delta x^2}\phi_{N+1} - \frac{2K}{\Delta x^2} y_{1,N} + \frac{K}{\Delta x^2} y_{1,N-1} + f(y_{1,N})
\end{aligned} \tag{24}
$$

the following state-space description is obtained

$$
\begin{pmatrix} \dot{y}_{1,1} \\ \dot{y}_{2,1} \\ \dot{y}_{1,2} \\ \dot{y}_{2,2} \\ \cdots \\ \dot{y}_{1,N-1} \\ \dot{y}_{2,N-1} \\ \dot{y}_{1,N} \\ \dot{y}_{2,N} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & & & \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} y_{1,1} \\ y_{2,1} \\ y_{1,2} \\ y_{2,2} \\ \cdots \\ y_{1,N-1} \\ y_{2,N-1} \\ y_{1,N} \\ y_{2,N} \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & & \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \cdots \\ v_{N-1} \\ v_N \end{pmatrix} \tag{25}
$$

By selecting measurements from a subset of points $x_j \ j \in [1, 2, \cdots, m]$, the associated observation (measurement) equation becomes

$$\begin{pmatrix} z_1 \\ z_2 \\ \cdots \\ z_m \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & & \\ 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix} \begin{pmatrix} y_{1,1} \\ y_{2,1} \\ y_{1,2} \\ y_{2,2} \\ \cdots \\ y_{1,N} \\ y_{2,N} \end{pmatrix} \tag{26}$$

Thus, in matrix form one has the following state-space description of the system

$$\begin{aligned} \dot{\tilde{y}} &= A\tilde{y} + Bv \\ \tilde{z} &= C\tilde{y} \end{aligned} \tag{27}$$

Setting $a = \frac{K}{Dx^2}$ and $b = -\frac{2K}{Dx^2}$, the initial description of the system given in (25) is rewritten as follows

$$\begin{pmatrix} \dot{y}_{1,1} \\ \dot{y}_{2,1} \\ \dot{y}_{1,2} \\ \dot{y}_{2,2} \\ \cdots \\ \dot{y}_{1,N-1} \\ \dot{y}_{2,N-1} \\ \dot{y}_{1,N} \\ \dot{y}_{2,N} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ b & 0 & a & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ a & 0 & b & 0 & a & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 0 & b & 0 & a & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & & & & & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & a & 0 & b & 0 & a & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & a & 0 & b & 0 \end{pmatrix} \begin{pmatrix} y_{1,1} \\ y_{2,1} \\ y_{1,2} \\ y_{2,2} \\ \cdots \\ y_{1,N-1} \\ y_{2,N-1} \\ y_{1,N} \\ y_{2,N} \end{pmatrix}$$
$$+ \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & & \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \cdots \\ v_{N-1} \\ v_N \end{pmatrix} \tag{28}$$

The associated control inputs are defined as

$$\begin{aligned} v_1 &= \frac{K}{\Delta x^2}\phi_0 + f(y_{1,1}) \\ v_2 &= f(y_{1,2}) \\ v_3 &= f(y_{1,3}) \\ &\cdots \\ v_{N-1} &= f(y_{1,N-1}) \\ v_N &= \frac{K}{\Delta x^2}\phi_{N+1} + f(y_{1,N}) \end{aligned} \tag{29}$$

By selecting measurements from a subset of points x_j $j \in [1, 2, \cdots, m]$, the associated observation (measurement) equation remains as in (26), i.e.

$$\begin{pmatrix} z_1 \\ z_2 \\ \cdots \\ z_m \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & & \\ 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix} \begin{pmatrix} y_{1,1} \\ y_{2,1} \\ y_{1,2} \\ y_{2,2} \\ \cdots \\ y_{1,N} \\ y_{2,N} \end{pmatrix} \tag{30}$$

For the linear description of the system in the form of (27) one can perform estimation using the standard Kalman filter recursion. First, the discrete-time equivalents of matrices A, B and C are computed using common discretization methods. These are denoted as A_d, B_d and C_d, respectively. Next, the discrete-time Kalman filter can be decomposed into two parts: i) time update (prediction stage), and ii) measurement update (correction stage).

Measurement update

$$\begin{aligned} K(k) &= P^-(k){C_d}^T[C_d \cdot P^-(k){C_d}^T + R]^{-1} \\ \hat{y}(k) &= \hat{y}^-(k) + K(k)[z(k) - C_d\hat{y}^-(k)] \\ P(k) &= P^-(k) - K(k)C_dP^-(k) \end{aligned} \tag{31}$$

Time update

$$\begin{aligned} P^-(k+1) &= A_d(k)P(k){A_d}^T(k) + Q(k) \\ \hat{y}^-(k+1) &= A_d(k)\hat{y}(k) + B_d(k)u(k) \end{aligned} \tag{32}$$

Therefore, by taking measurements of $\phi(x, t)$ at time t at a small number of measuring points $j = 1, \cdots, n_1$ it is possible to estimate the complete state vector, i.e., to get values of ϕ in a mesh of points that covers efficiently the variations of $\phi(x, t)$. By processing a sequence of output measurements of the system, one can obtain local estimates of the state vector $\hat{y}$. The measuring points can vary in time provided that the observability criterion for the state-space model of the PDE holds.

The proposed derivative-free nonlinear Kalman filter is of improved precision because unlike other nonlinear filtering schemes, e.g., the extended Kalman filter, it does not introduce cumulative numerical errors due to approximative linearization of the system's dynamics. Besides, it is computationally more efficient (faster) because it does not require the calculation of Jacobian matrices and partial derivatives (Fig. 2).

3.3 Derivative-free nonlinear Kalman filtering

As mentioned above, for the system of (6) and (27), state estimation is possible by applying the derivative-free nonlinear Kalman filter. The system is first turned into discrete-time form using common discretization methods and then the recursion of the linear Kalman filter described in (31) and (32) is applied.

Unlike the extended Kalman filter (EKF), the proposed filtering method does not attempt to solve the problem of nonlinear estimation for nonlinear PDEs by performing approximate linearizations which require the computation of Jacobian matrices, and which are valid only near specific points (thus finally introducing numerical error). The concept of

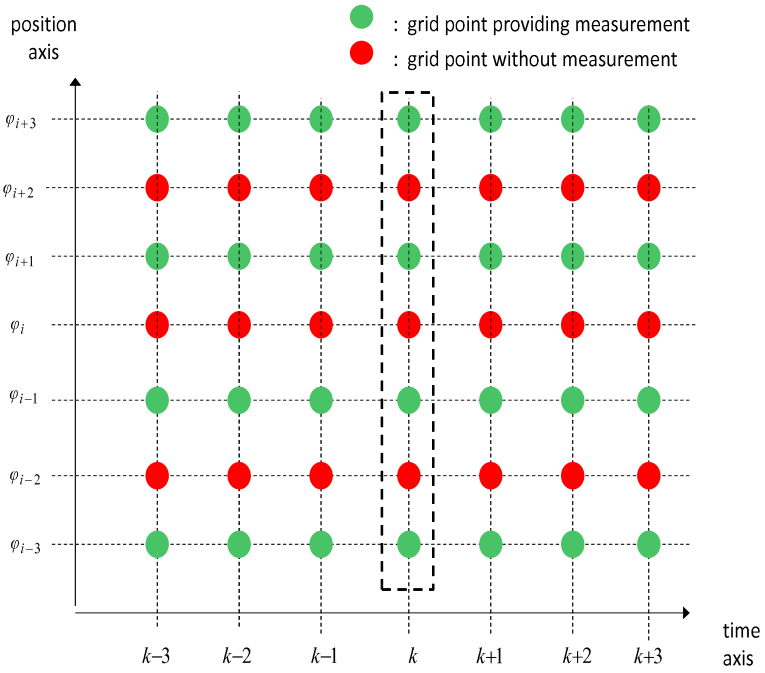

Fig. 2 Grid points for measuring $\phi(x, t)$

the proposed filtering method is as follows: First, the nonlinear wave PDE (e.g., the sine-Gordon wave PDE) is decomposed into a set of ordinary nonlinear differential equations. Actually, a nonlinear differential equation is associated with each point of the discretization of the spatial axis of the wave PDE. Next, the nonlinear differential equations are transformed into linear ones by a change of coordinates (diffeomorphism) which is in accordance with differential flatness theory. State estimation is performed for the equivalent set of the linear differential equations which finally describes the initial nonlinear wave dynamics. Such a transformation stands for an exact linearization approach which neither requires the computation of Jacobian matrices nor introduces numerical error. Finally, by applying the inverse transformation one obtains state estimates for the initial model of the nonlinear wave PDEs.

4 Equivalence between Kalman filters and regressor models

4.1 Equivalence between the standard Kalman filter and linear regressor models

For the purpose of parametric change detection it is convenient to turn the Kalman filter model of distributed parameter systems into equivalent ARMAX (autoregressive moving average model with auxiliary input) models. An ARMAX model is an input-output model of the form

$$A(z)Y_k = C(z)U_k + B(z)\{\epsilon_k\}. \tag{33}$$

A, B, C are polynomial matrices in the backwards shift operator z^{-1}:

$$\begin{aligned} A(z) &= A_0 - \sum_{i=1}^{p} A_i z^{-i} \\ B(z) &= \sum_{j=0}^{q} B_j z^{-j} \\ C(z) &= \sum_{l=1}^{L} C_l z^{-l} \end{aligned} \tag{34}$$

such that A has a non-singular constant term A_0 and where ϵ_k is a white noise sequence with covariance matrix R. A state-space model and particularly the Kalman filter estimator can be written in the form of an ARMAX model. For linear systems, the Kalman filter (for the single-input case) can be written in the form [24]

$$\begin{pmatrix} \hat{x}_1(k+1) \\ \hat{x}_2(k+1) \\ \cdots \\ \cdots \\ \hat{x}_n(k+1) \end{pmatrix} = \begin{pmatrix} \alpha_1 & 1 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & 1 \\ \alpha_n & \cdot & \cdot & \cdot & 0 \end{pmatrix} \begin{pmatrix} \hat{x}_1(k) \\ \hat{x}_2(k) \\ \cdots \\ \cdots \\ \hat{x}_n(k) \end{pmatrix} + \begin{pmatrix} g_1 \\ \cdot \\ \cdot \\ \cdot \\ g_n \end{pmatrix} U_k + \begin{pmatrix} \kappa_1(k) \\ \cdot \\ \cdot \\ \cdot \\ \kappa_n(k) \end{pmatrix} \epsilon_k \tag{35}$$

$$\hat{Y}(k) = (10 \cdot \cdot 0)\hat{X}(k-1) + JU_k + \epsilon_k \tag{36}$$

Using successive substitutions this can be rewritten as a time-varying ARMAX model:

$$A(z)Y_k = C(z)U_k + B(k, z)\epsilon_k \tag{37}$$

where

$$\begin{aligned} A(z) &= 1 - \alpha_1 z^{-1} - \cdots - \alpha_n z^{-n} \\ C(z) &= g_1 z^{-1} + \cdots + g_n z^{-n} + JA(z^{-1}) \\ B(\kappa, z) &= 1 + [\kappa_1(k-1) - \alpha_1]z^{-1} + \cdots + [\kappa_n(k-n) - \alpha_n]z^{-n} \end{aligned} \tag{38}$$

Matrix $B(\kappa, z)$ is time-varying because the Kalman filter gain K_k is time-varying. But, under the conditions of the stability theorem, K and B are asymptotically constant. Thus, the ARMAX description of the Kalman filter becomes

$$A(z)Y_k = C(z)U_k + B(z)\epsilon_k \tag{39}$$

This approach also holds for multi-input systems and one can transform again the state-space representation into an ARMAX model.

5 Change detection with the local statistical approach

5.1 The global χ^2 test for change detection

Parametric change detection for distributed parameter systems is based on the processing of the residuals, i.e., of the differences between the outputs of the PDE model and the outputs of the associated Kalman filter. First, the residual e_i is defined as the difference between the Kalman filter output $\hat{y}_i$ and the physical system output y_i, i.e., $e_i = \hat{y}_i - y_i$. It is more formal to define the residual as the difference between the Kalman filter output and the exact model

output, where the exact model replaces the physical system and has the same number of parameters as the Kalman filter (see Fig. 3). The partial derivative of the residual square is:

$$H(\theta, y_i) = \frac{1}{2}\frac{\partial e_i^2}{\partial \theta} = e_i \frac{\partial \hat{y}_i}{\partial \theta}. \tag{40}$$

The local statistical approach to fault diagnosis can be used for checking if the parameters of the system which is described by the PDE remain at their nominal values, or if they have deviated from them. Based on a small parametric disturbance assumption, the proposed Fault Detection and Isolation (FDI) method aims at transforming complex detection problems concerning a parameterized stochastic process into the problem of monitoring the mean of a Gaussian vector. The local statistical approach consists of two stages : i) the global test which indicates the existence of a change in some parameters of the distributed parameter system, ii) the diagnostics tests (sensitivity or min-max) which isolate the parameter affected by the change. The method's stages are analyzed first, following closely the method presented in [23, 24].

As shown in Fig. 3 the concept of this parametric change detection technique is as follows: there is a Kalman filter (ARMAX) model that represents the unchanged PDE dynamics. At each time instant the output of the aforementioned reference model is compared to the output of the Kalman filter (ARMAX) model that represents the changed dynamics of the PDE. The difference e_i between these two output measurements is called the residual. The statistical processing of a sufficiently large number of residuals through an FDI method provides an index-variable that is compared against a fault threshold and which can give early indication about deviation of the PDE model from its fault-free condition. Under certain conditions (detectability of changes) the proposed FDI method enables also the fault isolation, i.e., to identify the source of fault within the distributed parameter system.

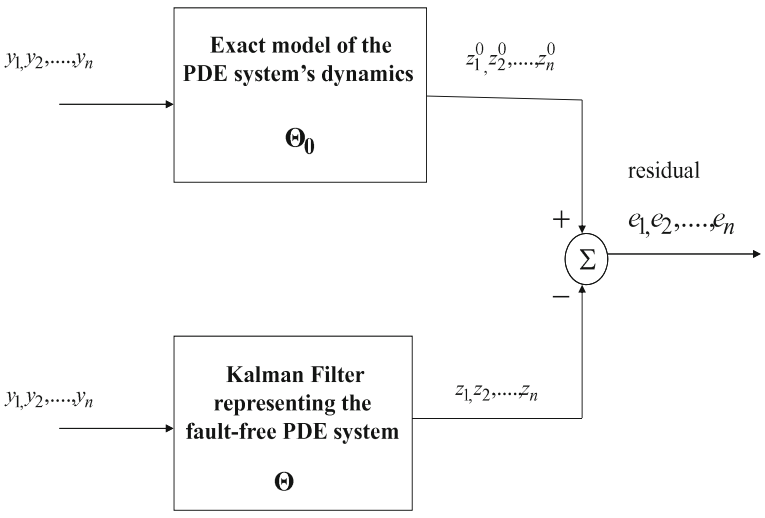

Fig. 3 Residual between the output of the distributed parameter system and the Kalman filter that models the PDE dynamics in the fault-free case

Considering the representation of the Kalman filter as an ARMAX model, the partial derivative of the residual square is:

$$H(\theta, \hat{y}_i) = \frac{1}{2}\frac{\partial e_i^2}{\partial \theta} = e_i \frac{\partial \hat{y}_i}{\partial \theta} \tag{41}$$

where θ is the vector of the model's parameters. The vector H having as elements the above $H(\theta, \hat{y}_i)$ is called the primary residual. The gradient of the output with respect to the ARMAX model parameters are given by

$$\frac{\partial \hat{y}}{\partial w_i} = x_i \tag{42}$$

Next, having calculated the partial derivatives of (42), the rows of the Jacobian matrix J are found by

$$J(\theta_0, \hat{y}_k) = \left.\frac{\partial \hat{y}_k(\theta)}{\partial \theta}\right|_{\theta=\theta_0} \tag{43}$$

where θ_0 represents the nominal value of the parameters. The problem of change detection with the χ^2 test consists of monitoring a change in the mean of the Gaussian variable which for the one-dimensional parameter vector θ is formulated as

$$X = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} e_k \frac{\partial \hat{y}_k}{\partial \theta} \sim N(\mu, \sigma^2) \tag{44}$$

where $\hat{y}_k$ is the output of the Kalman filter (ARMAX) model generated by the input pattern x_k, e_k is the associated residual and θ is the vector of the model's parameters. It is noted that X is the monitored parameter for the FDI test, which means that when the mean value of X is 0 the system is in the fault-free condition, while when the mean value of X has moved away from 0 the system is in a faulty condition. For a multivariable parameter vector θ should hold $X \sim N(M\delta\theta, S)$, where S denotes the covariance matrix of X. Given a set of data of N measurements, the statistical FDI method enables to decide if the system's parameters θ_* remain consistent with their nominal values θ_0 (or if they have deviated from them). The notation is introduced only for the convenience of problem formulation, and its actual value does not need to be known. Then the model validation problem amounts to make a decision between the two hypotheses:

$$\begin{aligned} H_0 &: \theta_* = \theta_0 \\ H_1 &: \theta_* = \theta_0 + \frac{1}{\sqrt{N}}\delta\theta \end{aligned} \tag{45}$$

where $\delta\theta \neq 0$. It is known from the Central Limit Theorem that, for a large data sample, the normalized residual given by (44) asymptotically follows a Gaussian distribution when $N \to \infty$ [23–28]. More specifically, the hypothesis that has to be tested is:

$$\begin{aligned} H_0 &: X \sim N(0, S) \\ H_1 &: X \sim N(M\delta\theta, S) \end{aligned}$$

where M is the sensitivity matrix (see (46)), $\delta\theta$ is the change in the parameter vector and S is the convariance matrix (see (47)). The product $M\delta\theta$ denotes the new center of the

monitored Gaussian variable X, after a change on the system's parameter θ. The sensitivity matrix M of $\frac{1}{\sqrt{N}}X$ is defined as the mean value of the partial derivative with respect to θ of the primary residual defined in 41, i.e. $E\{\frac{\partial}{\partial\theta}H(\theta, \hat{y}_k)\}$ and is approximated by [8]:

$$M(\theta_0)\simeq\frac{\partial}{\partial\theta}\frac{1}{N}\sum_{k=1}^{N}H(\theta_0, \hat{y}_k)\simeq\frac{1}{N}J^T J. \tag{46}$$

The covariance matrix S is defined as $E\{H(\theta, y_k)H^T(\theta, \hat{y}_{k+m})\}$, $m = 0, \pm1, \cdots$ and is approximated by [28]:

$$\begin{aligned} S = \simeq&\sum_{k=1}^{N}[H(\theta_0, \hat{y}_k)H^T(\theta_0, \hat{y}_k)] + \\ &+\sum_{m=1}^{I}\frac{1}{N-m}\sum_{k=1}^{N-m}[H(\theta_0, \hat{y}_k)H^T(\theta_0, \hat{y}_{k+m}) + \\ &\qquad + H(\theta_0, \hat{y}_{k+m})H^T(\theta_0, \hat{y}_k)] \end{aligned} \tag{47}$$

where an acceptable value for I is 3. The decision tool is the likelihood ratio $s(X) = ln\frac{p_{\theta_1}(x)}{p_{\theta_0}(x)}$, where $p_{\theta_1}(X) = e^{[X-\mu(X)]^T S^{-1}[X-\mu(X)]}$ and $p_{\theta_0}(X) = e^{X^T S^{-1}X}$. The center of the Gaussian distribution of the changed system is denoted as $\mu(X) = M\delta\theta$ where $\delta\theta$ is the change in the parameters vector. The *Generalized Likelihood Ratio* (GLR) is calculated by maximizing the likelihood ratio with respect to $\delta\theta$ [28]. This means that the most likely case of parameter change is taken into account. This gives the global χ^2 test t:

$$t = X^T S^{-1}M(M^T S^{-1}M)^{-1}M^T S^{-1}X. \tag{48}$$

Since X asymptotically follows a Gaussian distribution, the statistics defined in (48) follow a χ^2 distribution with n degrees of freedom. Mapping the change detection problem to this χ^2 distribution enables the choice of the change threshold. Assuming that the desired probability of false alarm is α, then change threshold λ should be chosen from the relation

$$\int_{\lambda}^{\infty}\chi_n^2(s)ds = \alpha, \tag{49}$$

where $\chi_n^2(s)$ is the probability density function (p.d.f.) of a variable that follows the χ^2 distribution with n degrees of freedom.

5.2 Parametric change isolation with the sensitivity test

The parametric change detection method should be able to find out, among the complete set of parameters of the PDE, which are the ones that are subject to change with respect to their nominal values. A first approach to change isolation is to focus only on a subset of the parameters while considering that the rest of the parameters remain unchanged [28]. The parameters vector η can be written as $\eta = [\phi, \psi]^T$, where ϕ contains those parameters to be subject to the isolation test ,while ψ contains those parameters to be excluded from the isolation test. M_ϕ contains the columns of the sensitivity matrix M which are associated with the parameters subject to the isolation test. Similarly M_ψ contains the columns of M that are associated with the parameters to be excluded from the sensitivity test.

Assume that, among the parameters η, it is only the subset ϕ that is suspected to have undergone a change. Thus η is restricted to $\eta = [\phi, 0]^T$. The associated columns of the

sensitivity matrix are given by M_ϕ and the mean of the Gaussian to be monitored is $\mu = M_\phi \phi$, i.e.,

$$\mu = MA\phi, \quad A = [0, I]^T. \tag{50}$$

Matrix A is used to select the parameters that will be subject to the fault isolation test. The rows of A correspond to the total set of parameters while the columns of A correspond only to the parameters selected for the test. Thus the fault diagnosis (χ^2) test of (48) can be restated as:

$$t_\phi = X^T S^{-1} M_\phi (M_\phi^T S^{-1} M_\phi)^{-1} M_\phi^T S^{-1} X. \tag{51}$$

5.3 Parametric change isolation with the min-max test

In this approach the aim is to find a statistic that will be able to detect a change on the part ϕ of the parameters vector η and which will be robust to a change in the non-observed part ψ [28]. Assume the vector partition $\eta = [\phi, \psi]^T$. The following notation is used:

$$M^T S^{-1} M = \begin{pmatrix} I_{\varphi\varphi} & I_{\varphi\psi} \\ I_{\psi\varphi} & I_{\psi\psi} \end{pmatrix} \tag{52}$$

$$\gamma = \begin{pmatrix} \varphi \\ \psi \end{pmatrix}^T \cdot \begin{pmatrix} I_{\varphi\varphi} & I_{\varphi\psi} \\ I_{\psi\varphi} & I_{\psi\psi} \end{pmatrix} \cdot \begin{pmatrix} \varphi \\ \psi \end{pmatrix} \tag{53}$$

where S is the previously defined covariance matrix. The min-max test aims to minimize the non-centrality parameter γ with respect to the parameters that are not suspected for change. The minimum of γ with respect to ψ is given for:

$$\psi^* = \arg\min_\psi \gamma = \varphi^T (I_{\varphi\varphi} - I_{\varphi\psi} I_{\psi\psi}^{-1} I_{\psi\varphi}) \varphi \tag{54}$$

and is found to be

$$\begin{aligned} \gamma^* &= \min_\psi \gamma = \varphi^T (I_{\varphi\varphi} - I_{\varphi\psi} I_{\psi\psi}^{-1} I_{\psi\varphi}) \varphi \\ &= \begin{pmatrix} \varphi \\ -I_{\psi\psi}^{-1} I_{\psi\varphi} \varphi \end{pmatrix}^T \begin{pmatrix} I_{\varphi\varphi} & I_{\varphi\psi} \\ I_{\psi\varphi} & I_{\psi\psi} \end{pmatrix} \begin{pmatrix} \varphi \\ -I_{\psi\psi}^{-1} I_{\psi\varphi} \varphi \end{pmatrix} \end{aligned} \tag{55}$$

which results in

$$\gamma^* = \varphi^T \{[I, -I_{\varphi\psi} I_{\psi\psi}^{-1}] M^T \Sigma^{-1}\} \, \Sigma^{-1} \{\Sigma^{-1} M [I, -I_{\varphi\psi} I_{\psi\psi}^{-1}]\} \varphi \tag{56}$$

The following linear transformation of the observations is considered

$$X_\phi^* = [I, -I_{\varphi\psi} I_{\psi\psi}^{-1}] M^T \Sigma^{-1} X \tag{57}$$

The transformed variable X_ϕ^* follows a Gaussian distribution $N(\mu_\phi^*, I_\phi^*)$ with mean

$$\mu_\varphi^* = I_\varphi^* \varphi \tag{58}$$

and with covariance

$$I_\varphi^* = I_{\varphi\varphi} - I_{\varphi\psi} I_{\psi\psi}^{-1} I_{\psi\varphi} \tag{59}$$

The max-min test decides between the hypotheses

$$H_0^* : \mu^* = 0$$

$$H_1^* : \mu^* = I_\varphi^* \varphi$$

and is described by

$$\tau_\varphi^* = X_\varphi^{*T} I_\varphi^{*-1} X_\varphi^*. \tag{60}$$

The stages of fault detection and isolation (FDI), for the PDE system, with the use of the local statistical approach, are summarized in Table 1.

Remark 1 The previously analyzed results show that Kalman filtering for the nonlinear wave PDE (such as the one met in the Peyrard-Bishop-Dauxois DNA model) can be performed by transforming the PDE model into an equivalent state-space description. The latter transformation is based on a change of coordinates (diffeomorphism), according to differential flatness theory. In the next section, the article shows the equivalence between the Kalman filter for the wave PDE and ARMAX models. This equivalent representation in the ARMAX form enables us to apply the local statistical approach to change detection for finding parametric changes in the wave PDE. The purpose of the statistical change detection test is to find out if the parameters of the wave PDE remain consistent with their nominal values or if they had deviated from them.

6 Simulation tests

6.1 Nonlinear filtering for the dynamics of the DNA molecule

The proposed filtering scheme was tested in estimation and fault diagnosis for a wave equation of the form of (16) under unknown boundary conditions. Nonlinear 1D wave-type partial differential equations of this type appear in models of coupled oscillators. One can consider for example the nonlinear PDE [29, 30]

$$\frac{\partial \phi}{\partial t^2} = K \frac{\partial^2 \phi}{\partial x^2} + f(\phi) \tag{61}$$

where c, ϵ and l are constants. This type of PDE appears in the DNA dynamics model of Peyrard-Bishop-Dauxois. Equation (61) describes the motion of an array of pendula

Table 1 Stages of the local statistical approach for FDI

1. Generate the residuals partial derivative given by (41)
2. Calculate the Jacobian matrix J given by (43)
3. Calculate the sensitivity matrix M given by (46)
4. Calculate the covariance matrix S given by (47)
5. Apply the χ^2 test for change detection of (48)
6. Apply the change isolation tests of (51) or (60)

each of which is coupled to its nearest neighbors by a torsional spring with a coupling coefficient K. The angle $x_i = \phi_i$ of the ith pendulum and the vertical axis evolves according to (61).

To perform state estimation of the distributed parameter system of (61) a grid consisting of $n = 50$ points was considered. The number of measurement points was $n_1 = 25$. In general, the number of measurements of the state variable $x_1 = \phi(x, t)$ which can be used by the estimation algorithm is $n_1 \leq n$, where n is the number of grid points, and the criterion to select the number of grid points where measurements will be taken is to maintain the system's observability.

In Fig. 4 the monitored wave function $\phi(x, t)$ and the associated first derivative in time $\dot{\phi}(x, t)$ are depicted. Indicative results about the estimation obtained at local grid points is given in Fig. 5 and in Fig. 8. It was assumed that changed dynamics was generated by one specific node of the PDE system (e.g., node 85 monitoring output 22 of the PDE system). This implied that locally at this node the spring coefficient deviated from its nominal value (Figs. 6, 7 and 8).

The experimental results show that state estimates in the vicinity of the faulty node (node giving output 22, i.e., state vector element 85) exhibit significant deviations comparing to the estimated values of the state vector. As moving far from the faulty node (e.g. state vector elements 61 to 64) the estimated and the real values of the state vector elements exhibit smaller differences. Thus, the comparison of the recorded measurements against the estimated values from the derivative-free nonlinear Kalman filter provides a clear indication about the faulty node. Thus it becomes possible to isolate this node from the rest of the set of nodes.

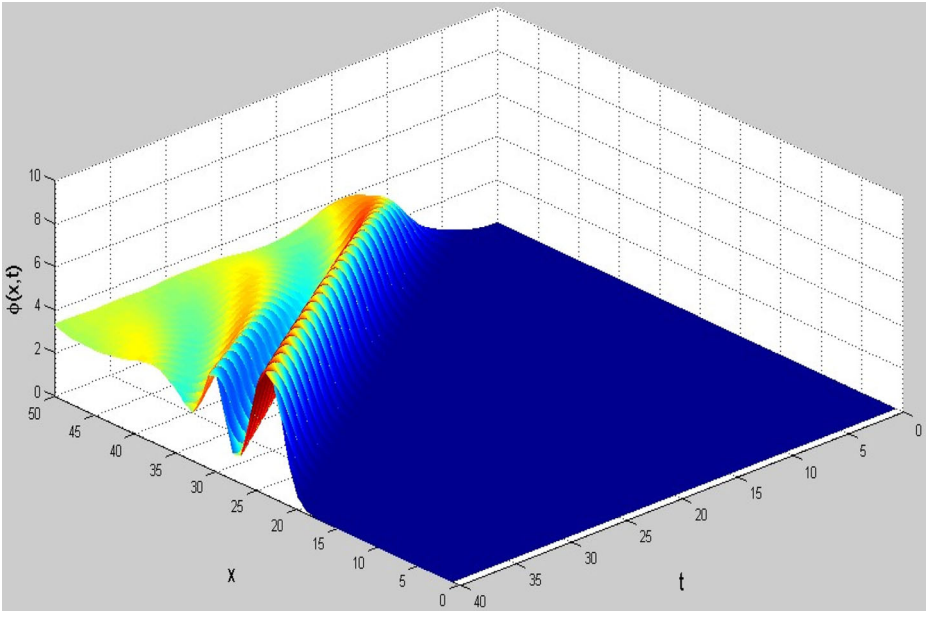

Fig. 4 The monitored wave function $\phi(x, t)$

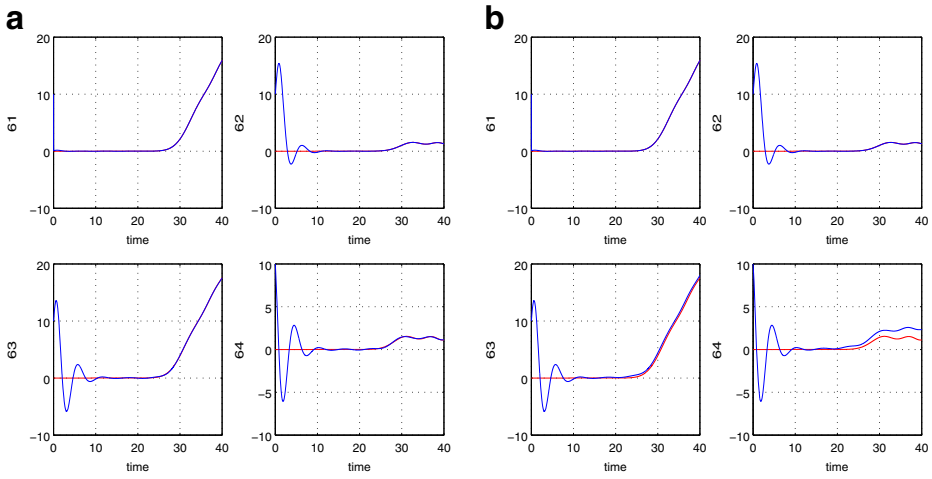

Fig. 5 Monitoring of state vector elements y_{61} to y_{64} of the DPS (**a**) when all nodes are fault-free (**b**) when a fault appears at the node providing output 22, i.e., state variable y_{85}

6.2 Detection of incipient changes in the dynamics of the DNA molecule

It is also important to detect incipient changes in the coefficients of the distributed parameter model. It will be shown that it is possible to detect a global change of the wave coefficient K in the Peyrard-Bishop-Dauxois PDE model of the DNA. To this end the the following state-space equation of the distributed parameter system is used. The state-space equation is written in the form of an ARMAX model which enables fault diagnosis with the use of the local statistical approach.

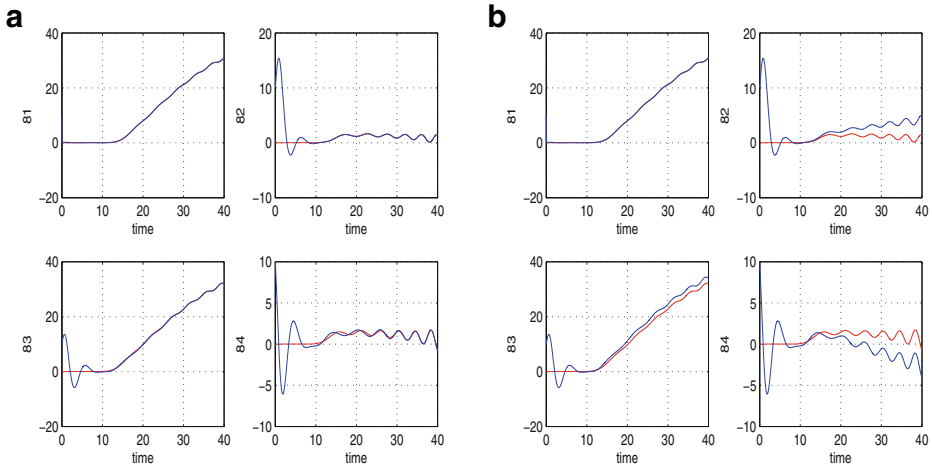

Fig. 6 Monitoring of state vector elements y_{81} to y_{84} of the DPS (**a**) when all nodes are fault-free (**b**) when a fault appears at node providing output 22, i.e., state variable y_{85}

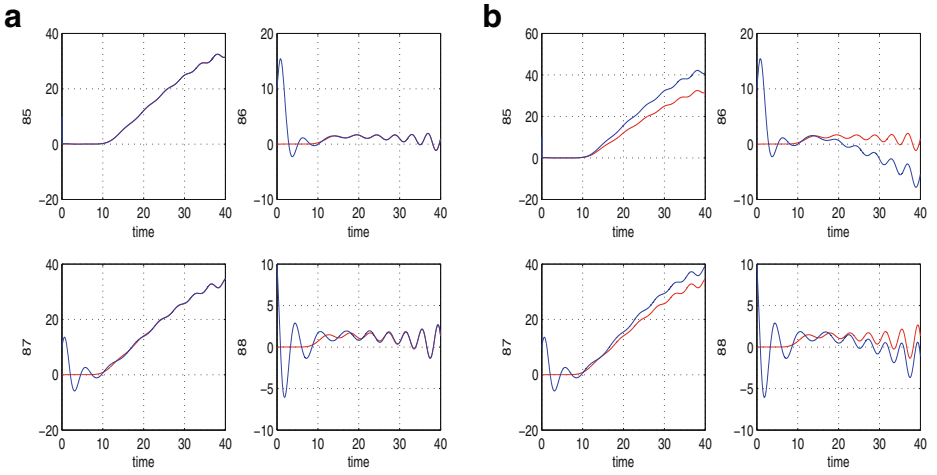

Fig. 7 Monitoring of state vector elements y_{85} to y_{88} of the DPS (**a**) when all nodes are fault-free (**b**) when a fault appears at node providing output 22, i.e., state variable y_{85}

Without loss of generality it is assumed that coefficient K remains the same at all points of the grid. Using only the last subsystem in description of dynamics of the PDE one has

$$\begin{aligned} \dot{y}_{1,N} &= y_{2,N} \\ \dot{y}_{2,N} &= \frac{K}{\Delta x^2}\phi_{N+1} - \frac{2K}{\Delta x^2}y_{1,N} + \frac{K}{\Delta x^2}y_{1,N-1} + f(y_{1,N}). \end{aligned} \tag{62}$$

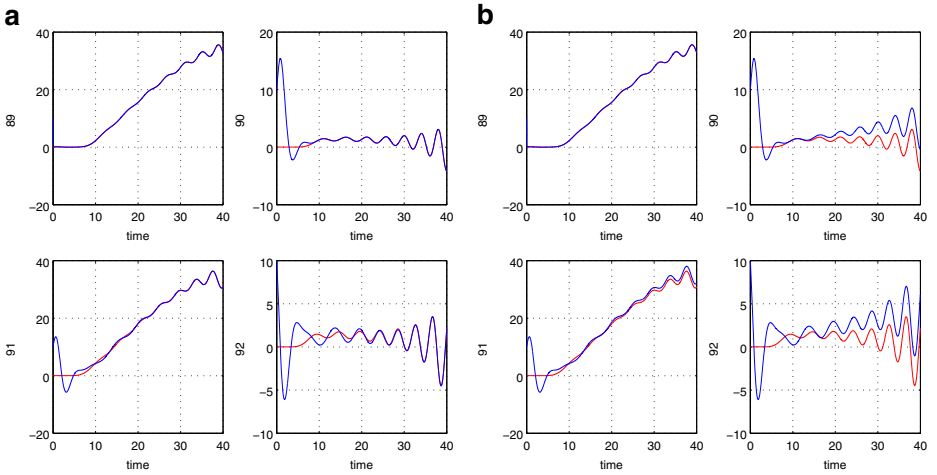

Fig. 8 Monitoring of state vector elements y_{89} to y_{92} of the DPS (**a**) when all nodes are fault-free (**b**) when a fault appears at node providing output 22, i.e., state variable y_{85}

Defining $v_N = \frac{K}{\Delta x^2}\phi_{N+1} + \frac{K}{\Delta x^2} y_{1,N-1} + f(y_{1,N})$ the following discrete-time description of the system is obtained

$$\begin{pmatrix} y_{1,N}(k+1) \\ y_{2,N}(k+1) \end{pmatrix} = \begin{pmatrix} 1 & T_s \\ -\frac{2K}{Dx^2} T s & 1 \end{pmatrix} \begin{pmatrix} y_{1,N}(k) \\ y_{2,N}(k) \end{pmatrix} \begin{pmatrix} 0 \\ T_s \end{pmatrix} v_N(k) \tag{63}$$

$$z_{1,N}(k) = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} y_{1,N}(k) \\ y_{2,N}(k) \end{pmatrix} \tag{64}$$

The associated ARMAX model is found to be

$$z_{1,N}(k+2) = 2z_{1,N}(k+1) - (1 + \frac{T_s^2 2K}{Dx^2}) z(k) + v_N(k). \tag{65}$$

In a similar manner, the discrete-time model of the Kalman filter is written as

$$\begin{pmatrix} \hat{y}_{1,N}(k+1) \\ \hat{y}_{2,N}(k+1) \end{pmatrix} = \begin{pmatrix} 1 & T_s \\ -\frac{2K}{Dx^2} T s & 1 \end{pmatrix} \begin{pmatrix} \hat{y}_{1,N}(k) \\ \hat{y}_{2,N}(k) \end{pmatrix} + \\ + \begin{pmatrix} 0 \\ T_s \end{pmatrix} v(k) + \begin{pmatrix} \kappa_1(k) \\ \kappa_2(k) \end{pmatrix} \hat{e}(k) \tag{66}$$

$$\hat{z}(k) = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} \hat{y}_{1,N}(k) \\ \hat{y}_{2,N}(k) \end{pmatrix} \tag{67}$$

and the associated ARMAX model is found to be

$$\hat{z}_{1,N}(k+2) = 2\hat{z}_{1,N}(k+1) - (1 + T_s^2 \frac{2K}{Dx^2}) \hat{z}_{1,N}(k) \\ + T_s v_N(k) + \kappa_1(k) \hat{e}(k+1) + (\kappa_1(k) - \kappa_2(k) T_s) \hat{e}(k) \tag{68}$$

where $\hat{e}(k)$ is the estimation error (innovation). The output of the ARMAX model can be also written in the product form

$$\hat{z}_{1,N}(k+1) = w(k) \cdot X^T(k) \tag{69}$$

where the weights vector is defined as

$$w(k) = \left(2, \ -(1 + T_s^2 \frac{2K}{Dx^2}), \ T_s, \ \kappa_1(k), \ \ (\kappa_1(k) - \kappa_2(k) T_s) \right) \tag{70}$$

and the regressor vector is defined as

$$X(k) = \left(\hat{z}_{1,N}(k), \ \hat{z}_{1,N}(k-1), \ v_N(k-1), \ \hat{e}(k), \ \hat{e}(k-1) \right). \tag{71}$$

Indicative results about the performance of the global χ^2 in detection of incipient changes of parameter K of the nonlinear wave PDE are depicted in Fig. 9. The fault threshold is set equal to the number of parameters in the associated ARMAX model, i.e., $\eta = 5$. It can be observed that the proposed FDI method was capable of detecting changes in parameter K which were less than 1% of the coefficient's nominal value. For small deviations from the parameter's nominal value the χ^2 test obtained a value that was several times larger than the fault threshold.

Remark 2 The contribution to biology of the article's methods on nonlinear PDE filtering and parametric change detection is summarized as follows. The paper considers that the

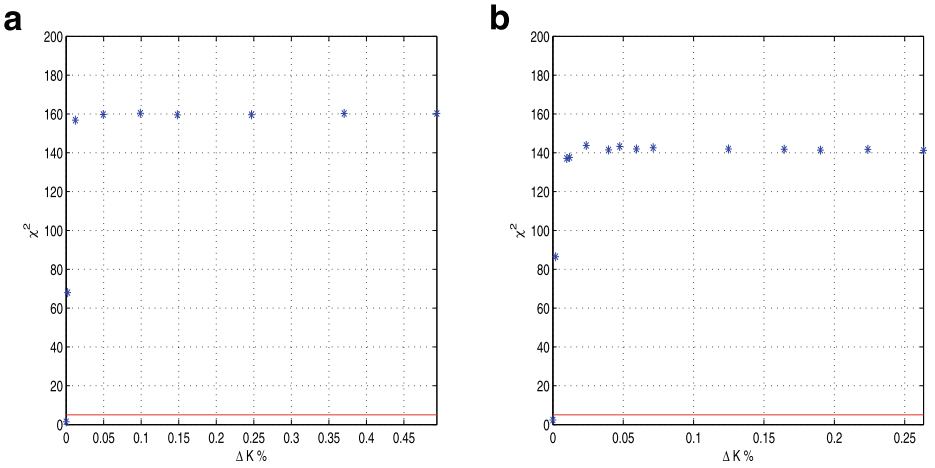

Fig. 9 Detection of incipient changes in the coefficient K of the nonlinear wave equation using the χ^2 test (**a**) nominal value $K = 0.04050$ (**b**) nominal value $K = 0.05050$

dynamics of the DNA molecule is represented by a set of coupled nonlinear oscillators and the associated motion is equivalent to a wave-type nonlinear partial differential equation. Parametric changes in the DNA structure imply also changes in the wave-dynamics. Thus by measuring specific oscillatory characteristics of the DNA molecule and by processing them with the local statistical approach to fault diagnosis it is possible to detect changes in the DNA structure. Such changes can be the result of a disease or of pharmaceutical treatment (see [31–33]). For example, one can obtain information about the effects that specific chemotherapy drugs have on the DNA molecule.

Remark 3 Fault diagnosis is equivalent to parametric change detection and change isolation, with the difference that the parameter change is considered to have a negative effect on the system's condition, that is to be a fault. In the case of change detection for the parameters defining the wave-type dynamics of the DNA molecule one can find out if there is variation of their coupling strength parameters (hydrogen bonds) from their nominal values. Should the nominal values be associated with the healthy condition of the DNA molecule then any deviation from these parameters can be interpreted as a fault, leading to a disease condition. On the contrary, there may be cases in which the deviation of coupling strength parameters from their initial values can be desirable. This happens for instance in the case of chemotherapy treatment where the role of the chemotherapy drugs is to modify the structural properties of the DNA molecule.

Remark 4 The paper has dealt only with the detection of changes in the parameters of the DNA molecule (and of the associated nonlinear wave PDE) and not with the estimation of these parameters. However, the estimation problem is linked to the detection problem and the Kalman filter can be also used for parameter estimation in the least mean squares sense. As it has been shown, the DNA molecule dynamics takes the form of the state-space model of (25) and (26). In the case of parameter estimation one will consider in place of (25) a new state update equation, in which instead of the state variables vector the parameters vector will be used. The measurement equation given in (26) can be kept as it is. For this

modified state-space description one can perform again Kalman filtering, and the outcome of the filter's recursion will be the estimated parameters vector [21]. Finally, about possible approaches for obtaining measurements from the DNA molecule one can note fluorescence microscopy, optical tweezers and atomic force microscopy [34, 35].

Remark 5 Stochasticities in the form of additive input variables in the state-space model of the wave PDE are implied throughout the paper, and this also holds for (1) and (27). The purpose in using the Kalman filter for solving the state estimation problem, instead of a deterministic observer, is that when taking measurements at the various points of the spatial grid of the PDE, these measurements are affected by noise. The characteristics of this noise are determined by the process and measurement noise covariance matrices Q and R, which are described in the Kalman filter recursion of (31) and (32).

7 Conclusions

The paper has proposed state estimation and parametric change detection in PDE systems with a new nonlinear filtering approach, the so-called *derivative-free nonlinear Kalman filter*. In particular the paper is concerned with the Peyrard-Bishop-Dauxois model of the DNA dynamics which takes the form of a wave partial differential equation. The method is based into decomposition of the nonlinear partial differential equation that describes the dynamics of the distributed parameter system, into a set of nonlinear ordinary differential equations. Next, with the application of a change of coordinates (diffeomorphism) that is based on differential flatness theory, the local nonlinear differential equations are turned into linear ones. This enables to describe the PDE dynamics with a state-space equation that is in the linear canonical (Brunovsky) form. For the linearized equivalent of the PDE system it is possible to perform state estimation with the use of the standard Kalman filter recursion. Unlike other nonlinear filtering methods, such as the extended Kalman filter, the proposed approach does not require the computation of partial derivatives and Jacobian matrices. Moreover, it avoids the cumulative numerical errors which appear in distributed extended Kalman filtering and which are due to truncation of higher order terms in the Taylor expansion of the system's dynamical model. Thus, the proposed filtering method succeeds improved accuracy in the estimates of the PDE system which describes the DNA dynamics.

Next, the *local statistical approach to fault diagnosis* has been proposed for performing detection of incipient changes in the Peyrard-Bishop-Dauxois model of the DNA dynamics. To this end, statistical processing of the differences (residuals) between the Kalman filter's outputs and measurements from the PDE system that described the DNA dynamics have undergone statistical processing. Detection and isolation of parametric changes with the local statistical approach have two significant advantages. First, it provides a credible criterion (χ^2 test) to detect changes in the parameters of the PDE system. This criterion is more efficient than the normalized square error and mean error tests since it employs the modeling error derivative and records the tendency for change. Thus early change detection of parametric changes in the DNA molecule becomes possible. The second advantage is that it recognizes the parameters of the Peyrard-Bishop-Dauxois PDE model that have undergone a change. Thus fault isolation becomes possible as well. The efficiency of the derivative-free nonlinear Kalman filter in parametric change detection has been confirmed through simulation experiments in the case of the 1D-wave equation that was consider to describe the Peyrard-Bishop-Dauxois DNA dynamics.

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