

Inference of couplings between variables of a given system using causal wavelets, causal information, equations reconstruction, and other techniques

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ABSTRACT

To infer directional couplings from variables is a difficult problem in dynamical systems, especially when its variables are taken from the real world. Many approaches have been developed to infer such couplings directly from observational time series. The objective of the present study is to investigate the capabilities of a set of techniques in test situations where the dynamics are governed by either fully deterministic (ordinary differential) equations or partially deterministic equations (the same ones with a stochastic perturbation added, the deterministic part remaining dominant).

The studied system is based on two three-dimensional chaotic subsystems with very different dynamics, but similar structure, considering various couplings between them (none, unidirectional, bidirectional). One system is dissipative, and the other one is conservative. The time evolution produced by their variables is clearly correlated with one system, almost totally decorrelated with the other one. The following techniques, some of which are introduced in this study, are considered: simple/causal correlation, mutual/causal information, Granger causality index, cross/causal wavelet coherence, bivariate global modeling, and equation reconstruction techniques.

All the techniques are evaluated based on their ability to detect direct and indirect causal relationships. Most of them prove poorly capable of detecting direct couplings and are not really robust in the contexts with low variable correlation, external weak couplings, and stochastic perturbations. Applied to the current problems, the bivariate modeling and the equation reconstruction techniques, both based on a global modeling technique, appear to be the most effective approaches to infer causality. The detection of weak bidirectional couplings appears particularly challenging under noisy conditions. Causal detection is tested on a set of groundwater level observational time series, revealing deterministic but complex couplings between three sub-basins of the Se San River basin (Central Highlands, Vietnam).

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Inferring causal relationships between observed variables is a common, but often difficult, problem in open environments, where dynamics typically result from multiple and nested interactions. In this study, different approaches are tested in a context presenting a great diversity of dynamical relationships. Two chaotic systems with similar structure but very different dynamics are used for this purpose, coupled to each other under

different types of weak coupling. One system is highly dissipative and has a high level of correlation between its variables. Another is conservative and its variables are almost completely uncorrelated. The analyses reveal that most of the techniques tested here can detect which system a variable belongs to, but few of them are able to reconstruct the directional links between the variables. This also shows that most approaches are not applicable to

strongly decorrelated variables and poorly robust to noise. The bivariate global modeling technique and, more particularly, the equation reconstruction technique are found to be the most effective and robust approaches when applied to these contexts. These latter are proven effective in real-world applications by applying them to a set of groundwater level observation time series, revealing a complex coupling between three sub-basins in the Vietnamese Central Highlands.

I. INTRODUCTION

In physics and in most of the natural sciences, causality refers to the relationship between causes and effects with the principle that an effect cannot occur before the cause due to the arrow of time. Identifying causal relationships is a very fundamental step in science to understand the time evolution of any dynamics. Though, causal relations are—in practice—particularly challenging to investigate from observations.

The first difficulty is to define causation, which depends on the description of the dynamics. Two paradigms can be used to think and describe dynamical behaviors: determinism and stochasticity. By definition, a dynamic is deterministic if its state at time t entirely and uniquely defines the state at time $t + dt$ immediately after. A stochastic dynamic can be defined as a random process characterized by unpredictability, even in a very short term. In this paper, causality will be considered strong when it results from deterministic processes and weak when it results from stochastic processes. The main objective of this study will be to test and compare techniques for inferring causal couplings—in the strong sense—between variables of a given system.

Although deterministic, some dynamical systems can be unpredictable due to a high sensitivity to the initial conditions.^{1–4} This type of dynamical regime is called chaotic. This is an important assertion here since this means that, even under strong determinism, causality detection may have to cope with unpredictability.

Dynamical regimes such as chaotic and stochastic make the definition of a finalist causality particularly difficult. Indeed, if a very small perturbation of the system state may completely change the effect after a sufficiently long time, due to either high sensitivity or stochasticity, then any attempt to explain a final situation B at time $t + \Delta t \gg t$ as the causal effect of the situation A at time t may be illusory. For this reason, probabilistic definitions of causality have progressively been promoted.⁵ Unfortunately, such a point of view does not account for any underlying determinism, which is unsatisfying given that unpredictability can also result from deterministic processes. To have a proper description of the causal chain, the deterministic part should be distinguished from the stochastic part. Moreover, instead of focusing on a finalist view, a dynamical view of causation may advantageously be fostered.

For this reason, a general definition involving both the deterministic and the stochastic contributions such as

$$\frac{dX_t}{dt} = \mathcal{F}(X_t) + \mathcal{G}(X_t) \cdot \varepsilon_t \quad (1)$$

should be fostered, with X_t being the state of the system at time t , $\mathcal{F}$ being the vector field representing the deterministic laws of evolution, and $\mathcal{G}$ being the vector field defining the coupling of the system with a noise ε_t . For the present context, ε_t will be assumed to be a white noise of Gaussian distribution, and the coupling will be chosen such as $\mathcal{G} = 1$ in order to have a noise of Brownian type without any privileged direction and magnitude.

Determining the causal effect from situations A to B will consist in identifying all the deterministic and stochastic factors that have contributed to the evolution from state A to state B—all other things remaining equal (or equivalent). This work will focus here on deterministic causality. Determining the causal effect in the strong sense will consist in reconstructing the deterministic part $\mathcal{F}$ of Eq. (1), or a good approximation of it, also enabling to reconstruct the fluence diagram between the variables of X_t . In the present work, stochasticity will be used to blur the hidden determinism.

Numerous techniques have been introduced to detect unknown relationships directly from observational time series. The simple (linear) correlation (SC)⁶ is an emblematic example of this problem: Although commonly used as a preliminary step to investigate potential relationships between variables, it cannot apply to causality detection because its formulation is symmetric whereas causality is directional. It is also known to be very poorly adapted to nonlinear contexts.^{7–9} Although also symmetric in its definition, the Mutual Information (MI)⁹ may overcome some of these limitations since, in principle, it is sensitive also to dependencies that do not manifest themselves in the covariance.¹⁰ In such symmetric situations, the anteriority between events A and B may be used to investigate the who's who in a cause-and-effect perspective. However, this may only permit a qualitative detection of causality that may not allow to argue robustly for a causal link.

Some approaches^{11,12} have been developed to detect causality in deterministic contexts. The Takens' embedding theorem served this purpose, for which delay coordinates are used to reconstruct the phase space. The idea is to investigate whether it is possible to establish a directional correspondence between the phase space reconstructed from two observed variables. In practice, the use of a correspondence between different state spaces reconstructed by embedding from different variables does not depend on time (see Appendix A), which may generate difficulties when trying to detect directional relationships. Moreover, the possibility to reconstruct X from Y or Y from X will also depend on observability.¹³ Despite these limitations, some embedding approaches were proven useful in eliminating false connections¹⁴ and in detecting connections in highly complex causal networks.¹⁵

Based on wavelet transforms,¹⁶ cross wavelets¹⁷ can be used to get cross information between time series to detect localized correlation in both frequency and time.¹⁸ It has proven to be powerful to detect couplings when these are sufficiently strong enough to generate a certain level of synchronization, even temporarily.¹⁹ It can also provide phase information between signals, which may help in the detection of directional couplings.¹⁸ Interestingly, some early works have tried to define a wavelet for causation;²⁰ however, these apply to univariate time series only and, therefore, cannot be expected to detect a relationship between cause and effect, but rather breakups, shocks, or sudden changes.

The Granger causality²¹ is a modeling approach of causal detection. It takes its idea from Wiener²² and is based on predictability. Basically, the idea is that if variable X has an influence on Y , then information from X should improve the (short-term) forecasting of Y .

Equation reconstruction techniques can also be used to unveil causal relationships.^{23–26} Their aim is to obtain interpretable equations directly from observational time series. As such, it can be categorized as a data-driven or as a machine learning approach. Deep learning may be used for this purpose, but it is not mandatory and it may probably be suboptimal since an artificial neural network is not required to get equations from time series. Equation reconstruction takes its origin from electrical engineering and statistics^{27,28} for the problem of system identification²⁹ and from the theory of nonlinear dynamical systems³⁰ for the problems of state space reconstruction (from a subset of observations)³¹ and for the sensitivity to the initial conditions.^{32,33} Taken together, these fields have led to the development of the global modeling technique.³⁴

Equation reconstruction has recently acknowledged a boom of interest.^{35,36} However, most of the previously developed techniques are not adapted to detect causal relationships because either they require that all the system variables are observed,²⁵ which is rarely the case, or they were designed to model the dynamics from a single variable.^{32,33,37} Moreover, few of them were proven able to tackle problems directly based on observational time series taken from the real world.

Developed by one of us, the algorithms used in the present study belong to the global modeling approach: it aims to reproduce the original dynamics in the phase space as a whole, possibly from a sub-ensemble of observed variables. It can apply, in principle, whatever the number of variables is observed. It can, thus, be used to detect causal relationships between two variables (the minimum required to investigate causation) or more. Moreover, it has proven its applicability not only to theoretical cases but also to numerous problems of the real world in epidemiology and eco-epidemiology,^{24,38} hydrology and soil eco-hydrology,^{39,40} cave hydro-aerology,⁴¹ etc.

All the techniques tested in the study are introduced in Secs. II A–II D. For the techniques originally presenting a symmetry between the variables (correlation, mutual information, cross wavelets transform), a causal version will also be proposed by introducing a dissymmetry.

Both synthetic data sets and observational time series gathered from the real world are considered in the study, which are all presented in Sec. III. The results of the analyses are given in Sec. IV for the synthetic cases, without coupling (Sec. IV B) and then with unidirectional (Sec. IV C) and bidirectional coupling (Sec. IV D). The analyses of the observational time series are presented in Sec. IV E. A conclusive discussion is then provided in Sec. V.

II. THEORETICAL BACKGROUND

A. Continuous, cross, and causal wavelets transforms

The continuous wavelets transform (CWT)⁴² consists of applying a zero mean function localized in both time and frequency

(a wavelet), as bandpass filter to a time series. The Morlet wavelet

$$\Psi_0(\tau) = \pi^{-\frac{1}{4}} e^{i f_0 \tau} e^{-\frac{\tau^2}{2}}, \quad (2)$$

with τ and f_0 dimensionless time and frequency, and i such as $i^2 = -1$ was used in this analysis, with $f_0 = 6$ for a good balance between time localization and frequency identification. For a time series of uniform time step δt , the CWT is defined as

$$w_x^k(s) = \sqrt{\frac{\delta t}{s}} \sum_{k'=1}^N x_{k'} \Psi_0^* \left[(k' - k) \frac{\delta t}{s} \right], \quad (3)$$

where $*$ represents the complex conjugate, s is the scale factor defined as $\tau = s t$, and x_k refers to the k th element of the observed time series $x(t)$ of length N .

The cross wavelets transform (XWT)^{43,44} is defined for two signals $x(t)$ and $y(t)$, as the result of cross spectrum

$$W_{xy}(s, \tau) = X(s, \tau) Y^*(s, \tau), \quad (4)$$

with $X(s, \tau)$ being the wavelets coefficients of the CWT resulting from $x(t)$, $Y^*(s, \tau)$ being the conjugate wavelets coefficients of the CWT resulting from $y(t)$, s being the scaling factor, and τ being the temporal translation. The delay between the two time series, for a given time scale s at time t , can be estimated too as the phase

$$\phi = \arg(W_{xy}(s, t)). \quad (5)$$

The cross wavelet coherence (XWC) is then defined as

$$C_{xy}(t, f) = \frac{\| \langle W_{xy}(t, f) \rangle \|}{\| \langle W_{xx}(t, f) \rangle \|^{1/2} \| \langle W_{yy}(t, f) \rangle \|^{1/2}}, \quad (6)$$

where $\langle \cdot \rangle$ denotes a time–frequency smoothing function. Its value can vary between 0 and 1 corresponding to the minimum to maximum levels of local correlation at a given time and scale. In comparison to simple correlation, it can reveal similarities specific to a scale, for a temporary time.

The causal wavelets transform (KWT) is introduced here as a variant of the cross wavelet transform that we propose for the detection of causality and that we define as a cross wavelet transform applied to two specific variables: the first one being a time derivative. To replace one variable by its derivative in the XWT comes from the following reasoning: If x is deterministically governed (strong causality), with a contribution by y , then we will have $\dot{x} = f(y, z_1, \dots, z_n)$ with z_n being other causal terms. As a consequence, we will then have a strong relationship between $\dot{x}$ and $f(y, z_1, \dots, z_n)$ and we may also have a permanent relation between $\dot{x}$ and y if the relation between y and $f(y, z_1, \dots, z_n)$ is sufficiently simple. The KWT

$$W_{xy}(s, \tau) = X(s, \tau) Y^*(s, \tau) \quad (7)$$

is, thus, a specific case of the XWT, that is, with $X(s, \tau)$ being the wavelets coefficients of the CWT obtained from $\dot{x}(t)$ the temporal derivative of $x(t)$. The annotation $\dot{\cdot}$ is used to clearly distinguish the type of analysis since it can lead to specific properties (see Appendix B). Here also, the delay can be estimated as $\phi = \arg(W_{xy}(s, t))$ at given time t and scale s .

Although being a specific case of XWT, KWT is expected to enable a higher potential of coupling detection since being asymmetric and more specific in its principle: If one variable y acts on another variable x , it will generate variations on x and its variations in time, that is $\dot{x}(t)$, should be linked to y , although $x(t)$ and $y(t)$ may have different dynamics (therefore, KWT will not require any correlation between them). The causal wavelet coherence (KWC) is defined as

$$C_{xy}(t, f) = \frac{\| \langle W_{xy}(t, f) \rangle \|}{\| \langle W_{xx}(t, f) \rangle \|^{1/2} \| \langle W_{yy}(t, f) \rangle \|^{1/2}}. \quad (8)$$

A value close to 0 will reflect the absence of causality. To argue for causation, the coherence should be close to one ($C_{xy} \approx 1$) with a dephasing close to zero ($\phi_{xy} \approx 0$). However, self causation cannot be identified with these tools. Indeed, a causal coherence C_{xy} equal to 1 with a dephasing close to $\pi/2$ ($C_{xy} \approx 1$ and $\phi_{xy} \approx \pi/2$) may only reflect a self coherence without causation (see Appendix B, Proposition 2).

In Sec. IV, scalograms will be shown (e.g., Figs. 6–8 under free of noise conditions). These scalograms present the wavelet coherence (XWC, KWC) between different couples of variables in a (time, scale) plane representation. The yellow areas correspond to scale and time localizations associated with a high coherence. The arrows on these figures show the phase of the complex-valued XWT/KWT defined by Eqs. (4) and (7) (here, the horizontal arrows pointing to the right are read as 0° , while vertical arrows pointing upwards represent a $+90^\circ$ phase offset). On the vertical axis, the larger scales are represented on the higher part of each subplot individual figure.

For a signal $x(t)$ with Fourier transform equal to $X(\omega)$, it is well known that the derivative of x has a Fourier transform $FT[\dot{x}(t)] = i\omega X(\omega)$, which leads to a phase offset of 90° between $x(t)$ and $\dot{x}(t)$. A similar property holds approximately for the phase of the complex-valued cross-wavelet transform of $\dot{x}(t)$ and $x(t)$ at least when using a complex-valued Morlet wavelet (see Appendix B).

Hence, the following observations are expected: the XWT of positively correlated synchronous signals should lead to a good level of coherence (close to 1) and a phase offset close to 0° , while the phase offset should become equal to $\pm 180^\circ$ for anti-correlated signals in phase opposition. The XWT of two signals in phase quadrature, such as a signal and its derivative, can therefore lead to a high coherence at most scales and positions with a phase offset of $\pm 90^\circ$.

In the case of a strong causality, for example, $\dot{x} = ay$, the XWC (C_{xy}) and the KWC C_{xy} should differ, with a higher wavelet coherence in the second case since $\dot{x}(t)$ and $y(t)$ will differ by a multiplicative coefficient only, whereas $x(t)$ and $y(t)$ may be very different time series. For the same reason, they should also differ in their phase offset (90° and 0° , respectively, at least when no noise is present).

The analyses presented in the paper were performed using the Wavelet toolbox⁴⁵ that were compared to the results obtained with the Wavelet coherence toolbox.⁴⁶ Results were found to be very similar except a net smoothing at very short time scales in the latter case.

B. The global modeling technique

The global modeling technique aims to obtain continuous, discrete, or delayed equations from observational time series.^{33,34,47} The present work will focus on the continuous case, more precisely on equations of ordinary differential form (ODEs). Given a dynamical system governed by a set of ODEs

$$\begin{cases} \dot{x}_1 = f_1(x_1, x_2, \dots, x_n), \\ \dot{x}_2 = f_2(x_1, x_2, \dots, x_n), \\ \vdots \\ \dot{x}_n = f_n(x_1, x_2, \dots, x_n), \end{cases} \quad (9)$$

and given an ensemble of measurements $\{\mathbf{X}^{\text{obs}}\}$ of this system such as $\mathbf{X} = \mathbf{h}(\mathbf{x})$, with $\mathbf{h}$ being the measurement functions, it is expected to retrieve an ensemble of n equations

$$\begin{cases} \dot{X}_1 = \hat{F}_1(X_1, X_2, \dots, X_n) + \varepsilon_1, \\ \dot{X}_2 = \hat{F}_2(X_1, X_2, \dots, X_n) + \varepsilon_2, \\ \vdots \\ \dot{X}_n = \hat{F}_n(X_1, X_2, \dots, X_n) + \varepsilon_n, \end{cases} \quad (10)$$

with $\hat{F}_j$ being the n functions to be identified (in both structure and parameterization) that will be a good approximation of the original system (9) and ε_j being a residual noise. The degree d^j of explained determinism of variable j is defined as

$$d_{X_j}^o = 100 - \frac{\sigma_{\hat{X}_j - \hat{F}_j(X_1, X_2, \dots, X_n)}^2}{\sigma_{\dot{X}_j^{\text{obs}}}^2} \times 100. \quad (11)$$

When a subset of variables is observed, a generalized canonical form can be used. For instance, in the case of two variables X_1 and Y_1 related to x_i and x_j in the original system Eq. (9), the following form

$$\begin{cases} \dot{X}_1 = X_2, \\ \vdots \\ \dot{X}_m = \hat{F}_X(X_1, \dots, X_m, Y_1, \dots, Y_p) + \varepsilon_X, \\ \dot{Y}_1 = Y_2, \\ \vdots \\ \dot{Y}_p = \hat{F}_Y(X_1, \dots, X_m, Y_1, \dots, Y_p) + \varepsilon_Y, \end{cases} \quad (12)$$

can be used with X_2 to X_m and Y_2 to Y_p the successive derivatives of, respectively, the observed variables X_1 and Y_1 , $m + p$ the model dimension, and $\hat{F}_X$ and $\hat{F}_Y$ two functions to be identified.

The Generalized global Polynomial Modeling (GPoM) package version 1.4, developed at the *Centre d'Etudes Spatiales de la Biosphère*, was used for this purpose.⁴⁸ It involves two algorithms. The first one aims to perform a structure pre-selection, providing an ensemble of candidate models, each presenting the smallest residual error for a given number of monomials in the equations. The second algorithm aims to test the numerical integrability and the solution at the convergence. To be kept after integration, a model should be, at least: (1) numerically integrable, (2) nontrivial (as far as the original dynamic is not), and (3) its variables should reproduce the same order of magnitude as the original ones. It will not be necessary

to accurately reproduce the original dynamics in the phase space: a rough model should be sufficient to detect the main couplings and the main causal terms. More accurate models may be needed to detect weak couplings and causal terms of lower contribution.

A detailed protocol of its use can be found in Ref. 26. More specifically, when applied to bivariate modeling, the number of derivatives was supposed to be *a priori* unknown. When trying to detect a coupling between X_1 and Y_1 , all the combinations of m and p were tried and the model dimension $m + p$ was progressively increased (from 2 to a maximum 6) until a satisfying model could be obtained. Note that models of dimension two were systematically rejected. Indeed, as guaranteed by the theorem of Poincaré-Bendixson, a two-dimensional system can produce only period-1 oscillations or fixed points. Therefore, to reproduce the complexity of the R76 or NH systems, an additional dimension is required to reconstruct the original dynamic.

The possibility to obtain equations directly from observational time series will not only depend on the capacities of the used algorithm but also on the observability of the system as seen from a set of variables^{49,50} (Examples taken from multivariate embeddings⁵¹ are presented in Appendix E in the [supplementary material](#).)

C. Statistical indicators

Four statistical indices were also considered for comparison: (1) the simple correlation (SC)

$$C_{XY} = \frac{\text{Cov}(X, Y)}{\sigma_X \sigma_Y}; \quad (13)$$

(2) the causal correlation (KC)

$$C_{XY}^K = \frac{\text{Cov}(\dot{X}, Y)}{\sigma_{\dot{X}} \sigma_Y}; \quad (14)$$

(3) the Mutual Information (MI)^{6,10}

$$I_{XY} = \sum_{j,k}^N p_{XY}(j, k) \log \frac{p_{XY}(j, k)}{p_X(j) p_Y(k)}, \quad (15)$$

with N being the number of closest points (j, k) ; and (4) the Causal Information (KI)

$$I_{XY}^K = \sum_{j,k}^N p_{\dot{X}Y}(j, k) \log \frac{p_{\dot{X}Y}(j, k)}{p_{\dot{X}}(j) p_Y(k)}. \quad (16)$$

To replace one variable by its derivative in (SC) and (MI) to get, respectively, (KC) and (KI) follows the same reasoning as passing from (XWT) to (KWT) (see Sec. II A).

D. Granger causality index

The Granger causality was introduced in the 1960s to detect causal relations between couples of variables. To investigate the influence of variable X on variable Y , two Vector Auto Regressive

models are built. Model M_1

$$Y(t) = a_0 + \sum_{j=1}^p a_j Y(t - j\delta t) + \varepsilon(t), \quad (17)$$

based on variable Y exclusively, and model M_2

$$Y(t) = a_0 + \sum_{j=1}^p a_j Y(t - j\delta t) + \sum_{j=1}^p b_j X(t - j\delta t) + \eta(t), \quad (18)$$

based on both variables X and Y , where the a_j and b_j are the model parameters estimated empirically, p is the lag parameter, δt is the sampling time, and $\varepsilon(t)$ and $\eta(t)$ are centered white Gaussian noises. If X improves the prediction of Y , then the error of model M_2 should be lower than the one of model M_1 . The variances σ_1 and σ_2 are used to quantify the causality using the Granger Causal Index (GKI)

$$G_{XY} = \log \left(\frac{\sigma_\varepsilon^2}{\sigma_\eta^2} \right). \quad (19)$$

In practice, δt was chosen equal to the original data sampling.

III. DATA

A. Independent dynamical systems

Ideally, a coupling detection technique should be able to unveil deterministic coupling even if the dynamic is highly unpredictable and whatever the level of correlation between the observed variables. Two chaotic systems are characterized by similar structures (see Fig. 1), but very different dynamics were chosen for the study. Introduced by Otto E. Rössler in 1976, his eponym system⁵²

$$\begin{cases} \dot{x} = -y - z, \\ \dot{y} = x + a_1 y, \\ \dot{z} = a_2 + z(x - a_3), \end{cases} \quad (20)$$

is three-dimensional and strongly dissipative. It has seven terms including only one nonlinear. For the parametrization $(a_1, a_2, a_3) = (0.432, 2., 4.)$, it produces a phase-coherent chaos (Fig. 2) characterized by a relatively high correlation level between x and the two other variables ($C_{xy} = -0.412$; $C_{xz} = +0.643$; $C_{yz} = -0.123$). Its dynamic is said phase-coherent because a roughly constant pseudo-period is required to complete a revolution around the attractor.⁵³

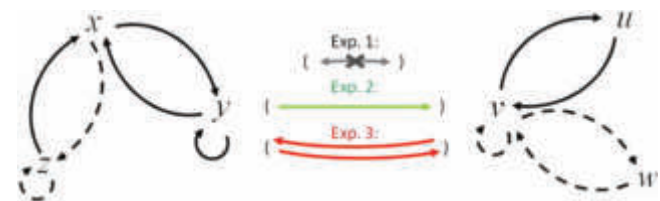


FIG. 1. Fluence diagram (in black) relating to Eq. (22) with the coupling coefficients relating to experimentations 1 (in gray), 2 (in green), and 3 (in red) summarized in Eq. (23).

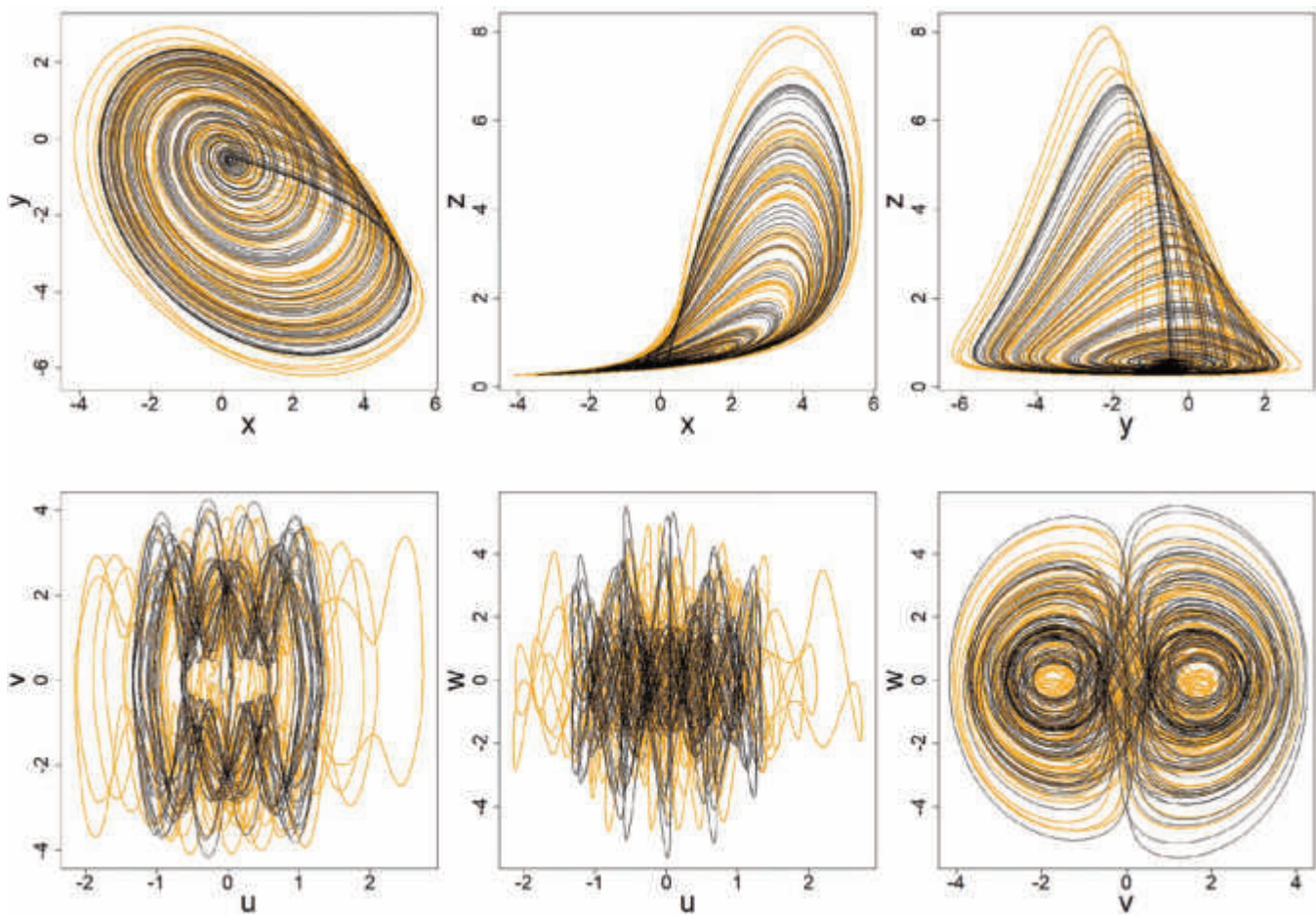


FIG. 2. Phase portraits of the Rössler (top line) and Nosé–Hoover (bottom line) systems, free of noise (in black), and with 0.01% dynamical noise (in orange), without coupling between the two systems.

Introduced ten years later, the Nosé–Hoover system^{54,55}

$$\begin{cases} \dot{u} = b_1 v, \\ \dot{v} = -u + vw, \\ \dot{w} = b_2 - v^2, \end{cases} \quad (21)$$

is also three-dimensional but conservative, and it has five terms only, including two nonlinear ones. For the parametrization $(b_1, b_2) = (0.2, 3)$, it produces a slow-fast behavior (Fig. 2) characterized by a quasicomplete decorrelation between its three variables ($C_{uv} = +0.025$; $C_{uw} = +0.142$; $C_{vw} = +0.016$). As a conservative system, different invariant sets can be obtained when using different initial conditions, as shown in Appendix F in the [supplementary material](#). Note, however, that, under external forcing or noisy perturbations, the system will not be isolated anymore. Therefore, the trajectory will not stay on any invariant set of the original NH system.

Without coupling, the two systems are independent and exhibit completely decorrelated cross portraits (Fig. 3). Time series generated by the two systems are shown in Fig. 4.

B. Coupled systems

To investigate the ability of the different techniques to detect weak couplings, coupling terms between the two systems were introduced in experiments including either unidirectional or bidirectional couplings. To test the robustness of the used techniques, simulations with dynamical noise were also performed. The six-dimensional R76-NH coupled system,

$$\begin{cases} \dot{x} = -y - z + \varepsilon_x, \\ \dot{y} = x + a_1 y + \kappa_{y \rightarrow y}(y - v) + \varepsilon_y, \\ \dot{z} = a_2 + z(x - a_3) + \varepsilon_z, \\ \dot{u} = b_1 v + \varepsilon_u, \\ \dot{v} = -u + vw + \kappa_{y \rightarrow v}(v - y) + \varepsilon_v, \\ \dot{w} = b_2 - v^2 + \varepsilon_w, \end{cases} \quad (22)$$

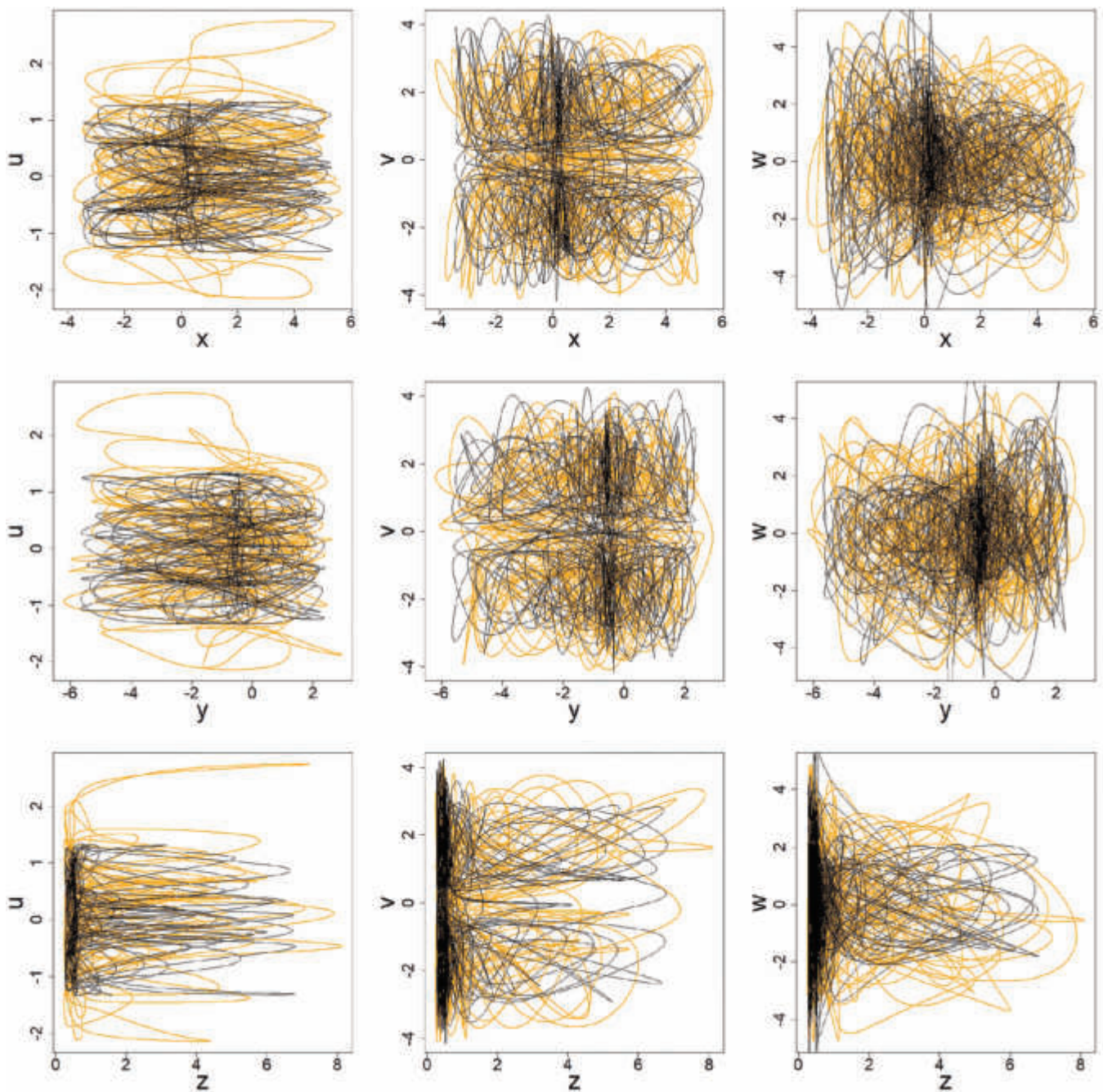


FIG. 3. Cross portraits of the Rössler and Nosé–Hoover systems without coupling between them, free of noise (in black) or with 0.01% dynamical noise (in orange).

was used with $\kappa_{y \rightarrow v}$ being the coupling parameter ensuring the action of the R76 system (through variable y) onto the NH system (on variable v), $\kappa_{v \rightarrow y}$ being the coupling parameter ensuring the action of the NH system (through variable v) onto the R76 system

(on variable y), and with ε_* being the centered Gaussian noise of percentage $p = \sigma_{\varepsilon_*}^2 / \sigma_{obs}^2 \times 100$. For $\kappa_{y \rightarrow v} = \kappa_{v \rightarrow y} = 0$, the two original three-dimensional systems (20) and (21) without coupling are retrieved. Three experiments will be considered, such as

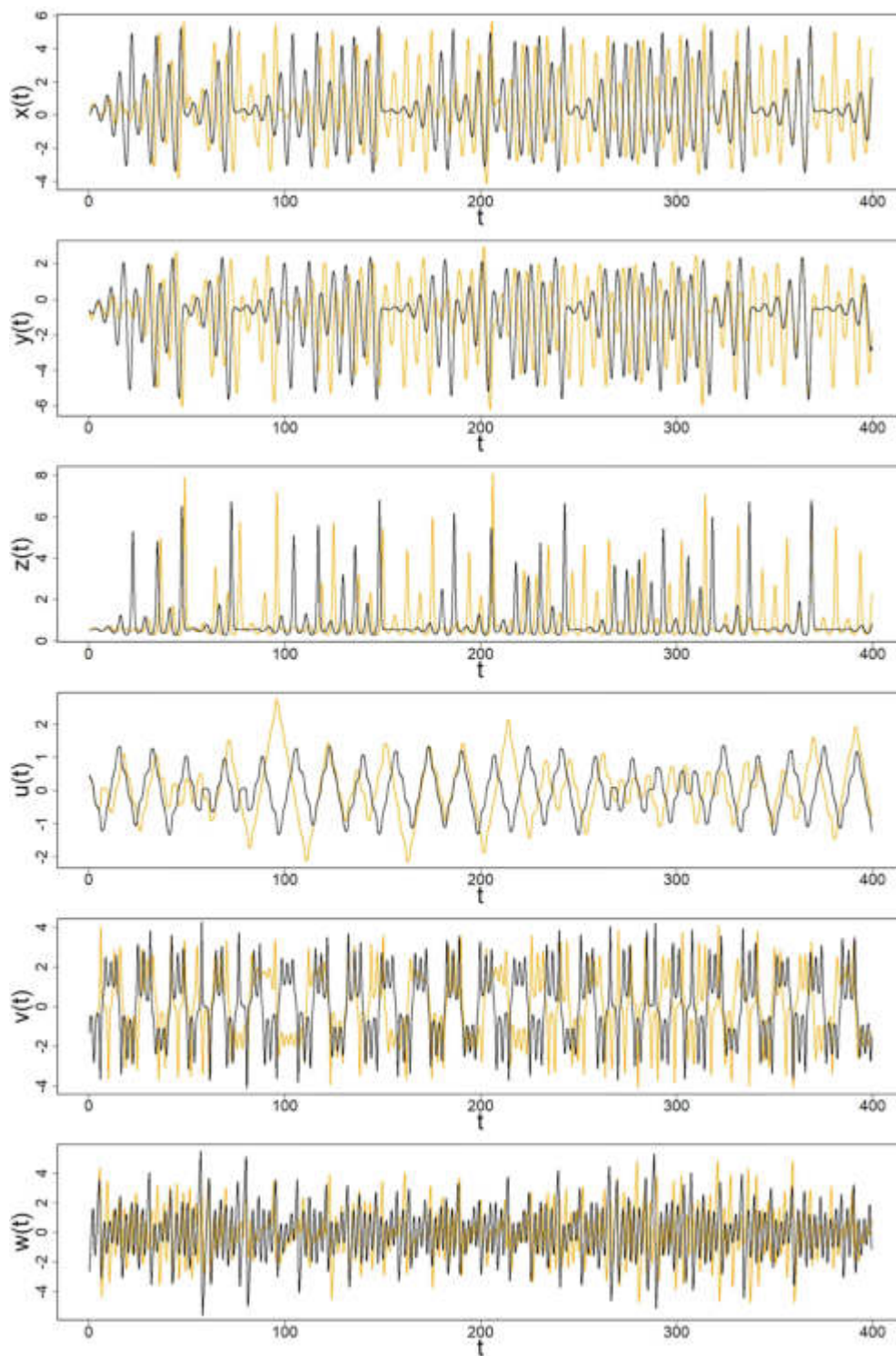


FIG. 4. Time series obtained by numerical integration of the Rössler and Nosé–Hoover systems without coupling, free of noise (in black), and with 0.01% dynamical noise (in orange).

$$\begin{cases} (1) & \kappa_{y \rightarrow v} = \kappa_{v \rightarrow y} = 0, \\ (2) & \kappa_{y \rightarrow v} = 0.8 \quad \& \quad \kappa_{v \rightarrow y} = 0, \\ (3) & \kappa_{y \rightarrow v} = \kappa_{v \rightarrow y} = 0.4, \end{cases} \quad (23)$$

free of perturbations to begin and then with a noise perturbation such as $p = 0.01\%$. In cases (2) and (3), the parameter values were chosen to generate a weak coupling, that is, sufficiently strong to modify the cross portraits close to a generalized synchronization,⁵⁶ but not enough to develop a clear synchronization between the coupled variables when considering the Lissajous plane, that is, cross portraits between the coupled variables.⁵⁷ The mean normalized synchronization error^{58,59} is commonly used to describe synchronization. It does not fully apply to the present analysis because the two systems are very different. Instead, the mean normalized synchronization error was reformulated as

$$E = \sum_i \frac{\sqrt{(v_i - y_i)^2}}{\sqrt{v_i^2 + y_i^2}}, \quad (24)$$

exclusively focusing on the coupled variables y and v . The coupling types are synthesized in Table I (see Appendix D in the supplementary material for more details).

TABLE I. Synchronization error E [see Eq. (24)] and coupling type.

	Experiment 1	Experiment 2	Experiment 3
Error E	0.88	0.66	0.78
Coupling type	None	Weak	Weak
Synchronization type	None	Generalized	Generalized

C. Environmental data set

To test the approaches under real conditions, a small set of environmental time series was also analyzed in the study. Three stations of groundwater level height from the *National Center for Water Resources Planning and Investigation* (NAWAPI) were considered on an 11-year long window for this purpose (Fig. 5). All are located in the Vietnamese Central Highlands, in the upper part of the Se San River basin (Kon Tum province, Vietnam).⁶⁰ Their coordinates are provided in Table II.

D. Experiments

In experiments (1)–(3), the analyses were first performed under free of noise conditions [$\varepsilon_* = 0$ in Eq. (22)]. The same analyses

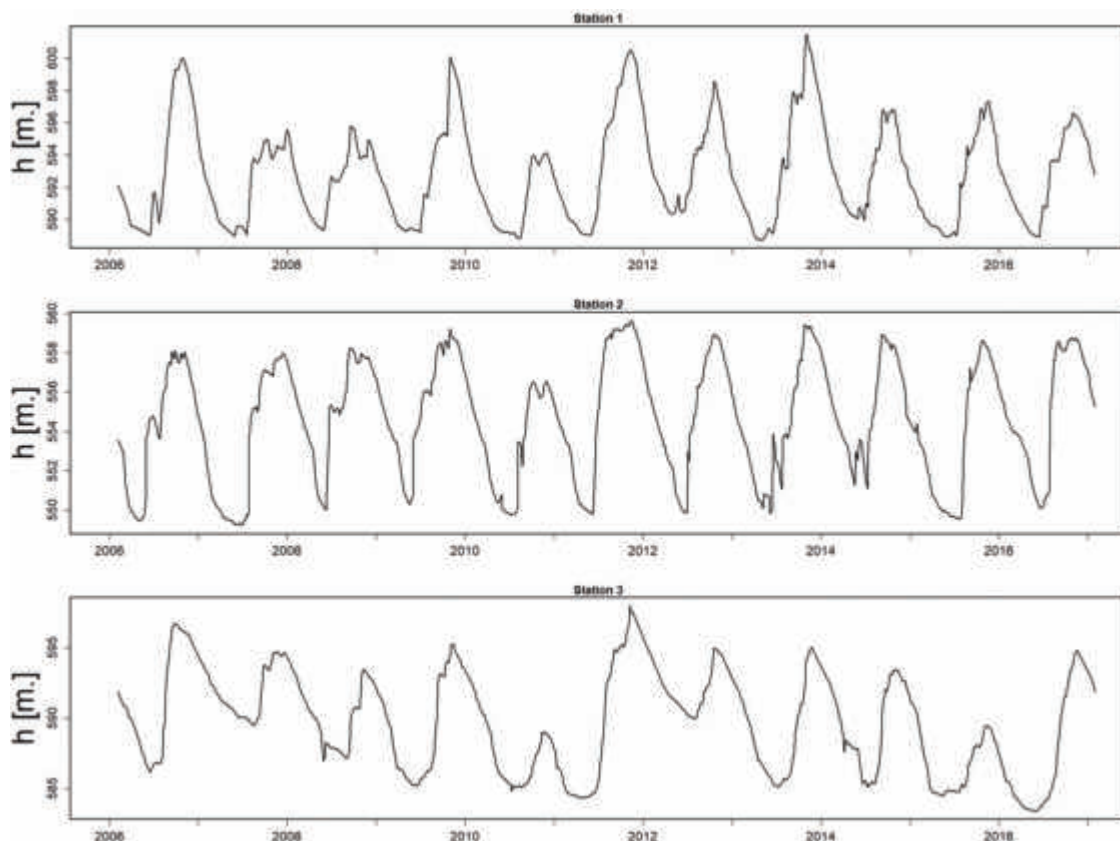


FIG. 5. Time series of groundwater level height, in meter above sea level, at three stations located in the Se San River basin (Central Highlands, Vietnam).

TABLE II. Coordinates of the three groundwater stations.

Height (m.a.s.l.)	Reference	Latitude (°N)	Longitude (°W)	Altitude (m)	Period (year)
h_1	LK137	14 603 103	107 884 645	607 498	2006–2017
h_2	LK140	14 417 464	107 970 804	563 026	2006–2017
h_3	LK63	14 175 687	107 871 595	599 217	2006–2017

were then performed again under stochastic perturbation such as $p = 0.01\%$.

For each experiment, the statistical indicators (SC, KC, MI, and KI) are estimated and the Granger Causality Index as well. The wavelet analyses are performed to generate the XWC and the KWC patterns. The global modeling is then applied considering the variables either two by two (bivariate modeling) or together all (equation reconstruction).

IV. RESULTS

A. Comparative results

The analyses were performed between the six variables (with their derivatives when required) for the three experiments, under both free of noise and noisy conditions. Detailed results for all the statistical indicators (SC, KC, MI, KI), the GKI, the bivariate modeling, and the equation reconstruction are all reported in Tables S2 and S3 in the [supplementary material](#), respectively, for free of noise and noisy conditions. The results of the wavelet analyses are shown in Figs. 6–8, and S8–S14, with additional details provided in Table S1 in the [supplementary material](#).

All these results are synthesized in Fig. 9 in confusion matrices to facilitate the comparison. In this synthesis, a coupling is considered detected even if indirect. Results concerning the detection of direct couplings are presented in Fig. S15 in the [supplementary material](#). The threshold of detection 0.4 was used for most of the criteria (SC, KC, XWC, and KWC). A different threshold of

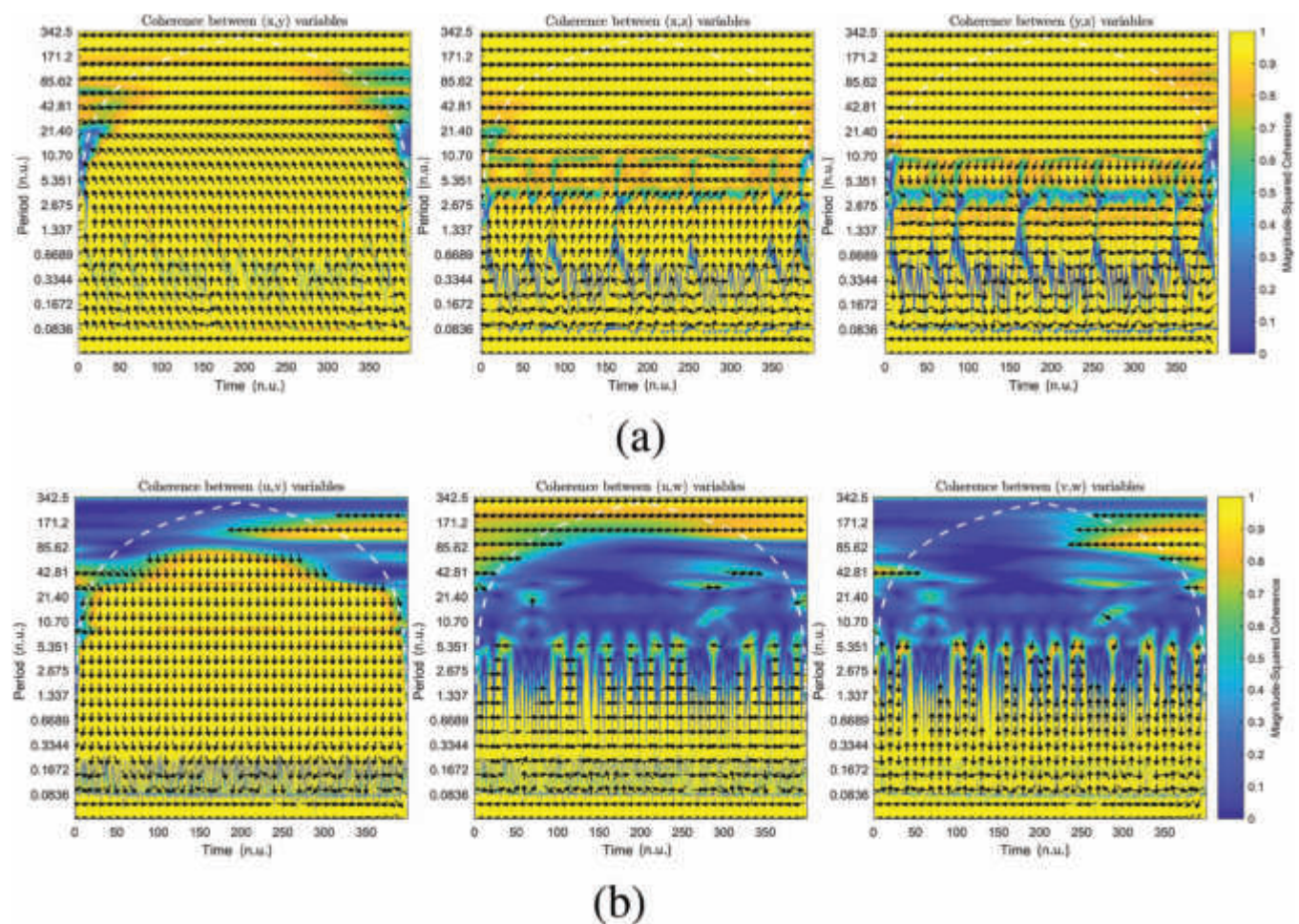


FIG. 6. Cross wavelet coherence XWC of the variables of the Rössler (a) and Nosé–Hoover (b) systems, free of noise. The definition of the cone of influence (dashed lines) is taken from Ref. 43 here and elsewhere. (a) XWC $C_{XY}(t, f)$ of (x, y) , (x, z) and (y, z) and (b) XWC $C_{XY}(t, f)$ of (u, v) , (u, w) and (v, w) .

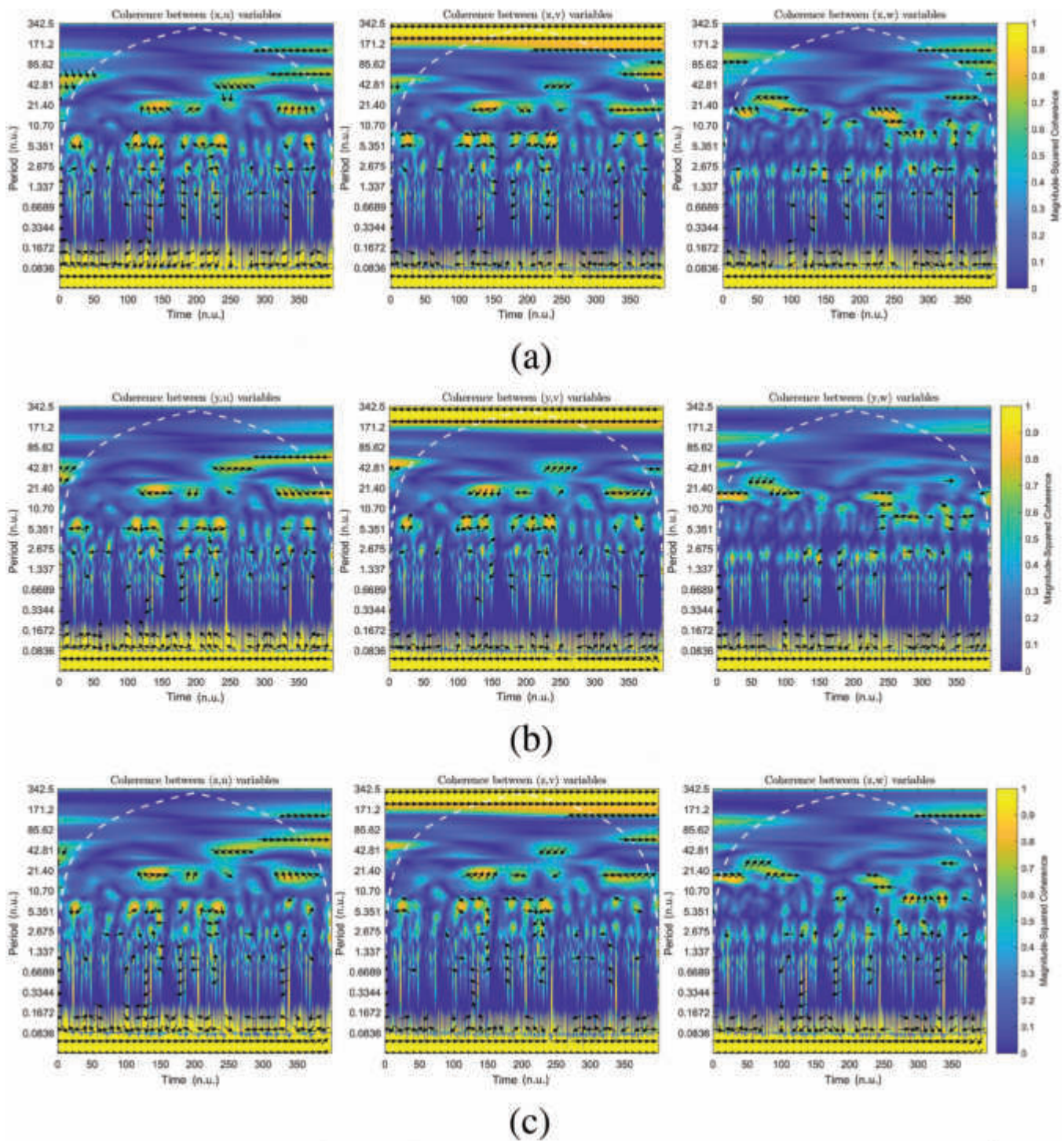


FIG. 7. Cross wavelet coherence of the variables interactions between Rössler variables x (a), y (b), and z (c) with the variables u , v , and w of the Nosé–Hoover system under free of noise conditions. (a) XWC $C_{XY}(t, f)$ of (x, u) , (x, v) , and (x, w) ; (b) XWC $C_{XY}(t, f)$ of (y, u) , (y, v) , and (y, w) ; and (c) XWC $C_{XY}(t, f)$ of (z, u) , (z, v) , and (z, w) .

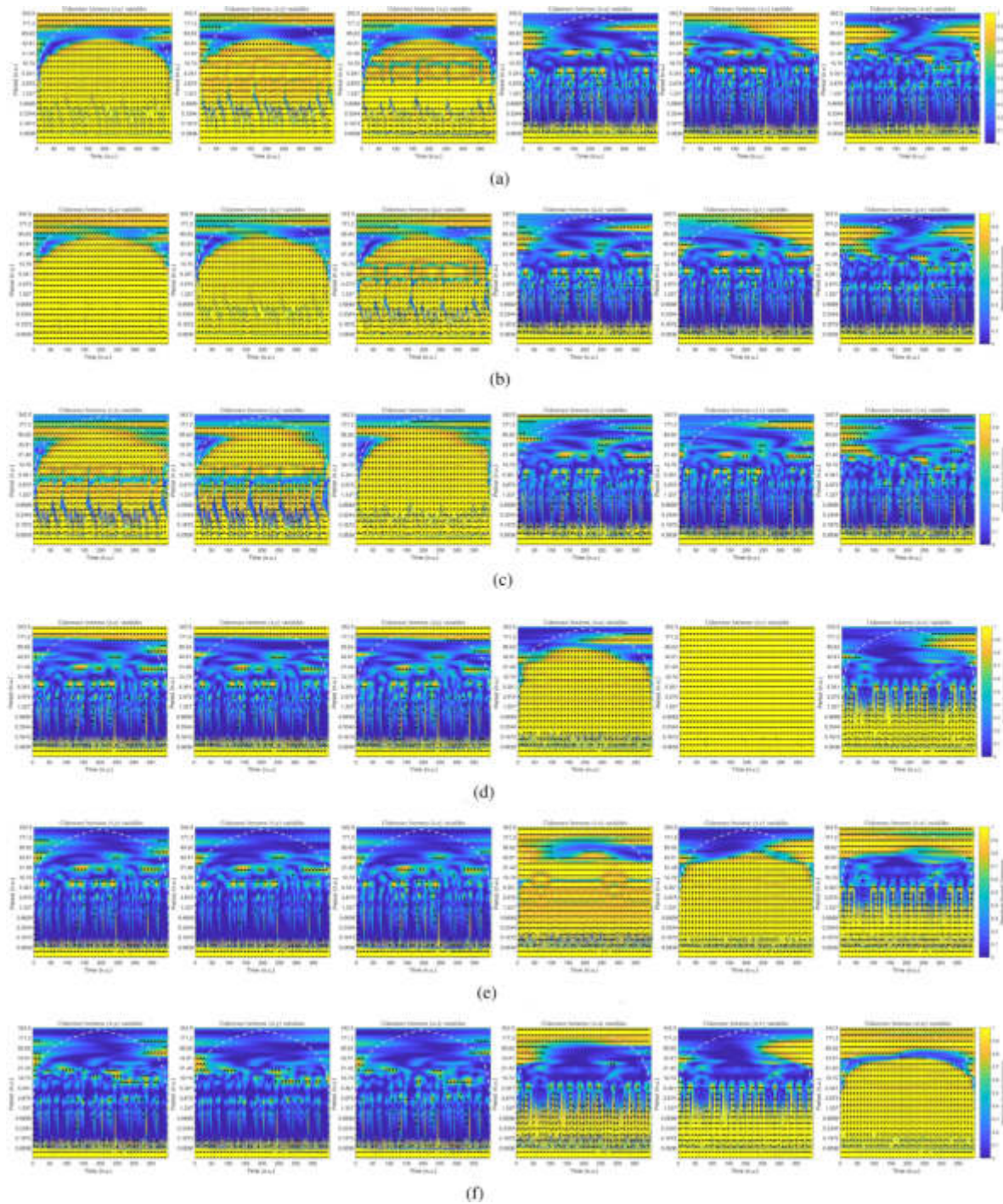


FIG. 8. Causal wavelet coherence (KWT) between the derivatives of the R66 and the NH variables $\dot{x}$ (a), $\dot{y}$ (b), $\dot{z}$ (c), $\dot{u}$ (d), $\dot{v}$ (e), $\dot{w}$ (f), and the original variables themselves of the two dynamical systems x, y, z, u, v , and w , under uncoupled ($\kappa_{y \rightarrow v} = \kappa_{v \rightarrow y} = 0$) and free of noise conditions. (a) Causal wavelet coherence $C_{\dot{x}\dot{y}}(t, f)$ of $(\dot{x}, x)$, $(\dot{x}, y)$, $(\dot{x}, z)$, $(\dot{x}, u)$, $(\dot{x}, v)$, and $(\dot{x}, w)$. (b) Causal wavelet coherence $C_{\dot{y}\dot{y}}(t, f)$ of $(\dot{y}, x)$, $(\dot{y}, y)$, $(\dot{y}, z)$, $(\dot{y}, u)$, $(\dot{y}, v)$, and $(\dot{y}, w)$. (c) Causal wavelet coherence $C_{\dot{z}\dot{y}}(t, f)$ of $(\dot{z}, x)$, $(\dot{z}, y)$, $(\dot{z}, z)$, $(\dot{z}, u)$, $(\dot{z}, v)$, and $(\dot{z}, w)$. (d) Causal wavelet coherence $C_{\dot{x}\dot{y}}(t, f)$ of $(\dot{u}, x)$, $(\dot{u}, y)$, $(\dot{u}, z)$ and $(\dot{u}, u)$, $(\dot{u}, v)$, and $(\dot{u}, w)$. (e) Causal wavelet coherence $C_{\dot{x}\dot{y}}(t, f)$ of $(\dot{v}, x)$, $(\dot{v}, y)$, $(\dot{v}, z)$ and $(\dot{v}, u)$, $(\dot{v}, v)$, and $(\dot{v}, w)$. (f) Causal wavelet coherence $C_{\dot{x}\dot{y}}(t, f)$ of $(\dot{w}, x)$, $(\dot{w}, y)$, $(\dot{w}, z)$ and $(\dot{w}, u)$, $(\dot{w}, v)$, and $(\dot{w}, w)$.

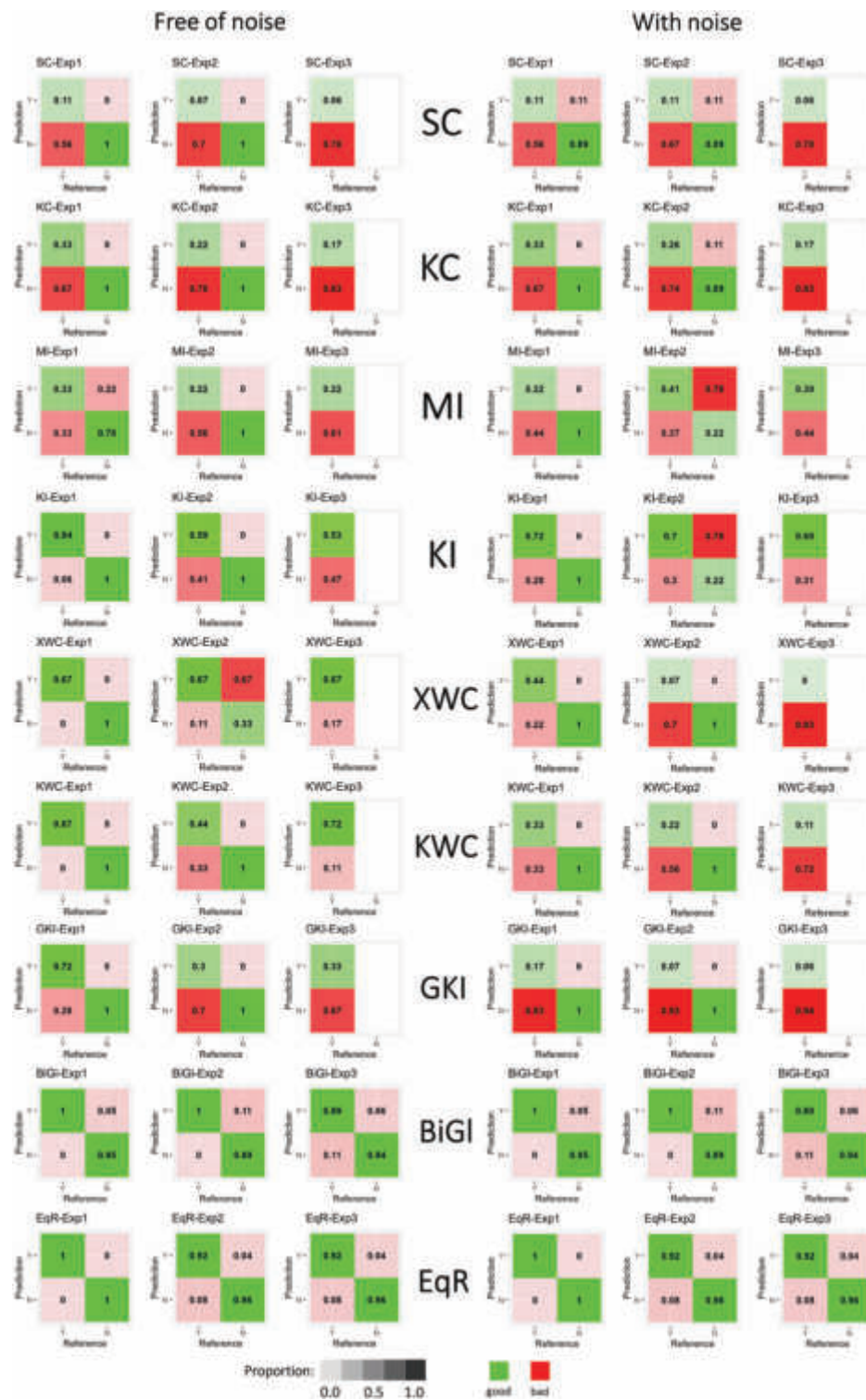


FIG. 9. Coupling detection. This figure synthesizes the results obtained with all the techniques (each row) and for all the experiments, either under free of noise conditions (left three panels with no-, uni- and bi-directional couplings) or with $p = 0.01\%$ of noise perturbation (right three panels with no-, uni- and bi-directional couplings). The techniques are Simple Correlation (SC), Causal correlation (KC), Mutual Information (MI), Causal Information (KI), Cross Wavelet Coherence (XWC), Causal Wavelet Coherence (KWC), Granger Causal Index (GKI), Bivariate Global modeling technique (BiGI), and Equation Reconstruction (EqR) techniques (lines 1–9). In each case, the results are presented as a confusion matrix considering all the links involved among the variables of the studied systems. Green color is used for proper detection (true positive, true negative), and red color for wrong detection (false positive, false negative). The level is given by the color transparency: few true detection (pale green), few false detection (pale red), high level of true detection (intense green), and high level of false detection (intense red).

0.2 was used for MI, KI, and GKI to account for the nonlinear relation between correlations and information indices. No criterion was necessary for the bivariate modeling and the equation reconstruction.

The confusion matrices enable us to distinguish four situations: (1) couplings and (2) absence of coupling properly detected (true positive and true negative) are plotted in green; (3) couplings and (4) absence of coupling wrongly detected (false positive and false negative) are in red. In the plots, the color lightness varies in proportion of the total number of positive or negative couplings detected among all the experiments. Self-influence was not taken into account in Fig. 9 to facilitate the comparison between the different techniques (but it was in Fig. S15 in the [supplementary material](#)).

The analyses show that the simple correlation (SC) and the causal correlation (KC) are systematically biased, generating numerous false negative detections, even under free of noise conditions. The mutual information (MI) is less biased but its results are also quite sensitive to noise. The causal information (KI) is significantly better under free of noise conditions but poorly able to detect weak couplings (uni- or bi-directional) under noisy conditions. The cross wavelet coherence (XWC) seems able to detect the couplings among the systems quite well when these are separated, but this ability is lost once the systems are weakly coupled, and it then becomes particularly sensitive to noise perturbations. The causal wavelet coherence (KWC) appears better able to detect both separate systems and directional couplings, but it is poorly robust to noise. The Granger causality index (GKI) is particularly bad except for strong deterministic couplings under free of noise conditions. Note that in experiment 3, the bidirectional couplings put in place between the variables y and v make all the variables of the two systems become at least indirectly coupled. As a consequence, it becomes impossible to have cases (2) and (4), the right part of the confusion matrix is then kept white. It is no longer the case when direct coupling becomes detectable (see BiGI and EqR) for which values are, thus, provided.

Interestingly, in all these experiments, the noisy conditions do not simply degrade the detection. The reason for this is that noise will propagate among the variables through numerical integrations, which may both foster the detection of some terms and degrade the detection of others.

The bivariate global modeling appears particularly good (with a proportion of bad detections lower than 11%) and robust to noisy conditions in all the experiments.

Also based on the global modeling technique but considering that all the variables are available, the equation reconstruction (EqR) appears quite efficient to reconstruct almost all the direct couplings in full detail, complete parameterization, and self-influence of the variables also included ([supplementary material](#), Fig. S15). Among them, the bidirectional weak couplings appear to be particularly challenging. This approach can also be used to estimate the contribution of each term. Moreover, its robustness to measurement noise, initial condition change, and time series length was also successfully passed with this approach.

These results are given in detail in Subsections IV B–IV D, considering the three experiments separately, and focusing on the most relevant results. As a consequence, the approaches presenting the most pronounced biases (SC, KC, MI, KI, and GKI fully documented

in Tables S2 and S3 in the [supplementary material](#)) will be mostly put aside in the following Secs. IV B–IV D.

B. Independent systems (experiment I)

In the first experiment, the six-dimensional system separates in two independent systems as resumed by the fluence relations (Fig. 1) deduced from Eqs. (20) and (21) in which linear (L) and nonlinear (NL) terms are distinguished by plain or dashed arrows, respectively.

The XWC analysis of the six variables taken two by two reveals a high level of coherence at all scales between variables (x, y, z) for the R76 system but only between u and v for the NH system as shown in Fig. 6 (to illustrate the interpretation of cross wavelet graphs, an example is shown and explained with details in Appendix G.1 in the [supplementary material](#)). Between u and w and between v and w , high levels of coherence are found only at short timescales. The couplings are, thus, clearly detected for the R76 system but poorly for the NH one, and this becomes even much more critical under noisy conditions (see [supplementary material](#), Fig. S10). The reason for that is that XWC is designed to detect correlations, not causality. The variables of the NH system being totally decorrelated, and the XWC fails to detect the relationships between its variables. It is actually why the NH system was chosen for this context: to challenge the ability to detect causality under poor correlation conditions. Very low levels of coherence are estimated when crossing the variables of the two systems (Fig. 7) and this result is confirmed under noisy conditions (see [supplementary material](#), Fig. S11).

For all the variables, high levels of coherence C (almost 1) are obtained at very short timescale ($s \leq 0.2$) because the signal is very smooth at these scales, under free of noise conditions. For this reason, these values should not be interpreted as a causation in the present situation (the same limitation will also be noted with the KWT). This observation shows that the causal effect may be localized on specific scale windows.

The phasing between the variables (given by the arrows) may provide information about causation. Indeed, a $\pm\pi/2$ delay may be the result of a causal effect, whereas a $0 \pm \pi$ delay may reflect a synchronization effect (see Propositions 1 and 2 in [Appendix B](#)). Unfortunately, inhomogeneous patterns are observed between most of the variables except between u and v for which a phasing of $-\pi/2$ is obtained at almost all scales that reveals the causal relationship of v on u made possible because the causation is unique and linear [$\dot{u} = b_1 v$ in Eq. (21)] so that we have $C_{uv} = C_{u \frac{\dot{u}}{b_1}} \approx 1$ with a $\pi/2$ delay. No clear phasing is observed between the other variables. For example, the XWC between x and y reveals a phase evolving from $\pi/2$ at scales lower than 2, to $3\pi/4$ and more at larger scales. Such patterns are difficult to interpret.

The KWC analysis does not require correlation as a precondition for causality detection. Moreover, it permits, in its principle, the detection of directional couplings thanks to its asymmetrical definition. By construction here, a causal effect should be characterized by a high coherence and a full phasing (0 or π depending on the variables signs) in the best situations, that is, when proportionality is expected between the observed variations (the derived variable) and the causal variable (see [Appendix B](#)). In practice, such a property may be blurred under nonlinear and/or multiple coupling conditions. The analysis clearly permits to distinguish the two

systems with high coherence levels ($C > 0.8$) between the variables (x, y, z) on one side, and between (u, v, w) on the other side; and low coherence levels ($0 < C < 0.4$) when crossing the variables of the two systems. This is particularly obvious under free of noise conditions (see Fig. 8) and still intelligible on localized window under noisy conditions (see [supplementary material](#), Fig. S12). However, the approach appears poorly able to distinguish direct from indirect causation [e.g., high coherence for (y, z) due to indirect influence]. The direct causation of variable v on variable u is specifically well detected (coherence level $C_{uv} = 1$ at all scales with no delay between the two signals $\phi = 0$), which explanation stems from the algebraic formulation of the dynamics of $\dot{u}$: the action of v is linear and with a unique term. Obviously, nonlinear links are a bit more difficult to detect which perturbs the detection of linear ones. As an example, the nonlinear action of w in equation ($\dot{v} = -u + vw$) is quite unclear. Similarly, the role of nonlinear term v^2 in the last equation ($\dot{w} = b_2 - v^2$) is not clearly highlighted. A more specific (nonlinear) analysis would be required to detect such terms as illustrated in [Appendix C](#) (see Fig. 20). The detection of self-influence also appears impossible since systematically positive with a delay $\pm\pi/2$ (see [Appendix B](#)).

The bivariate modeling can serve either to reconstruct original equations when all the variables of a given equation are available or to detect couplings between them when only a subset is available. The analyses with the modeling approach (bivariate and multivariate) were performed under both free of noise and noisy conditions. The results being found robust to the stochastic perturbations, and only the analyses of the noisy simulations are presented here. The right couplings were detected among all the variables of each of the two systems using appropriate embeddings. For the dynamics of R76, the model

$$\begin{cases} \dot{x} = X_2, \\ \dot{X}_2 = -0.899 - 0.977x - 2.574y + 0.607xy, \\ \quad -2.024X_2 + 0.634xX_2 - 0.167y^2 + 0.154X_2^2, \\ \dot{y} = 0.431y + 0.998x, \end{cases} \quad (25)$$

was obtained from the variables x and y . The second equation of R76 ($\dot{y} = x + a_1y$) is correctly reproduced, and thus the causality between x and $\dot{y}$ is found, including the self-influence of y . The influence of y on the evolution of x is obtained through $\dot{X}_2 = \ddot{x}$ but it cannot be stated if this influence is direct or indirect. For this reason, the coupling is considered detected but uncharacterized (and annotated **u** in Table S2 in the [supplementary material](#)). Note that the form of $\dot{X}_2$ matches with the theoretical expression with two additional monomials ($-0.167y^2$ and $0.154X_2^2$). Nothing else can be exhibited. No model was obtained with the embedding $(x, y, \dot{y})$ because observability equals zero in this latter case (see [supplementary material](#), Appendix E).

The model obtained from $x(t)$ and $z(t)$

$$\begin{cases} \dot{x} = X_2, \\ \dot{X}_2 = -1.808 - 1.027x + 4.012z + 0.3980X_2 - 0.9077xz, \\ \dot{z} = 1.858 - 3.652z + 0.9230xz, \end{cases} \quad (26)$$

also reveals the existence of a coupling between these two variables. The algebraic structure of this reformulation is exactly retrieved

[no spurious or lacking terms, see Eq. (6) in Appendix E in the [supplementary material](#)]. The influence of z on $\dot{x}$ cannot be interpreted as a direct influence because this influence is performed through $\dot{X}_2$ (in other terms, the first equation of the R76 system $\dot{x} = -y - z$ cannot be reconstructed, here, due to the absence of y). The causal influence of z on x are, thus, also considered detected but uncharacterized. Conversely, the equation for the variations of z [in Eq. (26)] can be interpreted because it is exclusively based on observed variables, enabling to retrieve the original equation structure $\dot{z} = b + z(x - c)$ [in Eq. (20)]. The variations of z are caused by a nonlinear term in xz and a linear contribution of z (and the constant term is also detected). The causal influence of x on z is, thus, perfectly detected and its self-influence as well.

Finally, the model from $y(t)$ and $z(t)$

$$\begin{cases} \dot{y} = Y_2, \\ \dot{Y}_2 = -1.010y - 1.003z + 0.4269Y_2, \\ \dot{z} = 1.595 - 3.209z - 0.4606yz + 0.8167zY_2, \\ \quad -0.0378z^2 + 0.02y, \end{cases} \quad (27)$$

unveils a coupling between these two terms but it cannot be interpreted as direct couplings since these are hidden by the absence of variable x which influence on y is, thus, performed through $\dot{Y}_2 = \ddot{y}$. The theoretical structure is rather well retrieved here again except two spurious terms with small coefficients $-0.0378z^2$ and $0.02y$ [see Eq. (E4) in Appendix E in the [supplementary material](#)]. An alternative embedding may have been used here $(y, z, \dot{z})$ [see Eq. (E7) in Appendix E in the [supplementary material](#)]. However, no satisfying model was obtained due to its low level of observability, and also because it is required to approximate the theoretical equations by a polynomial (and by default, GPoM uses polynomial forms). Anyway, this alternative embedding would not have brought additional information in terms of coupling.

The same analyses were performed with the variables of the NH system. The model obtained from $u(t)$ and $v(t)$

$$\begin{cases} \dot{u} = 0.1996v, \\ \dot{v} = V_2, \\ \dot{V}_2 = -0.2618 + 0.01880V_2 - 0.009845V_2^2 \\ \quad + 3.590v + 0.03559vV_2^2 + 0.02260v^2 \\ \quad - 0.9210v^3 + 0.08717u + 0.01256uV_2^2 \\ \quad + 0.07428uvV_2 - 0.03964uv^2 + 0.02023u^2V_2 \\ \quad - 0.09079u^2v + 0.1256u^3, \end{cases} \quad (28)$$

reveals the coupling between the two variables, with a direct influence of v on the variations of u , but the reverse influence remains uncharacterized, being performed through $\dot{V}_2 = \ddot{v}$; the model for $u(t)$ and $w(t)$

$$\begin{cases} \dot{u} = U_2, \\ \dot{U}_2 = -0.005092w + 0.8441U_2w - 0.1952u, \\ \dot{w} = 2.872 - 25.85U_2^2, \end{cases} \quad (29)$$

reveals couplings between these two variables, which cannot be interpreted as a direct influence since performed through

$\dot{U}_2 = \ddot{u}$. The theoretical structure is almost retrieved [that is, with one additional term of very small amplitude in the second equation $-0.005\,092w$, see Eq. (E8) in Appendix E in the [supplementary material](#)]. The model obtained from $v(t)$ and $w(t)$

$$\begin{cases} \dot{v} = V_2, \\ \dot{V}_2 = 1.4213V_2w - 0.2465vV_2^2 - 0.4753v^3, \\ \dot{w} = 3.0223 - 0.0412vV_2w - 1.0303v^2, \end{cases} \quad (30)$$

also detects the coupling between these two variables. The theoretical form is not very well retrieved here, with one term in v replaced by the spurious term $-0.2465vV_2^2$ in the second equation. A spurious term of small amplitude ($-0.0412vV_2w$) is found in the third equation preventing an interpretation in terms of direct causality [the theoretical Eq. (E10) is provided in Appendix E in the [supplementary material](#)]. No couplings were detected between the cross variables of the R76 and the NH systems, as expected.

Equation reconstruction. The global modeling technique was also applied considering the six variables of the two systems at the

same time. The following model

$$\begin{cases} \dot{x} = -1.003z - 1.005y, \\ \dot{y} = 0.431y + 0.998x, \\ \dot{z} = 1.858 - 3.652z + 0.923xz, \\ \dot{u} = 0.2v, \\ \dot{v} = 0.863vw - 0.979u, \\ \dot{w} = 2.964 - 1.086v^2, \end{cases} \quad (31)$$

was obtained that corresponds to the original set of algebraic equations with an error on the parameters varying from 0.3% to 13.7%. Several projections of its phase portraits are provided in [Fig. 10](#).

Models with more than 12 terms (up to 15 terms) were also obtained. All were based on the same 12-term minimal structure [Eq. (31)] with additional terms of small amplitude that did not improve the model dynamics. These models were rejected for lack of parsimony.

The degree of detected determinism was estimated using Eq. (11). Its estimates vary from 94.8% for the dynamics of v to 99.0%

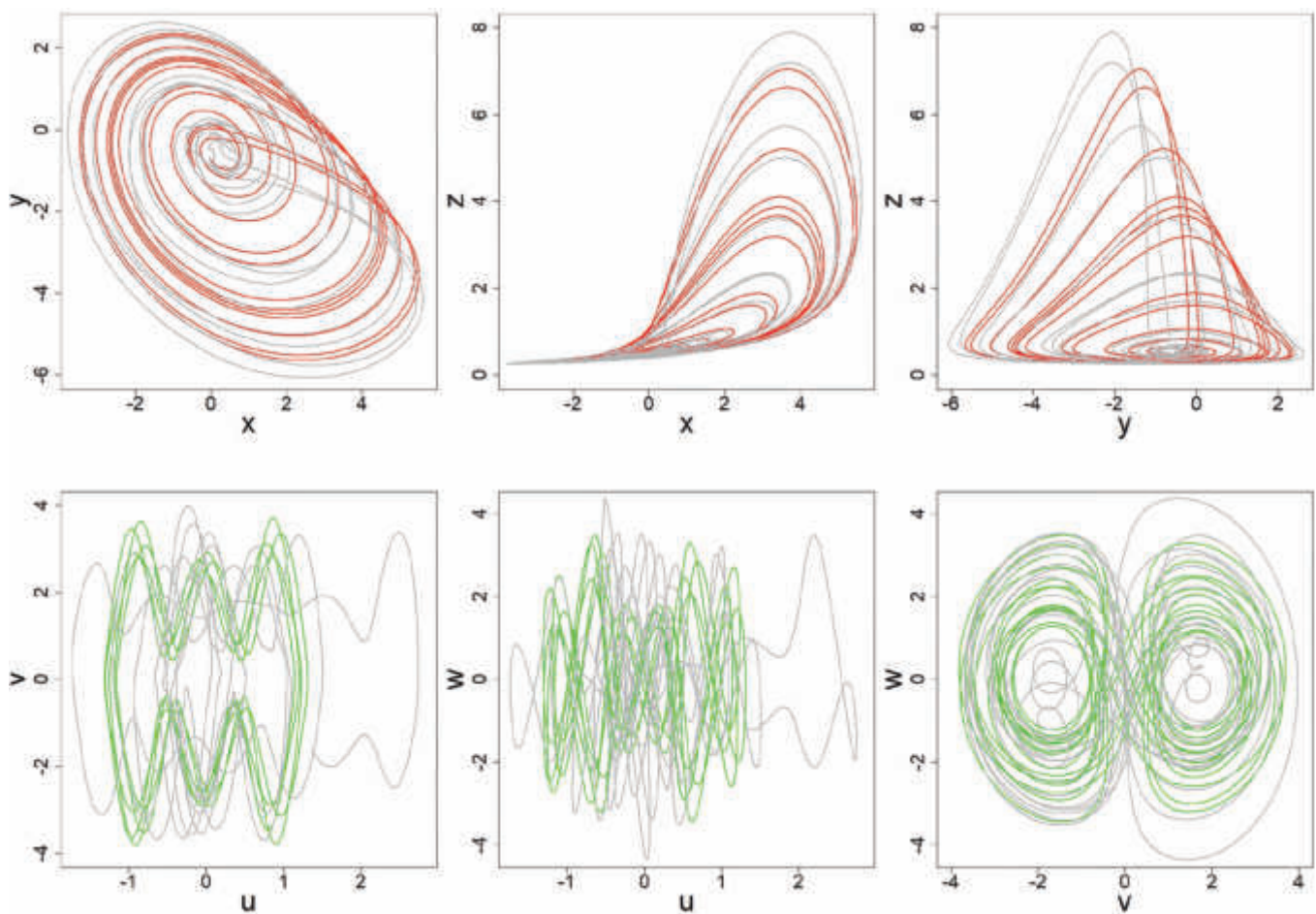


FIG. 10. Phase portraits of the global models (in color) obtained for the Rössler (top line) and Nosé–Hoover (bottom line) systems. The original phase portrait (with 0.01% dynamical noise without coupling) is also reported in the background for comparison (in gray).

TABLE III. Relative terms contribution estimated under noisy perturbations ($p = 0.01\%$) from the reconstructed equations (in bold) and degree of explained determinism d° (in %) [see Eq. (11)]. Box values correspond to false negative or false positive.

	x	y	z	u	v	w	v^2	w^2	xz	vw	d°
Experiment 1											
$\dot{x}$	0	74.1	25.9	0	0	0	0	0	0	0	99.0
$\dot{y}$	86.0	14.0	0	0	0	0	0	0	0	0	99.0
$\dot{z}$	0	0	46.4	0	0	0	0	0	53.6	0	98.3
$\dot{u}$	0	0	0	0	100	0	0	0	0	0	97.8
$\dot{v}$	0	0	0	12.9	0	0	0	0	0	87.1	94.8
$\dot{w}$	0	0	0	0	0	0	100	0	0	0	95.1
Experiment 2											
$\dot{x}$	0	70.6	29.4	0	0	0	0	0	0	0	99.1
$\dot{y}$	85.5	14.5	0	0	0	0	0	0	0	0	99.1
$\dot{z}$	0	0	46.1	0	0	0	0	0	53.8	0	98.1
$\dot{u}$	0	0	0	0	100	0	0	0	0	0	97.6
$\dot{v}$	0	22.9	0	3.6	15.2	0	0	0	0	58.2	95.5
$\dot{w}$	0	0	0	0	0	0	99.6	0.4	0	0	96.1
Experiment 3											
$\dot{x}$	0	93.1	6.9	0	0	0	0	0	0	0	98.4
$\dot{y}$	81.7	0	0	0	18.3	0	0	0	0	0	98.2
$\dot{z}$	0	0	47.8	0	0	0	0	0	52.2	0	94.7
$\dot{u}$	0	0	0	0	100	0	0	0	0	0	97.8
$\dot{v}$	0	3.4	0	10.8	5.8	0	0	0	0	80.0	95.3
$\dot{w}$	0	0	0	0	0	0	99.5	0.5	0	0	96.1

for x and y (see Table III). The contribution of the different algebraic terms to the deterministic causation was also estimated (also provided in Table III to be compared with the original contribution presented in Table S4 in the supplementary material). The causation of x mostly results from y and is slightly overestimated (74% instead of 72%); It is also due to z but slightly underestimated (26% instead of 28%). The variations of y are well estimated: mostly caused by x (86%) with a minor influence of y on itself (14%). The variations of z are also very well estimated: they are caused for a half (54%) by the nonlinear effect of xz and for another half (46%) by the linear effect of z itself alone. The variations of u are only caused by v . The variations of v are indeed mostly caused by the nonlinear effect of uw , although slightly underestimated (87% instead of 95%) with a small effect of v itself. Finally, the variations of w are only nonlinear and indeed exclusively caused by v^2 .

C. Experiment 2: Uni-directional coupling

The same series of analyses was applied to the two systems with uni-directional coupling from R76 to NH ($\kappa_{y \rightarrow v} = 0.8$ & $\kappa_{v \rightarrow y} = 0$). Only minor differences were observed when using all the statistical estimators. Similarly, the XWC (not shown) and the KWT (see supplementary material, Figs. S8 and S9) did not permit to distinguish any clear effect. In all these cases, the coupling between the two systems was not very clear and their direct couplings were difficult to detect.

The bivariate modeling was found to be able to detect quite similar results among both the R76 variables and the NH variables (not shown). Considering the cross variables between the two systems, most of the models were rejected because the cross portraits did not reveal any structure. Only three candidate models were not rejected. All the three models were based on variables y and v (the models from the other variables were all rejected). The (y, v) projection of their cross portraits is shown in Fig. 11.

The five-dimensional model

$$\begin{cases} \dot{y} = Y_2, \\ \dot{Y}_2 = Y_3, \\ \dot{Y}_3 = 0.4752 + 0.0731Y_3^2 - 1.153Y_2 - 0.1848Y_2^2, \\ \quad - 0.3476y + 0.1948yY_2 - 0.1155y^2, \\ \dot{v} = V_2, \\ \dot{V}_2 = 0.4384 - 0.3074V_2 + 3.6288v - 0.9518v^3, \\ \quad + 0.7553Y_2 + 0.6274y, \end{cases} \quad (32)$$

was selected among these three models [see Fig. 11(c)] that also showed the closest correlation to the original cross portrait. This model enables the detection of a directional coupling from R76 to NH (term $+0.6274y$ in the last equation).

Models from the other cross variables were all rejected, either because no model was obtained or because the obtained models exhibited inconsistencies with the original portraits. By themselves,

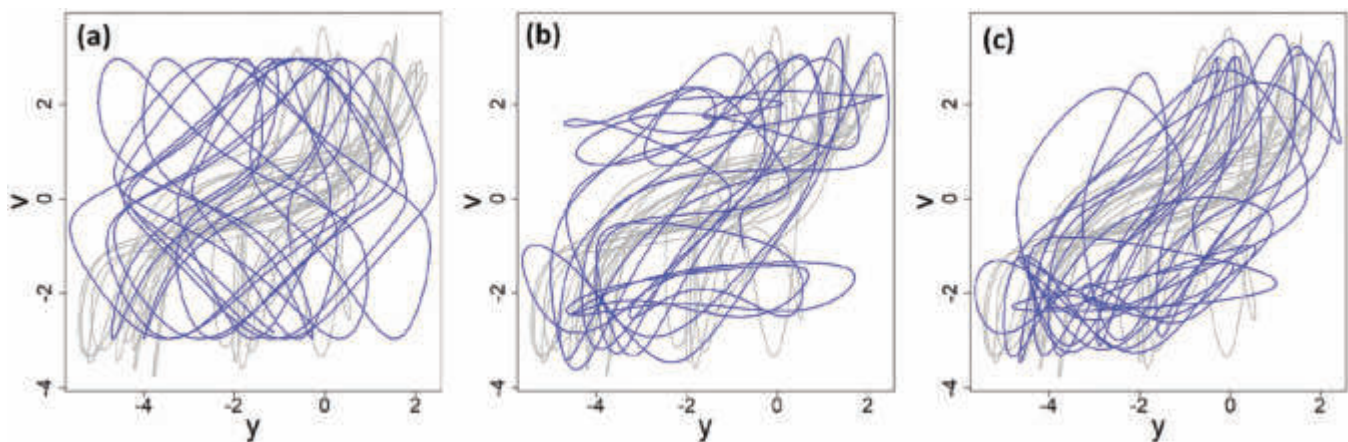


FIG. 11. Cross portraits of three models (in blue) obtained from variables y and v for the coupling between the Rössler and Nosé–Hoover systems (Experiment 2 with $p = 0.1\%$ of dynamical noise) with original cross portrait in the background (in gray). Model (a) and others with similar cross portraits (not shown) were rejected straightforward, and among the remaining two models (b) and (c), the latter was selected.

Eq. (32) cannot be used to interpret the couplings between y to v as a direct influence because derivatives are involved (Y_2 , Y_3 , and V_2). However, it can still be interpreted as a directional coupling from the R76 system (observed from variable y) to the NH system (observed from v); the variables y and v appear to be the most direct coupling among all the cross variables since none of the other variables enabled to reconstruct any coupling.

The equation reconstruction. When applying the global modeling technique to the six variables together, a 12-term model enabled to detect the structure of the two systems. However, this model did not produce satisfying cross portraits when compared to the original ones, in particular when considering the variables y and v [Fig. 12(a)]. Indeed, a very different level of correlation was estimated between the model variables y and v (6.9%) in comparison

to the original ones (72.6%). This 12-term model was, thus, rejected and the model search was pursued up to 15 terms. Numerous models were able to reproduce satisfyingly the three-dimensional projections (x, y, z) and (u, v, w), but a single set of equations

$$\begin{cases} \dot{x} = -0.9990z - 0.9966y, \\ \dot{y} = 0.4323y + 0.9998x, \\ \dot{z} = 1.8493 - 3.6242z + 0.9161xz, \\ \dot{u} = 0.1997v, \\ \dot{v} = 0.8835vw - 0.9910u + 0.7505y - 0.7424v, \\ \dot{w} = 3.0553 - 1.0674v^2 - 0.0582w^2, \end{cases} \quad (33)$$

was able to reproduce well both the portraits of the R76 and NH systems (Fig. 13) and their cross portrait (y, v) [Fig. 12(b)], with a

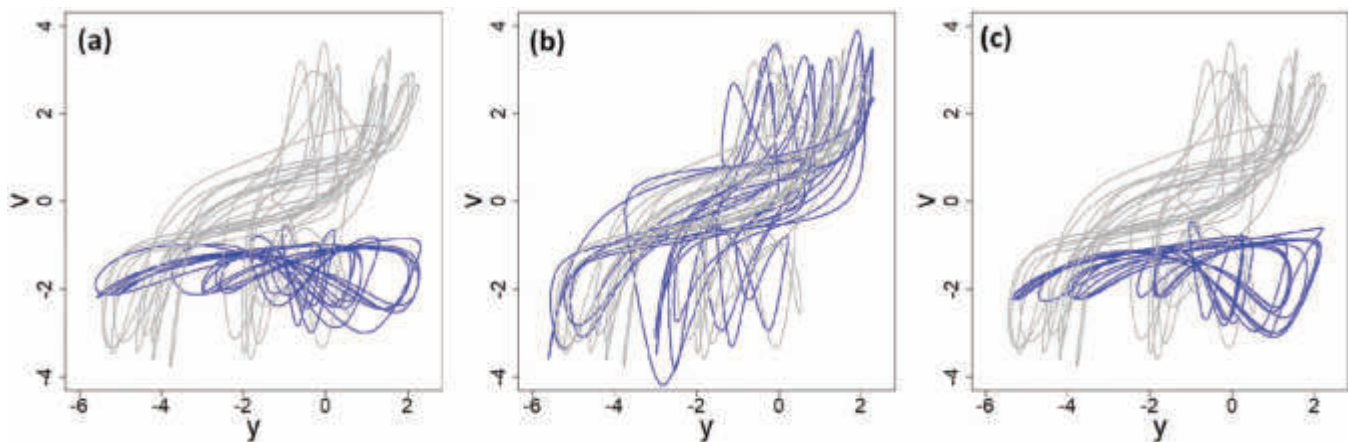


FIG. 12. Cross portraits (y, v) of three models (in blue) obtained between R76 and NH under unidirectional coupling ($\kappa_{y \rightarrow v} = 0.8$ & $\kappa_{v \rightarrow y} = 0$) with dynamical noise ($p = 0.01\%$). Models (a) and (c) were rejected, model (b) was selected. The original phase portrait is also reported in the background (in gray).

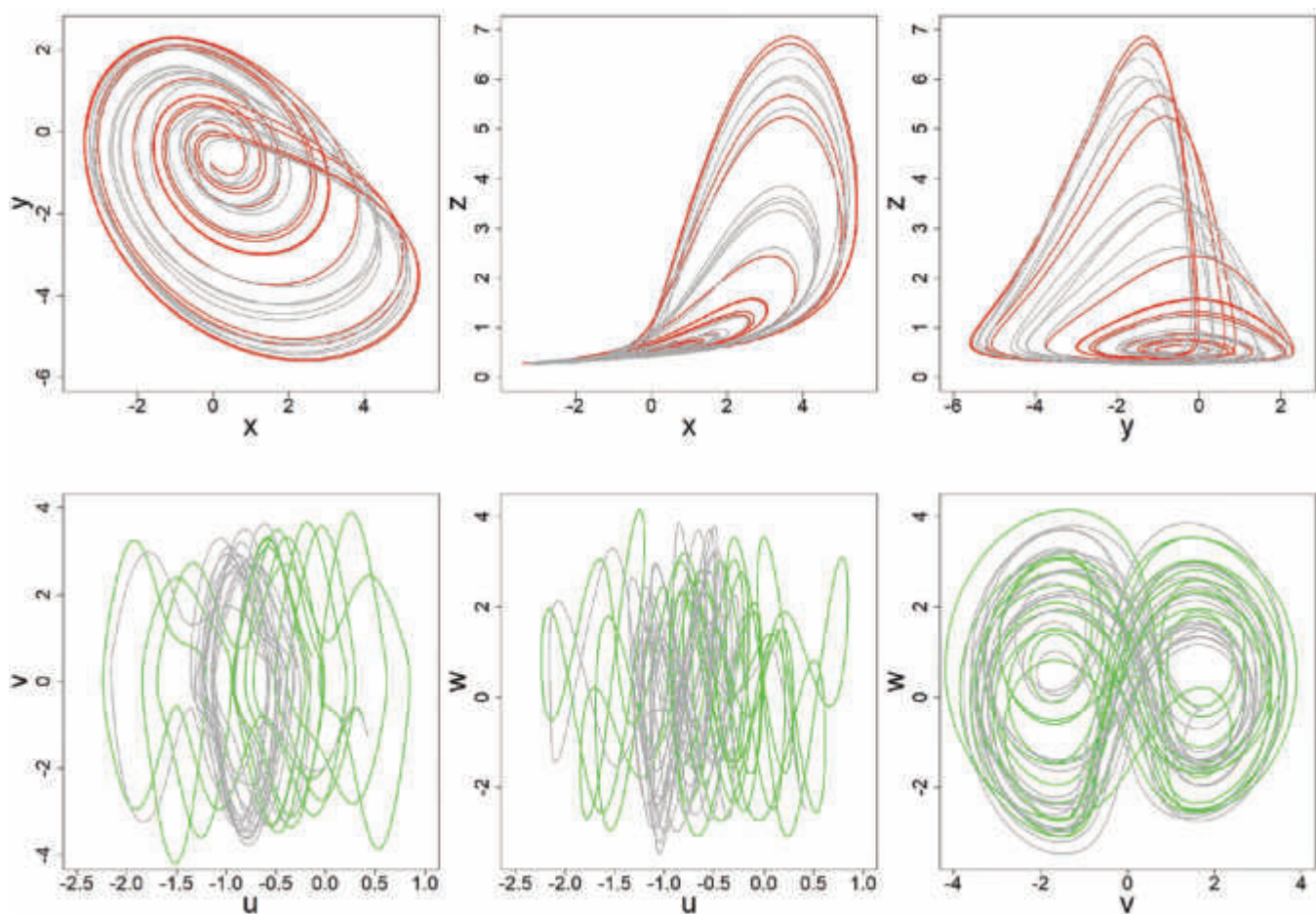


FIG. 13. Phase portraits of the models obtained for the R76 (top line) and NH (bottom line) systems under unidirectional coupling ($\kappa_{y \rightarrow v} = 0.8$ & $\kappa_{v \rightarrow y} = 0$) with $p = 0.01\%$ of dynamical noise; original portraits also reported for comparison (in gray).

correlation very similar to the original data (69.4%). Except one spurious term of small amplitude in the last equation ($-0.0582w^2$), the original system is retrieved with its linear coupling in the equation for variable v , the error on the parameters varying from 0.1% to 11.7%. The original coupling $+0.8(y - v)$ is retrieved ($+0.7505y - 0.7424v$) with an error of 7.2%. Among the other (rejected) models, the highest level of correlation between y and v did not overpass 19.6% at best [Fig. 12(c)].

D. Experiment 3: Bi-directional couplings

The same series of analysis was performed again considering the case with bi-directional coupling. As shown in [supplementary material](#) Table S2 (and S3 for noisy conditions), the bidirectional coupling generates information transferred into both directions between the two systems, which tends to blur even more the

readability of the results when trying to reconstruct the causal network between the variables with most of the approaches.

The *XWC* and the *KWC* analyses led to similar results among the variables of each system but when considering the interactions between the two systems, and couplings were detected in all directions between all the variables and it was impossible to distinguish direct couplings from indirect ones. This situation was even reinforced under noisy conditions.

The *bivariate modeling* was here again able to detect similar results among both the R76 variables and the NH variables (not shown). However, considering the cross variables, no robust model is able to reproduce the observed coupling was obtained: all were rejected.

Equation reconstruction enabled to obtain numerous models reproducing the R76 and NH portraits satisfyingly but only three of them reproduced the cross portrait (y, v) reasonably well

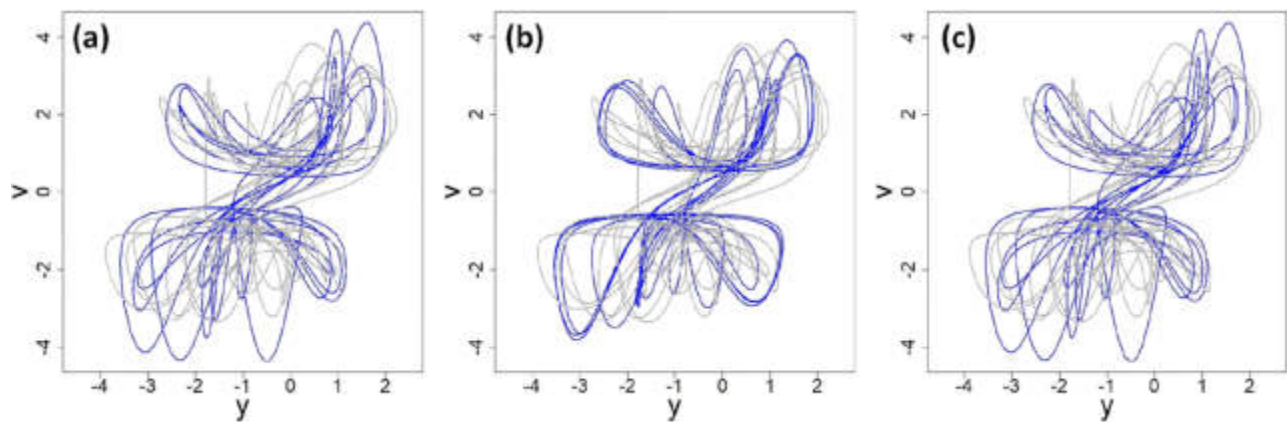


FIG. 14. Cross portraits of three models (in blue) obtained for the Rössler and Nosé-Hoover systems under bidirectional coupling ($\kappa_{y \rightarrow v} = \kappa_{v \rightarrow y} = 0.4$) with dynamical noise ($p = 0.01\%$). Correlations between y and v were estimated for each model giving 0.35, 0.37, and 0.35, respectively, to be compared to the original correlation of 0.39. Models (a) and (c) were rejected, and model (b) was selected. The original phase portrait is also reported in the background (in gray).

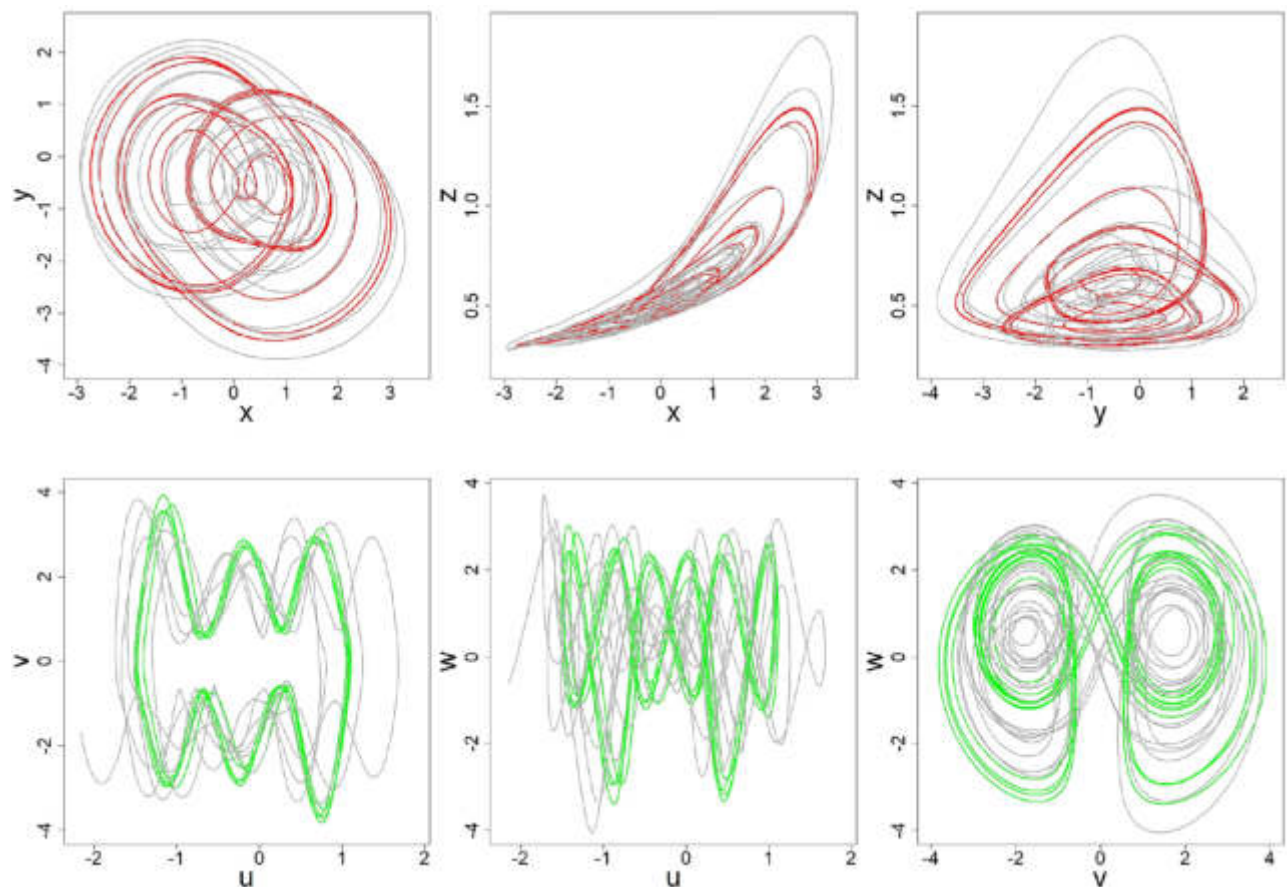


FIG. 15. Phase portraits of the models selected for the R76 (top line) and NH (bottom line) systems under bidirectional coupling ($\kappa_{y \rightarrow v} = \kappa_{v \rightarrow y} = 0.4$) with dynamical noise ($p = 0.01\%$); original portraits also reported for comparison (in gray).

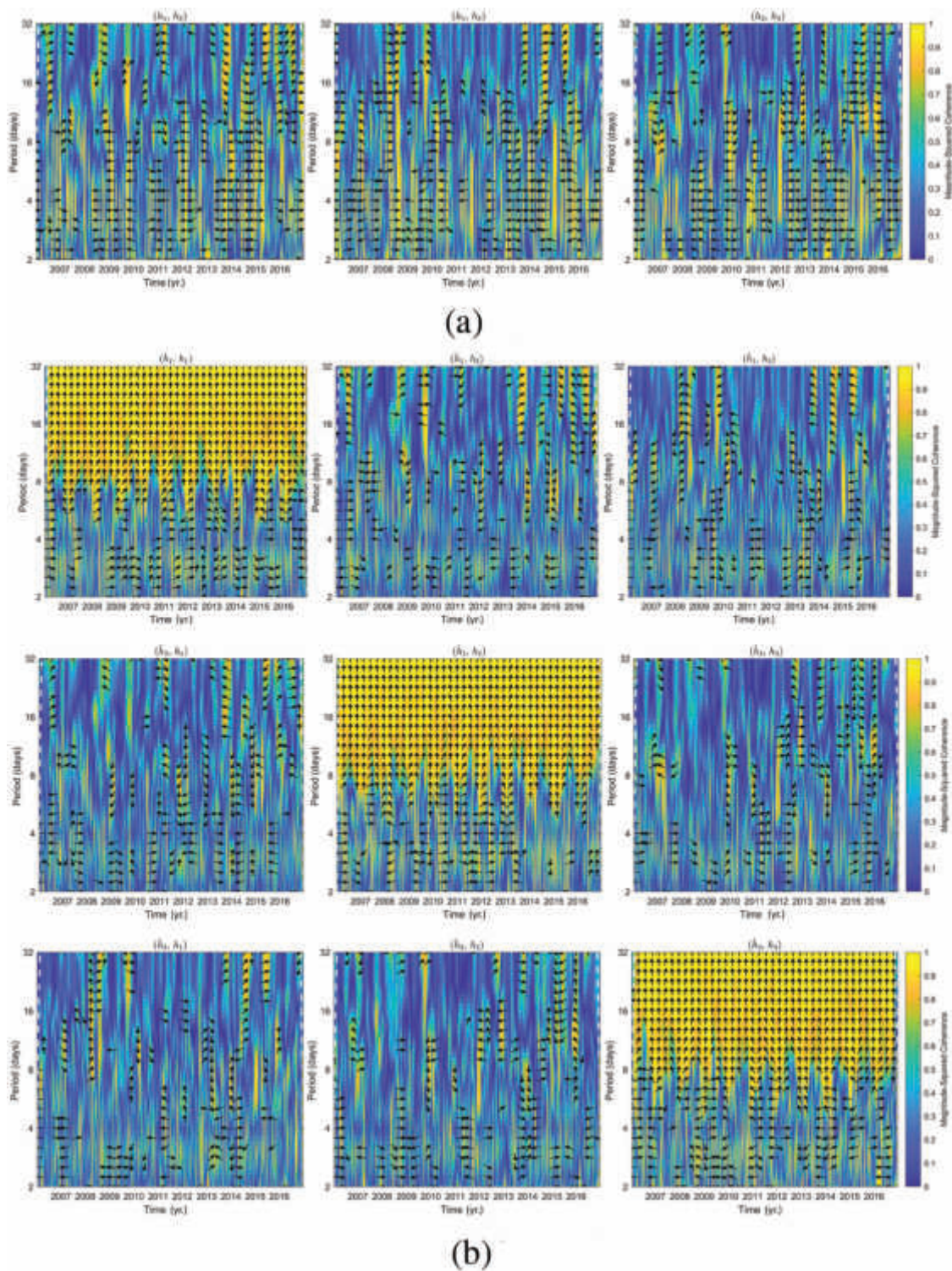


FIG. 16. XWT (a) and KWT (b) analyses of the groundwater height measured at three piezometric stations $h_1(t)$, $h_2(t)$, and $h_3(t)$. (a) XWC $C_{XY}(t, f)$ of (h_1, h_2) , (h_1, h_3) , and (h_2, h_3) . (b) KWC $C_{XY}(t, f)$ between h_1 , h_2 , and h_3 .

(see Fig. 14). The model

$$\begin{cases} \dot{x} = -1.0119z - 1.0024y, \\ \dot{y} = 0.4016v + 0.9878x, \\ \dot{z} = 1.85 - 3.683z + 0.9307xz, \\ \dot{u} = 0.1999v, \\ \dot{v} = 0.8772vw - 0.9873u + 0.3415y - 0.3467v, \\ \dot{w} = 3.1354 - 1.0752v^2 - 0.067w^2, \end{cases} \quad (34)$$

for which projections of portrait are shown in Figs. 15 and 14(b), enabled to get a correlation between y and v equal to 0.37, that is, the closest to the original one (0.39) in comparison to the other two models (0.35 and 0.36). Except one spurious term of smaller amplitude in the last equation ($-0.0670w^2$), the original system is retrieved with an error on the parameters varying from 0.1% to 14.6%. The bidirectional coupling is detected in the selected model: one in the equation for variable y (term $0.4016v$) and the other one in the equation for v (the terms $0.3415y - 0.3467v$). The original coupling $\kappa_{y \rightarrow v}(y - v)$ is retrieved with a parameter error of $\sim 14\%$.

The other coupling $\kappa_{v \rightarrow y}(v - y)$ is only partially retrieved since only the term in v is unveiled (with an error of 0.4%) while the original term in y is not detected. As expected, these bidirectional coupling terms do not generate a full synchronization between the two variables but a generalized synchronization very similar to the original one. Note that a single directional coupling only was detected from NH to R76 in the two other candidate models [Figs. 14(a) and 14(c)]. Additional test of robustness were also performed to challenge the equation reconstruction technique under measurement noise conditions, shorter time series length, and changes in the initial conditions (provided in Appendix F in the [supplementary material](#)).

TABLE IV. Results from environmental data. Correlations greater than 0.4, and information greater than 0.2 are in bold (diagonal values excepted when not significant).

	h_1	h_2	h_3		h_1	h_2	h_3
Intercorrelation C_{XY}				Causal correlation $C_{\dot{X}Y}$			
h_1	1	0.89	0.69	$\dot{h}_1$	0.00	0.01	0.02
h_2	0.89	1	0.67	$\dot{h}_2$	0.00	0.00	0.02
h_3	0.69	0.67	1	$\dot{h}_3$	0.30	0.34	0.21
Mutual information I_{XY}				Causal information $I_{\dot{X}Y}$			
h_1	3.69	1.09	0.51	$\dot{h}_1$	0.04	0.00	0.14
h_2	1.09	3.69	0.49	$\dot{h}_2$	0.02	0.00	0.07
h_3	0.51	0.49	3.69	$\dot{h}_3$	0.07	0.05	0.13
XWT coherence C_{XY}				KWT coherence $C_{\dot{X}Y}$			
h_1	1	0.40	0.40	$\dot{h}_1$	0.67	0.34	0.33
h_2	0.40	1	0.38	$\dot{h}_2$	0.48	0.67	0.31
h_3	0.40	0.38	1	$\dot{h}_3$	0.32	0.32	0.67
Bivariate models				Equation reconstruction			
$\dot{h}_1$	u	NL	...	$\dot{h}_1$	NL	NL	...
$\dot{h}_2$	NL	u	...	$\dot{h}_2$	NL	NL	NL
$\dot{h}_3$	...	...	...	$\dot{h}_3$	NL	NL	...

E. Application to a set of environmental time series

Estimating and foreseeing the volume of water resources at short and long time scales is an important problem in the Viet-

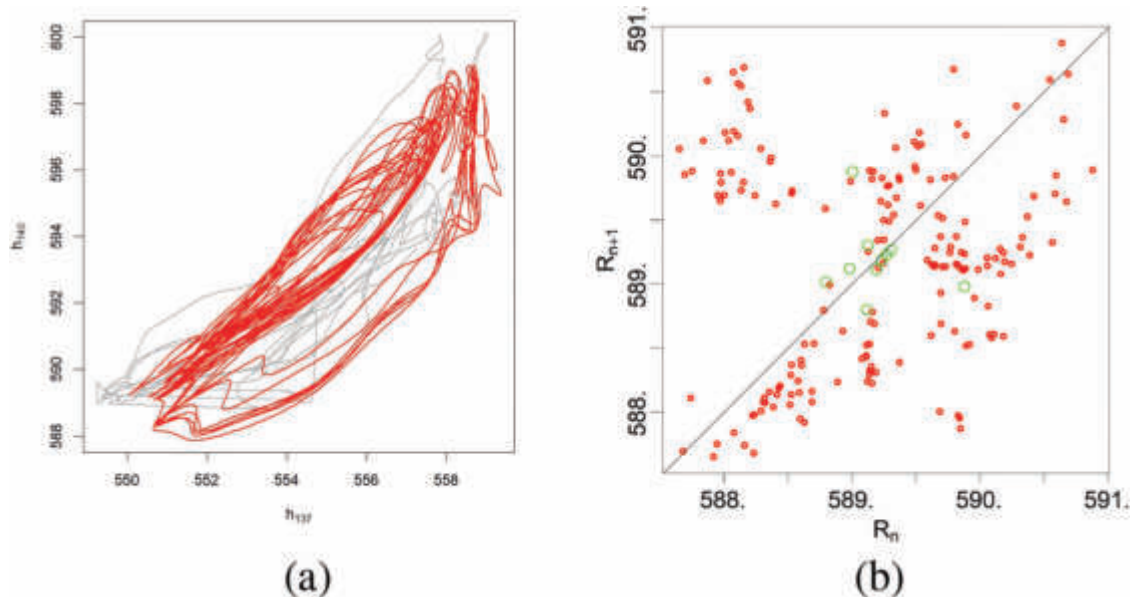


FIG. 17. Model (in red) and original (in the background in gray or green) phase portraits in (h_1, h_2) projection (a) and first return map along the h_2 direction (b) (both in m.a.s.l.). (a) Phase portrait. (b) First return map.

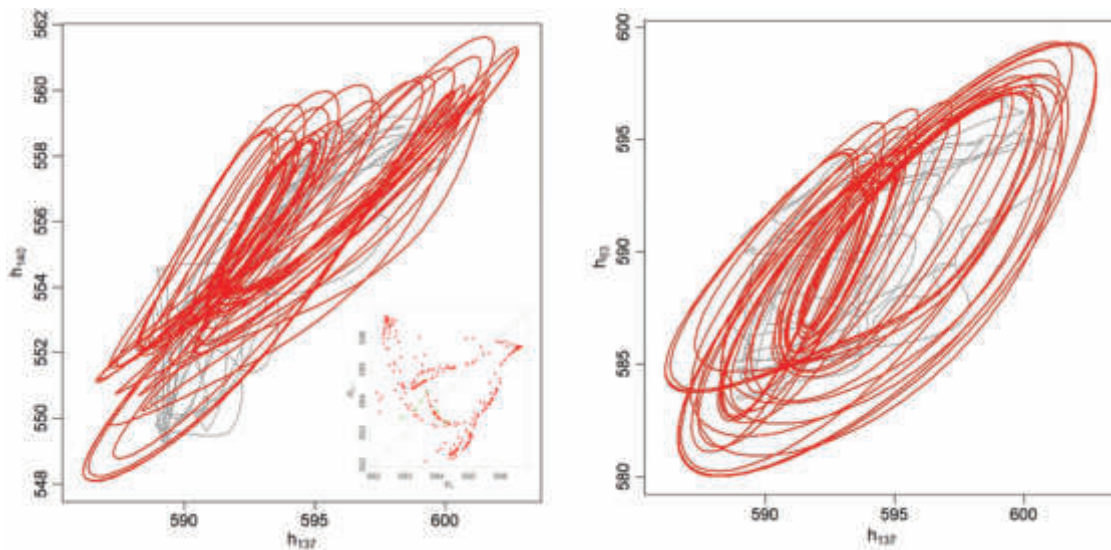


FIG. 18. Model (red) and original (gray in the background) phase portraits in (h_1, h_2) projection (left) and (h_1, h_3) projection (right).

name Central Highlands.^{60,61} Though, water fluxes in aquifers are difficult to understand and monitor in fractured rocks and in karstic systems where the underground connection network can be very complex and is generally poorly known. In practice, it is common to monitor the groundwater level in an ensemble of wells spatially distributed. In the present study, three time series of groundwater level measured in the Se San River basin are considered (see Fig. 5). The various indicators and techniques presented in Secs. IV A–IV D were all applied again to this data set to investigate the potential coupling among the three time series (see Table IV).

The XWC did not enable to detect any clear patterns although higher values of coherence were more often found at scales between 3 and 5 days [Fig. 16(a)] and with a mean value of coherence close to $C = 0.4$, suggesting a possible coupling among the three.

The KWC was also found difficult to interpret for the same reason [Fig. 16(b)]. Similarly, a higher recurrence of high levels of coherence was found, but on a smaller band centered on a scale at three days. High levels of self coherence (values close to 1) with a $\pm\pi/2$ phase were observed in the three cases at long time scales ($\gtrsim 8$ days), but these cannot be interpreted as self causal (see Appendix B for a demonstration). The mean values were all found to be higher than $C = 0.3$ with one value significantly higher suggesting an influence of h_1 on h_2 ($C_{h_2h_1} = 0.48$). A more in-depth analysis

would be required to investigate the causation based on wavelets.

The bivariate modeling was then applied to the three time series taken two by two. A single model was obtained between stations 1 and 2. The conditions requested for a causal interpretation were all satisfied. (1) The model was found robust to numerical integration and its robustness was tested on a long period (more than twice the observation time length). (2) It was proven to be nontrivial. Indeed, this model is four-dimensional and surprisingly rich dynamically (see Fig. 17 and supplementary material, Fig. S16). Its first return map [Fig. 17(b)] confirms this complexity. (3) It also reproduces satisfyingly the order of magnitude of the observed variables. This model, thus, strongly argues for a deterministic coupling between the two variables although it cannot be interpreted as direct coupling due to the numerous derivatives involved in its formulation [see supplementary material, Eq. (J1)].

The equation reconstruction. The selection conditions were obtained with a single model involving the three stations of groundwater height: (1) Its numerical integrability was checked on a sufficiently long period. (2) Its dynamic is non trivial as proven by its phase portrait and its complex first return map (see Fig. 18). (3) The modeled and observed variables have the same order of magnitude. This model

$$\begin{cases} \dot{h}_1 = 207.2 - 1.643h_2 + 2.279 \times 10^{-3}h_2^2 + 0.8380h_1 - 1.223 \times 10^{-5}h_1h_3 - 1.488 \times 10^{-3}h_1h_2, \\ \dot{h}_2 = -34.91 + 0.3702h_3 - 6.386 \times 10^{-4}h_3^2 - 0.5699h_2 - 8.744 \times 10^{-4}h_2h_3 + 1.943 \times 10^{-3}h_2^2 + 0.2830h_1 \\ \quad + 1.451 \times 10^{-3}h_1h_3 - 1.804 \times 10^{-4}h_1h_2 - 1.101 \times 10^{-4}h_1^2, \\ \dot{h}_3 = 312.2 + 0.2135h_3 - 2.423h_2 - 3.965 \times 10^{-4}h_2h_3 + 0.004951h_2^2 + 0.9952h_1 - 0.004768h_1h_2 + 0.001394h_1^2, \end{cases} \quad (35)$$

TABLE V. Relative terms contribution (in bold when greater than 4%) and degree of explained determinism (in %).

	h_1	h_2	h_3	h_1^2	h_2^2	h_3^2	$h_1 h_2$	$h_1 h_3$	$h_2 h_3$	d°
$\dot{h}_1$	5.9	21.3	0.0	0.0	50.3	0.0	22.5	0.002	0.0	20.0
$\dot{h}_2$	0.59	2.2	1.4	0.13	31.9	5.7	28.8	22.3	6.9	19.1
$\dot{h}_3$	1.53	8.4	0.1	4.2	43.3	0.0	42.1	0.0	0.30	42.5

is three-dimensional, highly nonlinear and reveals a complex coupling between the three sub-basins.

The degree of explained determinism (see Table V) varies from one equation to another, it is 21.0% for variable h_1 , 19.1% for h_2 , and 42.5% for h_3 . These low magnitudes are explained by some missing contributions in the analysis. In particular, the rainfall input is not considered in the analysis, and neither the input/output of the other connected sub-basins located upstream, downstream, or aside. This lack of information may also explain the difficulty of the other approaches to detect any clear couplings.

Although the obtained model suggests complex bidirectional couplings among the three variables, the analysis of the relative contribution to the deterministic dynamics reveals the main influence of two terms (h_2^2 and $h_1 h_2$) on the groundwater height, at each of the three stations (see Table V).

V. CONCLUSION

Several techniques have been tested to infer causal couplings between variables of a given system involving two deterministic subsystems, thus producing causal relations in the strong sense.

Among these techniques, the simplest indicators (SC, KC, MI) and the GKI were found to be poorly able to unveil the causal relations, even under the simplest conditions here tested. Results were particularly poor when applied to the NH subsystem. The causal information (KI) proved to be a bit more efficient than the other indicators.

Two wavelet based techniques were also tested that presented significantly different results on the two sub-systems. The cross wavelet coherence (XWC) was found much more efficient to detect the causal influences among the variables of the R76 system than among that of the NH system. The reason directly derives from its formulation, which is designed to unveil local correlations in timescales and time. Introduced in the present work, the causal wavelet coherence (KWC), specifically designed to infer causal relations, was proven to be efficient to detect the causal influences not only for the R76 subsystem, but also for NH subsystem despite the totally decorrelated evolutions of its variables. Its limitation relying to nonlinearity was briefly addressed to show potential interest of the KWC to go further.

It was found that none of these techniques can be used to detect self causality, either simply due to their symmetric construction (SC, MI, XWC), or for analytic reasons (KWC), or due to their lack of robustness (GKI, KC, KI). All of them also revealed a strong sensitivity to noise and a poor ability to deal with multiple causal influences, and none of them were able to distinguish direct from indirect influence.

The global modeling technique was another approach tested here. It has proven to be quite efficient in all the studied contexts. This approach can be applied with at least two variables or with more when these are available. Two extreme situations were investigated (two or six observed variables).

When only a subset of variables is observed, the original equations can be retrieved only if all the variables involved in the causal coupling are available, but may not be retrieved in the general case. If some variables are missing, it may be possible to uncover couplings but it will not be possible to know if these are direct or indirect couplings and it may then be impossible to reconstruct the original fluence network among the variables. The good point here is that the equations will tell if they can, or not, be interpreted as direct coupling. As far as a derivative will be involved in a reconstructed equations, it should not be interpreted as a direct coupling unless other elements may permit to argue for it. These remarks are quite general: In the present work, the subsets of variables were all performed either considering the variables two by two or all of them at the same time. However, the same analyses may be performed considering a subset of three variables or more depending on what is available.

Applied when all the variables are observed, the global modeling was found especially powerful to retrieve the original sets of equations, thus permitting to get interpretable equations. The bidirectional weak couplings were found particularly tricky to uncover with this approach, especially under noisy conditions. Interestingly, it was also shown possible to estimate the contribution of the individual causal terms involved in the dynamics.

Applied to a dataset of groundwater level, the global modeling technique enabled to detect complex couplings between three stations and to unveil the main influence of one of the three stations in this dynamic.

SUPPLEMENTARY MATERIAL

See the [supplementary material](#) for a description of strong and weak couplings (Appendix D); an introduction to observability (Appendix E); sensitivity tests to initial conditions for conservative systems and to accumulated degraded conditions including, at the same time, sensitivity to the initial conditions, measurement noise, and shorter time series (Appendix F); an introduction to the interpretation of wavelet scalograms (Appendix G); Supplementary Figures S1–S16 (Appendix H); Supplementary Tables S2–S6 (Appendix I); and Eq. (J1) (Appendix J).

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Sylvain Mangiarotti: Conceptualization (lead); Formal analysis (lead); Funding acquisition (lead); Investigation (lead); Methodology (lead); Project administration (equal); Software (equal); Supervision (lead); Validation (equal); Visualization (equal); Writing – original draft (lead); Writing – review & editing (lead). **Mathis Neuhauser:** Investigation (equal); Validation (equal); Visualization (equal); Writing – review & editing (equal). **Ludovic Arnaud:** Conceptualization (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Validation (supporting); Visualization (supporting); Writing – review & editing (equal). **Thao Bach Nguyen:** Data curation (lead); Supervision (supporting); Visualization (supporting); Writing – review & editing (equal). **Sébastien Verrier:** Conceptualization (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Software (equal); Supervision (supporting); Validation (equal); Visualization (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

APPENDIX A: CAUSALITY BASED ON EMBEDDING TECHNIQUES

Embedding techniques enable to reconstruct a state space equivalent to the original state space based on a restricted number of variables.^{31,62,63} Its use to detect causality is problematic because it makes possible to reconstruct the dynamics of the complete system based on a restricted number of variables, even possibly a single one. In other words, if all the variables have all the information about the dynamics, how to determine what is causal?

Let us take the example of the Rössler system to exemplify this problem. Its original manifold $M_{(xyz)}$ is described by (x, y, z) . Equivalent manifolds can be reconstructed from x , y , or z , by using either derivatives or delayed variables. In the former case, we will get $M_{(x,\dot{x},\ddot{x})}$ a differential manifold reconstructed from x , $M_{(y,\dot{y},\ddot{y})}$ from y , or $M_{(z,\dot{z},\ddot{z})}$ from z . In the latter case, we will get delayed manifolds $M_{(x(t),x(t+\tau),x(t+2\tau))}$ from x and similarly $M_{(y(t),y(t+\tau),y(t+2\tau))}$ from y and $M_{(z(t),z(t+\tau),z(t+2\tau))}$ from z .

All these manifolds will be (in principle) equivalent. The differential case is more interesting here since enabling an analytic explanation. Indeed, using the Lie derivatives, algebraic relations can be established between the original Rössler system with its original variables x , y , and z and its jerk form

$$\ddot{X} = F_X(X, \dot{X}, \ddot{X}), \quad (A1)$$

with X being the observed variable and its derivatives

$$\begin{aligned} x &= f_x(x, \dot{x}, \ddot{x}) = x, \\ y &= g_x(x, \dot{x}, \ddot{x}) = -\frac{\dot{x}(a_3 - x) + \ddot{x} + a_2 + x}{a_1 + a_3 - x}, \\ z &= h_x(x, \dot{x}, \ddot{x}) = \frac{\ddot{x} + a_2 + x - a_1\dot{x}}{a_1 + a_3 - x}, \\ x &= f_y(y, \dot{y}, \ddot{y}) = \dot{y} - a_1y, \\ y &= g_y(y, \dot{y}, \ddot{y}) = y, \\ z &= h_y(y, \dot{y}, \ddot{y}) = a_1\dot{y} - \ddot{y} - y, \\ x &= f_z(z, \dot{z}, \ddot{z}) = a_3 + \frac{\dot{z} - a_2}{z}, \\ y &= g_z(z, \dot{z}, \ddot{z}) = -z - \frac{\ddot{z}}{z} + \frac{\dot{z}(\dot{z} - a_2)}{z^2}, \\ z &= h_z(z, \dot{z}, \ddot{z}) = z. \end{aligned} \quad (A2)$$

Note, however, that only the jerk form is unique when starting from a single observed variables, but the original three-dimensional form is not.⁶⁴ This will not be a problem for us here since our first goal with bivariate modeling is not to reconstruct the original systems from a restricted number of observed variables but to detect couplings between them.

The existence of similar functions is expected in the case of the delayed manifold although these cannot be formulated analytically. The important point here is that, although the relations between x , y , and z are originally dynamical, these can be reformulated into static relations by using derivatives or delayed variables, that is, taking advantage of an embedding. As a consequence, an embedding can be used to detect coupling properties but it may lose their direction and, thus, the causal relationships. Note, for example, that, although z does not contribute directly to the variations of y , and y does not contribute directly to the variations of z , it is possible to reformulate their (actually indirect) link by embedding and then to predict $z(t)$ from $y(t)$, and $y(t)$ from $z(t)$.

APPENDIX B: XWC AND KWC IN TWO SPECIFIC SITUATIONS

The *Morlet Wavelet* is defined as

$$\Psi_0(\tau) := \pi^{-\frac{1}{4}} e^{i f_0 \tau} e^{-\frac{\tau^2}{2}}, \quad (B1)$$

where τ is a dimensionless time and f_0 is the dimensionless frequency. In the context of features extraction, it is common to fix $f_0 = 6$ which is a good compromise to have both temporal and frequency localization. τ is define from the time t as $\tau = s.t$ introducing the *scale* parameter s .

The *Continue Wavelets transform* (CWT) of a signal $x(t)$ with *scale* s and *delay* t is defined as the convolution between the signal $x(t)$ and the rescaled Morley wavelet,

$$W_x(s, t) := x(t) \star \frac{\Psi_0^*\left(\frac{-t}{s}\right)}{\sqrt{s}} = \frac{1}{\sqrt{s}} \int_{-\infty}^{\infty} x(t') \Psi_0^*\left(\frac{t' - t}{s}\right) dt', \quad (B2)$$

where $\star$ represents the convolution product and $*$ represents the complex conjugate. When the signal $x(t)$ is discretized in N sample

x_k ,⁴³ it becomes

$$W_x^k(s) = \sqrt{\frac{\delta t}{s}} \sum_{k'=1}^N x_{k'} \Psi_0^* \left[(k' - k) \frac{\delta t}{s} \right]. \quad (\text{B3})$$

The Cross Wavelets Coherence (XWC) of two signals $x(t)$ and $y(t)$ is defined as

$$C_{xy} := \frac{\| \langle W_x(s, t), W_y^*(s, t) \rangle \|}{\| W_x(s, t) \|^{\frac{1}{2}} \| W_y(s, t) \|^{\frac{1}{2}}}, \quad (\text{B4})$$

where $\langle f(s, t) \rangle$ is a time–frequency smoothing function, which can be defined as $\langle f(s, t) \rangle = \frac{1}{\delta} \int_{t-\frac{\delta}{2}}^{t+\frac{\delta}{2}} f(s, t') dt'$ for a specific time window δ .⁴²

Proposition 1: The cross wavelet transform of a signal with itself has a coherence equal to 1 and a phase equal to 0.

Proof. From the definition (B4), taking $y(t) = x(t)$, it leads

$$C_{xx} = \frac{\| \langle W_x(s, t), W_x^*(s, t) \rangle \|}{\| \langle W_x(s, t) \|^{\frac{1}{2}} \| W_x(s, t) \|^{\frac{1}{2}}} \quad (\text{B5})$$

$$= \frac{\| \langle W_x(s, t) \|^2 \|}{\| W_x(s, t) \|^2} = 1 \quad (\text{B6})$$

and

$$W_{xx}(s, t) = w_x(s, t) w_x(s, t)^* = \| w_x(s, t) \|^2, \quad (\text{B7})$$

with $\phi = \arg(W_{xx}(s, t)) = 0$. $\square$

Proposition 2: The cross wavelets of a signal $x(t)$ with its time derivative $\dot{x}(t)$ has a (causal) coherence $C_{\dot{x}x}$ approximately equal to 1 and a phase close to $\frac{\pi}{2}$.

Proof. From the definition (3) and using the convolution property that allows the swapping of the derivative operator ($f \star g = f \star \dot{g}$), we have

$$W_{\dot{x}}(s, t) = \dot{x}(t) \star \frac{\Psi_0^* \left(-\frac{t}{s} \right)}{\sqrt{s}} = x(t) \star \frac{\dot{\Psi}_0^* \left(-\frac{t}{s} \right)}{\sqrt{s}}. \quad (\text{B8})$$

From the definition (B1), the derivative of the Morlet wavelet with respect to τ can be written as

$$\frac{d\Psi_0(\tau)}{d\tau} = \frac{d}{d\tau} \left(\pi^{-\frac{1}{4}} e^{if_0\tau} e^{-\frac{\tau^2}{2}} \right) \quad (\text{B9})$$

$$= \pi^{-\frac{1}{4}} \left(if_0 e^{if_0\tau} e^{-\frac{\tau^2}{2}} - \tau e^{if_0\tau} e^{-\frac{\tau^2}{2}} \right) \quad (\text{B10})$$

$$= \pi^{-\frac{1}{4}} (if_0 - \tau) e^{if_0\tau} e^{-\frac{\tau^2}{2}} \quad (\text{B11})$$

$$= (if_0 - \tau) \Psi_0(\tau). \quad (\text{B12})$$

The wavelet has 99.7% of its significant value when the variable τ is in the interval $[-3, 3]$. Therefore, on this interval, $f_0 > \tau$ and the derivative can be approximated as

$$\frac{d\Psi_0(\tau)}{d\tau} = (if_0 - \tau) \Psi_0(\tau) \simeq if_0 \Psi_0(\tau). \quad (\text{B13})$$

It follows that approximately the real part of the Morley wavelet (the imaginary part, respectively) is proportional to the imaginary part (the real part, respectively) of its derivative with respect to τ . This statement is illustrated in Fig. 19.

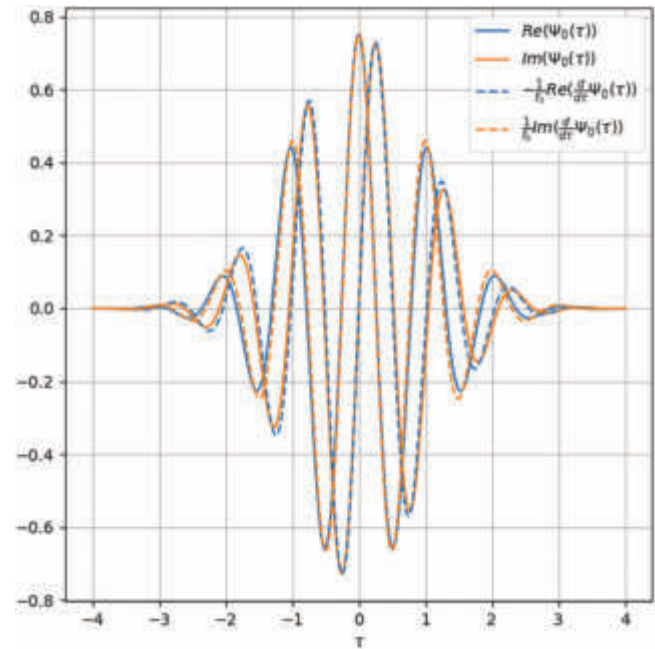


FIG. 19. Real (in blue) and imaginary (in orange) parts of the Morlet wavelet (plain lines) and their derivative with respect to τ (dashed lines).

To complete the proof, let us consider the derivative with respect to t using the chain rule with the same approximation

$$\dot{\Psi}_0^* \left(-\frac{t}{s} \right) = \frac{d}{dt} \left[\Psi_0^* \left(-\frac{t}{s} \right) \right] = \left(\frac{d}{dt} \left[\Psi_0 \left(-\frac{t}{s} \right) \right] \right)^*, \quad (\text{B14})$$

stating that $T = -\frac{t}{s}$, we have $\frac{dT}{dt} = -\frac{1}{s}$, and then

$$\dot{\Psi}_0^* \left(-\frac{t}{s} \right) = \left(\frac{d}{dt} [\Psi_0(T)] \right)^* \quad (\text{B15})$$

$$= \left(\frac{d}{dT} \Psi_0(T) \times \frac{dT}{dt} \right)^* = \left[\left(\frac{d}{dT} \Psi_0(T) \right) \times \left(-\frac{1}{s} \right) \right]^* \quad (\text{B16})$$

$$\simeq \left[if_0 \Psi_0(T) \times \left(-\frac{1}{s} \right) \right]^* = if_0 \Psi_0^* \left(-\frac{t}{s} \right) \times \left(+\frac{1}{s} \right), \quad (\text{B17})$$

given that $(ab)^* = a^*b^*$ and $(-if_0)^* = if_0$. Then, injecting it in the definition of the (CWT), we get

$$W_{\dot{x}}(s, t) = x(t) \star \frac{\dot{\Psi}_0^* \left(\frac{t}{s} \right)}{\sqrt{s}} \quad (\text{B18})$$

$$\simeq x(t) \star \left(\frac{if_0}{s} \right) \frac{\Psi_0^* \left(-\frac{t}{s} \right)}{\sqrt{s}} = \frac{if_0}{s} W_x(s, t). \quad (\text{B19})$$

We then have

$$W_{xx}(s, t) \simeq \left(\frac{if_0}{s} \right) w_x(s, t) w_x(s, t)^* \quad (\text{B20})$$

$$= \left(\frac{if_0}{s} \right) \|w_x(s, t)\|^2, \quad (\text{B21})$$

with $\phi = \arg(W_{xx}(s, t)) = \frac{\pi}{2}$. It is possible to approximately evaluate C_{xx} as

$$C_{xx} = \frac{\| \langle W_x(s, t), W_x(s, t)^* \rangle \|^2}{\langle \|W_x(s, t)\|^2 \rangle^{\frac{1}{2}} \langle \|W_x(s, t)\|^2 \rangle^{\frac{1}{2}}} \quad (\text{B22})$$

$$\simeq \frac{\| \langle \frac{if_0}{s} W_x(s, t), W_x(s, t)^* \rangle \|^2}{\langle \| \frac{if_0}{s} W_x(s, t) \|^2 \rangle^{\frac{1}{2}} \langle \| W_x(s, t) \|^2 \rangle^{\frac{1}{2}}} \quad (\text{B23})$$

$$\simeq \frac{\frac{f_0}{s} \| \langle W_x(s, t) \|^2 \rangle}{\frac{f_0}{s} \langle \| W_x(s, t) \|^2 \rangle} = 1 \quad (\text{B24})$$

that concludes the proof. $\square$

APPENDIX C: NONLINEAR CAUSAL WAVELET COHERENCE

Causal wavelet coherence may also be used to detect, at least, single nonlinear terms. Let us consider an equation of general form

$$\dot{X}_i = \alpha + \beta \prod_j X_j^{n_j}. \quad (\text{C1})$$

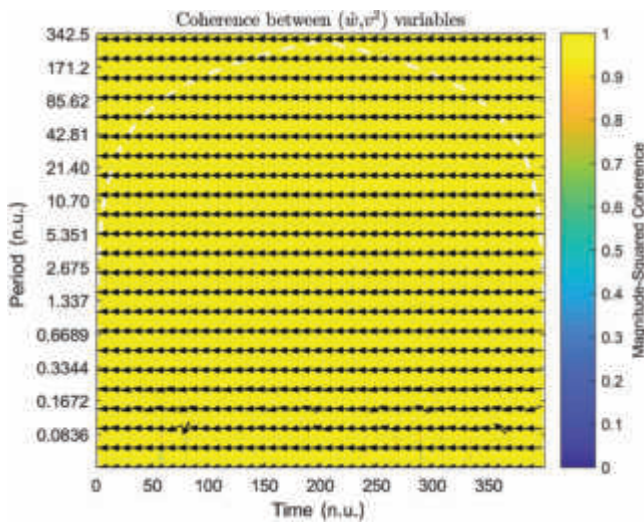


FIG. 20. Nonlinear Causal Wavelet Coherence applied to the detection of nonlinear terms [here v^2 in Eq. (21)] under free of noise conditions.

If we state $\dot{X} = \dot{X}_i$ and $Y(t) = \prod_j X_j^{n_j}(t)$, we get

$$C_{XY} = \frac{\| \langle W_X(s, t), W_{(X-\alpha)/\beta}^*(s, t) \rangle \|^2}{\langle \|W_X(s, t)\|^2 \rangle^{\frac{1}{2}} \langle \|W_{(X-\alpha)/\beta}(s, t)\|^2 \rangle^{\frac{1}{2}}} \quad (\text{C2})$$

$$= \frac{\frac{1}{\beta} \langle \|W_X(s, t)\|^2 \rangle}{\frac{1}{\beta} \langle \|W_X(s, t)\|^2 \rangle} = 1. \quad (\text{C3})$$

Applied to the third equation of NH system [Eq. (21)]

$$\dot{w} = b_2 - v^2, \quad (\text{C4})$$

the result $C_{wv^2} \approx 1$ with a 0 delay is indeed retrieved (see Fig. 20).

REFERENCES

- ¹H. Poincaré, "Les Méthodes Nouvelles de la Mécanique Céleste III." (Gauthier-Villard, Paris, 1899)
- ²E. N. Lorenz, "Deterministic non-periodic flow," *J. Atmos. Sci.* **20**(2), 130–141 (1963).
- ³R. H. Abraham and Y. Ueda, *The Chaos Avant-Garde: Memories of the Early Days of Chaos Theory* (World Scientific Publishing, Singapore, 2000).
- ⁴C. Letellier, L. F. Olsen, and S. Mangiarotti, "Chaos: From theory to applications for the 80th birthday of Otto E. Rössler," *Chaos* **31**(6), 060402 (2021).
- ⁵I. Drouot, "La causalité en philosophie et en sciences, 18ème-21ème siècles introduction," in *Statistique et causalité*, edited by Bertrand, Saporta et Thomas-Agnan, Technip "SFDS" (Paris, 2021).
- ⁶C. E. Shannon and W. Weaver, *The Mathematical Theory of Communication* (University of Illinois Press, 1949), ISBN 0-252-72548-4.
- ⁷R. Aggarwal and P. Ranganathan, "Common pitfalls in statistical analysis: The use of correlation techniques," *Perspect. Clin. Res.* **7**(4), 187–190 (2016).
- ⁸R. J. Janse, T. Hoekstra, K. J. Jager, C. Zoccali, G. Tripepi, F. W. Dekker, and M. van Diepen, "Conducting correlation analysis: Important limitations and pitfalls," *Clin. Kidney J.* **14**(11), 2332–2337 (2021).
- ⁹H. Fu, S. Tang, and X. Zhao, "Limitations of correlation coefficients in research on functional connectomes and psychological processes," *Hum. Brain Mapp.* **46**(10), e70287 (2025).
- ¹⁰A. Kraskov, H. Stögbauer, and P. Grassberger, "Estimating mutual information," *Phys. Rev. E* **69**(6), 066138 (2004).
- ¹¹G. Sugihara, R. May, H. Ye, C.-H. Hsieh, E. Deyle, M. Fogarty, and S. Munch, "Detecting causality in complex ecosystems," *Science* **338**, 496–500 (2012).
- ¹²M. Palús, A. Krakovská, J. Jakubík, and M. Chvosteková, "Causality, dynamical systems and the arrow of time," *Chaos* **28**, 075307 (2018).
- ¹³L. A. Aguirre, L. L. Portes, and C. Letellier, "Structural, dynamical and symbolic observability: From dynamical systems to networks," *PLoS One* **13**(10), e0206180 (2018).
- ¹⁴C. Lainscsek, S. S. Cash, T. J. Sejnowski, and J. Kurths, "Dynamical ergodicity DDA reveals causal structure in time series," *Chaos* **31**, 103108 (2021).
- ¹⁵C. Lainscsek, P. Salami, V. R. Carvalho, E. M. A. M. Mendes, M. Fan, S. S. Cash, and T. J. Sejnowski, "Network-motif delay differential analysis of brain activity during seizures," *Chaos* **33**, 123136 (2023).
- ¹⁶I. Daubechies, "The wavelet transform, time-frequency localization and signal analysis," *IEEE Trans. Inf. Theory* **IT-36**(5), 961–1005 (1990).
- ¹⁷P. C. Liu, "Wavelet spectrum analysis and ocean wind waves," in *Wavelets in Geophysics*, edited by E. Foufoula-Georgiou and P. Kumar (Academic Press, 1994), pp. 151–166.
- ¹⁸A. Grinsted, J. C. Moore, and S. Jevrejeva, "Application of the cross wavelet transform and wavelet coherence to geophysical time series," *Nonlinear Process. Geophys.* **11**(5/6), 561–566 (2004).
- ¹⁹M. Chavez and B. Cazes, "Detecting dynamic spatial correlation patterns with generalized wavelet coherence and non-stationary surrogate data," *Sci. Rep.* **9**(1), 7389 (2019).
- ²⁰H. H. Szu, B. A. Telfer, and A. W. Lohmann, "Causal analytical wavelet transform," *Opt. Eng.* **31**(9), 1825–1829 (1992).

- ²¹C. W. J. Granger, "Investigating causal relations by econometric models and cross-spectral methods," *Econometrica* **37**(3), 424–438 (1969).
- ²²N. Wiener, "The theory of prediction," in *Modern Mathematics for the Engineer*, edited by E. F. Beckenbach (McGraw-Hill, New York, 1956), pp. 125–139.
- ²³S. Mangiarotti, R. Coudret, L. Drapeau, and L. Jarlan, "Polynomial search and global modeling: Two algorithms for modeling chaos," *Phys. Rev. E* **86**, 046205 (2012).
- ²⁴S. Mangiarotti, "Low dimensional chaotic models for the plague epidemic in Bombay (1896–1911)," *Chaos, Solitons Fractals* **81**, 184–196 (2015).
- ²⁵S. L. Brunton, J. L. Proctor, and J. N. Kutz, "Discovering governing equations from data by sparse identification of nonlinear dynamical systems," *Proc. Natl. Acad. Sci.* **113**(15), 3932–3937 (2016).
- ²⁶S. Mangiarotti and M. Huc, "Can the original equations of a dynamical system be retrieved from observational time series?" *Chaos* **29**, 023133 (2019).
- ²⁷P. C. Young, "Parameter estimation for continuous-time models—A survey," *Automatica* **17**(1), 23–39 (1981).
- ²⁸D. C. Saha and G. P. Rao, *Identification of Continuous Dynamical Systems—The Poisson Moment Functionals (PMF) Approach* (Springer-Verlag, Berlin, 1983).
- ²⁹S. A. Billings, "Identification of nonlinear systems—A survey," *IEEE Proc. D* **127**(6), 272–285 (1980).
- ³⁰P. Bergé, Y. Pomeau, and C. Vidal, *L'ordre Dans le Chaos—Vers Une Approche Déterministe de la Turbulence* (Hermann, 1984) [Order Within Chaos: Towards a Deterministic Approach to Turbulence (Wiley-VCH, 1987)].
- ³¹F. Takens, "Detecting strange attractors in turbulence," *Lect. Notes Math.* **898**, 366–381 (1981).
- ³²L. A. Aguirre and S. A. Billings, "Dynamical effects of overparametrization in nonlinear models," *Physica D* **80**(1–2), 26–40 (1995).
- ³³G. Gouesbet and C. Letellier, "Global vector field reconstruction by using a multivariate polynomial L_2 -approximation on nets," *Phys. Rev. E* **49**(6), 4955–4972 (1994).
- ³⁴L. A. Aguirre and C. Letellier, "Modeling nonlinear dynamics and chaos: A review," *Math. Probl. Eng.* **2009**, 238960 (2009).
- ³⁵G. Camps-Valls, A. Gerhardus, U. Ninad, G. Varando, G. Martius, E. Balaguer-Ballester, R. Vinuesa, E. Diaz, L. Zanna, and J. Runge, "Discovering causal relations and equations from data," *Phys. Rep.* **1044**, 1–68 (2023).
- ³⁶N. Omejc, B. Gec, J. Brence, L. Todorovski, and S. Džeroski, "Probabilistic grammars for modeling dynamical systems from coarse, noisy, and partial data," *Mach. Learn.* **113**, 7689–7721 (2024).
- ³⁷C. Lainscek, C. Letellier, and I. Gorodnitsky, "Global modeling of the Rössler system from the z -variable," *Phys. Lett. A* **314**(5–6), 409 (2003).
- ³⁸S. Mangiarotti, M. Peyre, and M. Huc, "A chaotic model for the epidemic of Ebola virus disease in West Africa (2013–2016)," *Chaos* **26**, 113112 (2016).
- ³⁹S. Mangiarotti, Y. Zhang, and M. Leblanc, "Chaos theory applied to the modelling of Karst springs: First results from univariate time series," *Hydrogeol. J.* **27**, 2027–2043 (2019).
- ⁴⁰S. Mangiarotti, E. Fu, P. Jouquet, M. T. Tran, M. Huc, and N. Bottinelli, "Earthworm activity and its coupling to soil hydrology: A deterministic analysis," *Chaos* **31**(1), 013134 (2021).
- ⁴¹M. Sáez, D. Benavente, S. Cuezva *et al.*, "Scenarios for the Altamira cave CO₂ concentration from 1950 to 2100," *Sci. Rep.* **14**, 10359 (2024).
- ⁴²E. A. K. Cohen and A. T. Walden, "A statistical study of temporally smoothed wavelet coherence," *IEEE Trans. Signal Process.* **58**, 2964–2973 (2010).
- ⁴³C. Torrence and G. P. Compo, "A practical guide to wavelet analysis," *Bull. Am. Meteorol. Soc.* **79**(1), 61–78 (1998).
- ⁴⁴M. Farge, "Wavelet transforms and their applications to turbulence," *Annu. Rev. Fluid Mech.* **24**, 395–457 (1992).
- ⁴⁵M. Misiti, Y. Misiti, G. Oppenheim, and J.-M. Poggi (2004). "Wavelet toolbox for use with Matlab, User's guide version 3," The MathWorks, Inc. <https://www.mathworks.com/help/wavelet/index.html>.
- ⁴⁶See <http://www.glaciology.net/wavelet-coherence> for "Cross Wavelet and Wavelet Coherence Toolbox for Matlab."
- ⁴⁷C. Letellier, L. A. Aguirre, and U. S. Freitas, "Frequently asked questions about global modeling," *Chaos* **19**, 023103 (2009).
- ⁴⁸S. Mangiarotti, M. Huc, F. Le Jean, M. Chassan, and L. Drapeau (2023) "GPoM: Generalized polynomial modelling, CeCILL-2 licence, version 1.4 (2023, first version 2017)," Comprehensive R Archive Network. <https://CRAN.R-project.org/package=GPoM>.
- ⁴⁹C. Letellier and L. A. Aguirre, "Graphical interpretation of observability in terms of feedback circuits," *Phys. Rev. E* **72**, 056202 (2005).
- ⁵⁰C. Letellier, J. Maquet, and L. A. Aguirre, "How the choice of observable may influence the analysis of nonlinear dynamical systems," *Commun. Nonlinear Sci. Numer. Simul.* **11**(5), 555–576 (2006).
- ⁵¹L. A. Aguirre and C. Letellier, "Observability of multivariate differential embeddings," *J. Phys. A: Math. Gen.* **38**, 6311–6326 (2005).
- ⁵²O. E. Rössler, "An equation for continuous chaos," *Phys. Lett. A* **57**(5), 397–398 (1976).
- ⁵³J. D. Farmer, J. P. Crutchfield, H. Froeling, N. H. Packard, and R. S. Shaw, "Power spectra and mixing properties of strange attractors," *Ann. N.Y. Acad. Sci.* **357**, 453–471 (1980).
- ⁵⁴S. Nosé, "A molecular dynamics method for simulations in the canonical ensemble," *Mol. Phys.* **52**(2), 255–268 (1984).
- ⁵⁵W. G. Hoover, "Nonlinear conductivity and entropy in the two-body Boltzmann gas," *J. Stat. Phys.* **42**(3/4), 587–600 (1986).
- ⁵⁶L. Kocarev and U. Parlitz, "Generalized synchronization, predictability, and equivalence of unidirectionally coupled dynamical systems," *Phys. Rev. Lett.* **76**(11), 1816–1819 (1996).
- ⁵⁷J.-A. Lissajous, "Mémoire sur l'étude optique des mouvements vibratoires," *Ann. Chim. Phys., Troisième série* **51**, 147–231 (1857).
- ⁵⁸A. Buscarino, M. Frasca, M. Branciforte, L. Fortuna, and J. C. Sprott, "Synchronization of two Rössler systems with switching coupling," *Nonlinear Dyn.* **88**, 673–683 (2017).
- ⁵⁹S. Mangiarotti, I. Sendiña-Nadal, and C. Letellier, "Using global modeling to unveil hidden couplings in small grinsted motifs," *Chaos* **28**, 123110 (2018).
- ⁶⁰Socialist Republic of Vietnam, Data collection survey on water resources management in central highlands, Final Report, Main Report, April 2018, Japan International Cooperation Agency (JICA), Nippon Koei Co., Ltd.
- ⁶¹T. V. Tran, D. X. Tran, and D. B. Nguyen, "Agricultural drought in the Vietnamese Central Highlands at 1-km resolution: Monthly and annual datasets," *Data Brief* **48**(1), 109194 (2023).
- ⁶²H. Whitney, "Differentiable manifolds," *Ann. Math.* **37**(3), 645–680 (1936).
- ⁶³T. Sauer, J. A. Yorke, and M. Casdagli, "Embedology," *J. Stat. Phys.* **65**(3–4), 579–616 (1991).
- ⁶⁴C. Lainscek, "Nonuniqueness of global modeling and time scaling," *Phys. Rev. E* **84**, 046205 (2011).