1 Simulation of stochastic processes exhibiting any-range dependence and 2 arbitrary marginal distributions

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- Simulation of short and long-range dependent processes
- 12 Simulation of univariate and multivariate processes

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31 Abstract

32 Hydrometeorological processes are typically characterized by temporal dependence, short- or 33 long-range (e.g., Hurst behavior), as well as by non-Gaussian distributions (especially at fine 34 time scales). The generation of long synthetic time series that resemble the marginal and joint 35 properties of the observed ones is a prerequisite in many uncertainty-related hydrological studies, since they can be used as inputs and hence allow the propagation of natural variability 36 37 and uncertainty to the typically deterministic water-system models. For this reason, it has been 38 for years one of the main research topics in the field of stochastic hydrology. This work presents a novel model for synthetic time series generation, termed Symmetric Moving Average 39 40 (neaRly) To Anything (SMARTA), that holds out the promise of simulating stationary 41 univariate and multivariate processes with any-range dependence and arbitrary marginal distributions, provided that the former is feasible and the latter have finite variance. This is 42 43 accomplished by utilizing a mapping procedure in combination with the relationship that exists 44 between the correlation coefficients of an auxiliary Gaussian process and a non-Gaussian one, 45 formalized through the Nataf's joint distribution model. The generality of SMARTA is stressed through two hypothetical simulation studies (univariate and multivariate), characterized by 46 47 different dependencies and distributions. Furthermore, we demonstrate the practical aspects of the proposed model through two real-world cases, one that concerns the generation of annual 48 non-Gaussian streamflow time series at four stations, and another that involves the synthesis 49 50

of intermittent, non-Gaussian, daily rainfall series at a single location.

51 1 Introduction

52 Hydrometeorological time series (i.e., sequences of observations ordered in time) can be 53 considered the cornerstone of any water-related engineering study, although, such data are in 54 scarcity and often the available records don't have sufficient length for the task at hand (e.g., 55 reliability and risk-related studies). A historical record of such observations will rarely if ever 56 repeat in the future, which is the simplest manifestation of the high variability and uncertainty 57 that is naturally inherited therein. In this vein, it can be argued that embracing stochasticity in 58 hydrometeorological processes is a first step towards the development of uncertainty-aware 59 methodologies for water systems. Stochastic simulation, and the synthesis of long hydrometeorological time series, which are used in place of historical ones, can provide a 60 61 potential remedy to this situation. Synthetic time series are not predictions of future states, but rather constitute plausible realizations of the simulated process, that are, loosely speaking, 62 statistically equivalent with the parent information (i.e., historical data). Driving the typically 63 64 deterministic water-system simulation models with such realizations provides the means to assess their response in a probabilistic manner, under multiple, plausible scenarios. Nowadays, 65 synthetic data are used in a variety of studies, among them, the optimal planning and 66 management of reservoir systems (e.g., Celeste & Billib, 2009; Feng et al., 2017; Giuliani 67 et al., 2014; Koutsoyiannis & Economou, 2003; Tsoukalas & Makropoulos, 2015a, 2015b), 68 69 risk assessment of flood (e.g., Haberlandt et al., 2011; Paschalis et al., 2014; Qin & Lu, 70 2014; Wheater et al., 2005) and drought events (e.g., Herman et al., 2016), as well as water resources simulation under future climate conditions (e.g., Fatichi et al., 2011; Fowler et al., 71 72 2000; Kilsby et al., 2007; Nazemi et al., 2013). Thereby, the wide applicability of synthetic 73 time series and stochastic simulation highlight the need for simulation schemes that can 74 resemble the, intriguing and challenging to simulate, characteristics of hydrometeorological 75 processes.

76 A typical characteristic encountered in such processes is auto-dependence (persistence), either 77 short or long-range. The former, short-range dependence (SRD), has been extensively discussed in literature (e.g., Box et al., 2015) and implies an exponential autocorrelation 78 79 structure that diminishes after few time lags. On the contrary, the second, long-range

80 dependence (LRD), also known as long-term persistence (sometimes referred to as long-

81 memory), implies an auto-dependence structure that strongly extends for large lags (see, Beran, 82 1992). The latter behavior is also related to the so-called Hurst phenomenon, also known as

Joseph effect, fractional Gaussian noise (fGn), scaling in time or Hurst-Kolmogorov dynamics

84 (HK; Koutsoyiannis, 2011; Koutsoyiannis & Montanari, 2007); see also the review work of

85 Molz et al. (1997). Its discovery is usually credited to Hurst (1951), who while studying long

- 86 records of streamflow and other data noticed that extreme events tend to exhibit a clustering
- 87 behavior in terms of temporal occurrence. However, as pointed out by Koutsoyiannis (2011),
- 88 it was Kolmogorov (1940) who first proposed its mathematical description. Eventually, after
- the seminal work of Hurst and the extensive documentation of Mandelbrot and Wallis (1969a,
 1969b, 1969c) it is now acknowledged that LRD (and HK) processes are omnipresent in
- geophysics, hydrology, climate and other scientific disciplines (Beran, 1994; Koutsoyiannis,
 2002; O'Connell et al., 2016). The latter publications provide further examples and details

93 regarding the interpretation and identification of such behavior.

94 Regarding modelling and application of SRD or LRD in hydrological studies, the former type 95 (SRD) has been systematically studied and employed in numerous cases for the simulation of 96 a variety of hydrometeorological processes (Breinl et al., 2013; Brissette et al., 2007; Khalili 97 et al., 2009; Matalas, 1967; Mehrotra et al., 2015; Mhanna & Bauwens, 2012; Srikanthan 98 & McMahon, 2001; Srikanthan & Pegram, 2009; Thompson et al., 2007). On the other 99 hand, it is well recognized that proper representation of LRD is of high importance, especially 100 in reservoir-related studies, since their operation and regulation is performed in over-annual scale, where LRD is mostly encountered (Bras & Rodríguez-Iturbe, 1985; Iliopoulou et al., 101 102 2016; Koutsoyiannis, 2002). Other notable hydrology-related applications of LRD include 103 the stochastic simulation of precipitation or streamflow at finer time-scales, from monthly and daily (e.g., Detzel & Mine, 2017; Maftei et al., 2016; Montanari et al., 1997, 2000) to 10-104 105 second interval (e.g., Lombardo et al., 2012; Papalexiou et al., 2011), as well as the generation of synthetic storm hyetographs (e.g., Koutsoyiannis & Foufoula-Georgiou, 1993). 106 In general, SRD can be easily captured with the so-called AutoRegressive Moving Average 107 (ARMA) family of models, while we note that, even though such models have a long history 108 109 and are still popular, today the literature offers other powerful and flexible options (cf. Koutsoyiannis, 2016). On the other hand, LRD, hence HK behavior, requires the use of 110 111 alternative generation schemes (see, Bras & Rodríguez-Iturbe, 1985; O'Connell et al., 2016), such as fractional Gaussian noise models (Mandelbrot & Wallis, 1969a, 1969b, 112 1969c), fast fractional Gaussian noise (ffGn) models (Mandelbrot, 1971), broken line models 113 114 (Ditlevsen, 1971; Mejia et al., 1972) and Fractional AutoRegressive Integrated Moving-115 Average (FARIMA) models (Granger & Joyeux, 1980; Hosking, 1984). In contrast to the 116 abovementioned specialized simulation schemes, a notable exception, that can simulate any type of autocorrelation function of a process, is the Symmetric Moving Average (SMA) model 117

118 of Koutsoyiannis (2000, 2002, 2016), coupled with theoretical autocorrelation (or 119 autocovariance) structures. This flexibility is achieved by decoupling the parameter 120 identification of the autocorrelation structure and the generation mechanism (i.e., the model).

In addition to temporal dependence, hydrometeorological variables are often characterized by non-Gaussian and skewed distribution functions (partially attributed to the often non-negative nature of such processes), especially in fine time scales (e.g., daily or finer), where intermittency is omnipresent. The need to account for non-Gaussian distributions was early recognized by many researchers (e.g., Klemeš & Borůvka, 1974; Matalas & Wallis, 1976;

126 Matalas, 1967) and is currently remarked by the numerous large-scale statistical studies

127 conducted at various time scales (e.g., Blum et al., 2017; Cavanaugh et al., 2015; Kroll &

128 Vogel, 2002; McMahon et al., 2007; Papalexiou & Koutsoyiannis, 2013, 2016). Regarding

129 stochastic hydrology and simulation through linear stochastic models, many efforts have been

130 made towards that direction (i.e., simulating non-Gaussian processes) which can be broadly

131 classified in three main categories (Tsoukalas et al., 2018a): a) Explicit methods that are able to generate data from specific marginal distributions (e.g., Klemeš & Borůvka, 1974; 132 Lawrance & Lewis, 1981; Lombardo et al., 2012, 2017; Matalas, 1967) b) Implicit 133 134 approaches, pioneered by Thomas and Fiering (1963), that treat skewness via employing non-Gaussian white noise (typically from Pearson type-III distribution) for the innovation term 135 (Detzel & Mine, 2017; Efstratiadis et al., 2014; Koutsoyiannis, 1999, 2000; Lettenmaier 136 137 & Burges, 1977; Matalas & Wallis, 1976, 1971; Matalas, 1967; Todini, 1980). c) 138 Transformation-based approaches that employ appropriate functions (e.g., Box-Cox) in order to "normalize" the observed data; next simulate realizations using typical Gaussian stochastic 139 140 models and finally "de-normalize" the generated data in order to attain the process of interest 141 (e.g., Salas et al., 1980). However, as discussed in Tsoukalas et al. (2018a), most of these schemes exhibit a number of limitations that still remain unresolved. Particularly, approaches 142 143 of category (a) are limited to a narrow type of autocorrelation functions and non-Gaussian 144 distributions (e.g., Gamma or Log-Normal), while they are typically able to simulate only 145 univariate processes. On the other hand, approaches of category (b) are prone to the generation of negative values, provide an approximation of the marginal distributions, while encounter 146 147 difficulties when modelling highly skewed (univariate or multivariate) processes (Koutsoyiannis, 1999; Todini, 1980). It is noted thought, that some recent schemes are able 148 to capture moments higher than skewness (e.g., kurtosis), by the inclusion of additional model 149 parameters (Koutsoyiannis et al., 2018 and references therein). On top of these issues, only 150 151 few schemes (e.g., SMA) are able to model a variety of temporal correlation structures, while it is also possible to establish bounded dependence patterns which are far from natural ones 152 153 (Tsoukalas et al., 2018a, 2018b). Finally, regarding the schemes of category (c), they require 154 the specification of a non-trivial normalization function (due to the inadequacy of simple 155 transformations; such as, Box-Cox) that often entail several parameters (usually determined 156 through optimization techniques). Further to this, even if the latter function is properly 157 identified, it is acknowledged that they introduce bias in the simulated marginal and joint characteristics (Bras & Rodríguez-Iturbe, 1985; Salas et al., 1980 p. 73). 158

159 In this work, in an effort to simultaneously address these challenges and provide a flexible 160 method for synthetic time series generation, we introduce a generic, yet simple and 161 theoretically justified, explicit approach based on the simulation of univariate and multivariate stationary processes exhibiting any-range dependence and arbitrary marginal distributions. 162 More specifically, the proposed method can explicitly model the autocorrelation structure and 163 distribution of each individual process, provided that the former is feasible and the latter have 164 finite variance, while simultaneously it can preserve the lag-0 cross-correlation structure. The 165 166 main components of the method are, the SMA model of Koutsoyiannis (2000), a theoretical 167 autocorrelation structure and the pivotal concept of Nataf's joint distribution model (NDM, Nataf, 1962). The key idea of our approach lies in employing an auxiliary Gaussian stochastic 168 169 process, modelled using the SMA scheme, with such parameters that reproduce the target auto-170 (i.e., temporal; SRD or LRD) and lag-0 cross-correlation (i.e., spatial) coefficients of the process after its subsequent mapping to the actual domain via the target inverse cumulative 171 172 density functions (ICDFs). It is remarked that instead of SMA, any other linear stochastic model (e.g., ARMA-type) could be employed in order to mathematically describe the auxiliary 173 174 Gaussian process, yet, it is anticipated that the resulting simulation scheme will inherit its 175 properties regarding the simulation of univariate and multivariate processes, e.g., if the auxiliary model is capable of simulating SRD structures, the established simulation scheme 176 177 will also be SRD.

The latter rationale has also been employed within the scientific field of operations research and particularly by Cario and Nelson (1996), as well as, Biller and Nelson (2003) who proposed the AutoRegressive To Anything (ARTA) and the Vector AutoRegressive To 181 Anything (VARTA) methods respectively for the explicit simulation of stationary 182 autoregressive (AR) processes with arbitrary marginal distributions.

It is remarked that (to the extent of our knowledge) despite their wide acceptance, the 183 184 aforementioned approaches (and their variants) have been unknown to the hydrological community and have never been used for the simulation of hydrometeorological processes until 185 very recently. Nonetheless, it seems that presently, Nataf-based approaches are gaining 186 187 momentum. Particularly, using a similar rationale, Serinaldi and Lombardo (2017) introduced an approach for the synthesis of autocorrelated univariate binary processes, while, Papalexiou 188 189 (2018) provided a comprehensive treatment on the topic using autoregressive models and used, 190 for first time, mixed-type marginals enabling the modeling of intermittent processes like 191 precipitation. Finally, Tsoukalas et al. (2017, 2018a), employed the notion of NDM and 192 provided a generalization of the latter models (ARTA, VARTA), termed SPARTA (Stochastic 193 Periodic AutoRegressive To Anything), for the simulation of univariate and multivariate 194 cyclostationary (i.e., periodic) processes with arbitrary marginal distributions. Following the 195 same naming convention with the initial publications, and since our approach uses as an 196 auxiliary model the SMA scheme, the proposed method is termed Symmetric Moving Average 197 (neaRly) To Anything (SMARTA). Alternatively, given that the latter schemes make use of 198 the ICDF, which is generally a non-linear function, they can be viewed as a non-linear variation 199 of underlying linear stochastic models (e.g., AR or SMA). The use of the ICDF in the 200 abovementioned, Nataf-based, schemes ensures that the generated data will have the target 201 distribution but on the other hand it is recognized that the Pearson correlation coefficient 202 (which is used to express the dependencies in all linear stochastic models) is not invariant under 203 such non-linear monotonic transformations (Embrechts et al., 1999). Therefore, the main 204 challenge of such approaches, lies in identifying the "equivalent" correlations coefficients that 205 should be used within the generation procedure (Gaussian domain) in order to attain the target 206 correlation structure in the actual (i.e., real) domain. The latter relationship (i.e., that of 207 equivalent and target correlations) can be expressed theoretically through a double infinite 208 integral, which can be approximated with the use of numerical techniques such as the one 209 employed herein.

210 Further details about the proposed approach can be found in sections 2 and 3, where the latter 211 is further divided in four subsections. Particularly, section 2 presents some key concepts 212 regarding modeling of auto-dependence structure in general; while subsections 3.1 and 3.2 213 develop the theoretical background of the proposed approach; next, subsection 3.3 describes 214 the auxiliary SMA model and lastly, subsection 3.4 summarizes the overall approach and 215 provides the generation mechanism of SMARTA in step-by-step manner. The generality of 216 SMARTA is illustrated through a series of numerical examples, hypothetical (section 4) and 217 real-world (section 5), including the simulation of both univariate and multivariate time series. 218 Finally, in section 6 we synopsize and discuss the proposed modelling approach.

219 2 Modelling the auto-dependence structure

220 Before describing SMARTA, it is considered useful to provide a brief introduction to the tools 221 that allow the mathematical description of the auto-dependence structure of a stochastic 222 process. For a more thorough treatment, the interested reader is referred to the works of 223 Papoulis (1991) and Lindgren et al. (2013). To elaborate, let $\underline{x}_t, t \in \mathbb{Z}$ be a discrete-time stationary process, indexed using t, with finite variance $\sigma^2 := Var[\underline{x}_t]$ and autocorrelation 224 function $\rho_{\tau} := \operatorname{Corr}[\underline{x}_t, \underline{x}_{t+\tau}] = \rho_{|\tau|}$, where $\tau = 0, \pm 1, \pm 2, \dots$ denotes the time lag. The 225 autocovariance function (ACVF) of the process can be obtained by, $c_{\tau} := \text{Cov}[\underline{x}_t, \underline{x}_{t+\tau}] =$ 226 $\sigma^2 \rho_{\tau}$. It is reminded that a valid autocorrelation structure has to be positive definite (e.g., 227 Lindgren, 2013; Papoulis, 1991), which can be readily checked by formulating, and testing 228

for positive definiteness, the so-called $(n \times n)$ autocorrelation matrix **R**, whose $i^{\text{th}}, j^{\text{th}}$ elements are being determined by, $\mathbf{R}_{[i,j]} = \rho_{|i-j|}$.

Besides the ACF and ACVF, another particularly useful stochastic tool, is the climacogram (CG, Koutsoyiannis, 2010, 2016), which is typically depicted using a log-log plot, and expresses the variance of the aggregated $(\underline{X}_l^{(k)})$ or time averaged $(\underline{x}_l^{(k)})$ process at scale $k \in \mathbb{Z}^+$. We point out that the notation employed herein slightly differs from the typical one, since we restrict our attention to discrete-time processes. Assuming that \underline{x}_t denotes a discrete-time stationary process at the basic time scale k = 1, the discrete-time aggregated process at scale k > 1 can be obtained by,

$$\underline{X}_{l}^{(k)} \coloneqq \sum_{t=(l-1)k+1}^{\kappa l} \underline{x}_{t} \tag{1}$$

while the averaged discrete-time process is obtained by, $\underline{x}_{l}^{(k)} = \underline{X}_{l}^{(k)}/k$. Hence, the corresponding climacograms of the discrete-time aggregated and averaged process can be defined as $\Gamma^{(k)} \coloneqq \operatorname{Var}[\underline{X}_{l}^{(k)}]$ and $\gamma^{(k)} \coloneqq \operatorname{Var}[\underline{x}_{l}^{(k)}]$ respectively. Moreover, as shown by Beran (1994 p. 3), as well as by Koutsoyiannis (2010, 2016), the variance over scales (i.e., the CG) and the ACVF (and therefore ACF) are interrelated. Specifically, if the theoretical ACVF (or ACF), c_{τ} at the basic time scale (k = 1) is known, the corresponding theoretical discrete-time climacogram of the aggregated process can be calculated using the following equation,

$$\Gamma^{(k)} = c_0 k + 2 \sum_{\tau=1}^{k-1} (k-\tau) c_{\tau}$$
⁽²⁾

while the averaged one can be obtained by, $\gamma^{(k)} = \Gamma^{(k)}/k^2$. The recursive application of the following equation facilitates the calculation of the climacogram $\Gamma^{(k)}$,

$$\Gamma^{(k)} = 2\Gamma^{(k-1)} - \Gamma^{(k-2)} + 2c_{k-1}$$
(3)

248 It is noted that, $\Gamma^{(1)} = \gamma^{(1)} = c_0 = \sigma^2$, while $\Gamma^{(0)} = 0$. The inverse relationship that calculates

the ACVF of the aggregated discrete-time process $(\underline{X}_{l}^{(k)})$, denoted $C_{\tau}^{(k)} \coloneqq \text{Cov}[\underline{X}_{l}^{(k)}, \underline{X}_{l+\tau}^{(k)}]$, at time scale *k* given the theoretical climacogram is given by (Koutsoyiannis, 2017),

$$C_{\tau}^{(k)} = \frac{\Gamma^{(|\tau+1|k)} + \Gamma^{(|\tau-1|k)}}{2} - \Gamma^{(|\tau|k)}, \quad \tau \ge 0$$
(4)

Furthermore, the ACVF, $C_{\tau}^{(k)}$ at scale k is linked with the ACVF, c_{τ} , of the basic time scale k = 1, through the following relationship,

$$C_{\tau}^{(k)} = \sum_{t=1}^{k} \sum_{r=\tau k+1}^{(1+\tau)k} \operatorname{Cov}[\underline{x}_{t}, \underline{x}_{r}] = \sum_{t=1}^{k} \sum_{r=\tau k+1}^{(1+\tau)k} c_{|t-r|}, \quad \tau \ge 0$$
(5)

Analogously, the ACVF of the time averaged discrete-time process $(\underline{x}_l^{(k)})$ at scale *k*, denoted $c_{\tau}^{(k)} \coloneqq \text{Cov}[\underline{x}_l^{(k)}, \underline{x}_{l+\tau}^{(k)}]$, is obtained by $c_{\tau}^{(k)} = C_{\tau}^{(k)}/k^2$. Hence, the ACF of the aggregated discrete-time process at time scale *k* can be obtained by $\rho_{\tau}^{(k)} = C_{\tau}^{(k)}/\Gamma^{(k)}$, while the ACF of the time averaged discrete-time process by $\rho_{\tau}^{(k)} = c_{\tau}^{(k)}/\gamma^{(k)}$. Note that the ACF of the aggregated and time averaged process are identical, due to standardization of the corresponding ACVF with the variance. It is also noted that $C_0^{(k)} = \Gamma^{(k)}$ and $C_{\tau}^{(1)} = c_{\tau}$, while similarly, $c_0^{(k)} =$ $\gamma^{(k)}$ and $c_{\tau}^{(1)} = c_{\tau}$. 260 Undoubtedly, the most commonly-employed tool to characterize the auto-dependence structure 261 is the autocorrelation function (ACF). The literature offers a plethora of theoretical models in both continuous and discrete time (Dimitriadis & Koutsoyiannis, 2015; Gneiting, 2000; 262 263 Gneiting & Schlather, 2004; Koutsoyiannis, 2000, 2016; Papalexiou, 2018; Papalexiou et al., 2011), that can be easily combined with the proposed approach (see next section). In this 264 work we use the discrete-time Cauchy-type autocorrelation structure (CAS) of Koutsoyiannis 265 266 (2000) due to its simple and parsimonious form (a desired property in stochastic modelling), which however does not hinder its ability to model a wide range of short (ARMA-type) and 267 268 long-range dependence structures (including HK behavior). CAS is a two-parameter power-269 type autocorrelation structure which, in its simplest form, if the ACF has constant and positive 270 sign (as in the case of geophysical and hydrometeorological processes), is given by,

$$\rho_{\tau}^{\text{CAS}} = (1 + \kappa \beta \tau)^{-1/\beta}, \qquad \tau \ge 0 \tag{6}$$

where $\beta \ge 0$ and $\kappa > 0$ are parameters that control the degree of dependence (or persistence) of the process. It is remarked that the autocorrelation function of an HK (i.e., fGn) process consists a special case (or a very good approximation) of the latter model (i.e., Eq. (6)) whose theoretical ACF is given by,

$$\rho_{\tau}^{\mathrm{HK}} = \frac{1}{2} (|\tau - 1|^{2H} - 2|\tau|^{2H} + |\tau + 1|^{2H})$$
(7)

where *H* is the Hurst coefficient ($0 \le H \le 1$), which, loosely speaking, controls the degree of long-term dependence (or persistence) of the process. It has been shown that for large time lags and H > 0.5, the parameter β of CAS is related to the *H* coefficient of an HK ACF through the relationship $\beta = 1/(2 - 2H) > 1$, thus asymptotically resembling the right tail of latter theoretical model. More specifically, for $\beta > 1$ and when κ is set equal to κ_0 , see Eq. (8), CAS closely approximates the theoretical ACF of an HK process, even for small time lags.

$$\kappa = \kappa_0 := \frac{1}{\beta \left[\left(1 - \frac{1}{\beta} \right) \left(1 - \frac{1}{2\beta} \right) \right]^{\beta}}$$
(8)

In addition, the ACF of an SRD process (ARMA-type) can be obtained through CAS, by setting $\beta = 0$ and applying the L' Hôpital's rule. The resulting SRD ACF is given by,

$$\rho_{\tau}^{\text{SRD}} = \exp(-\kappa\tau) \tag{9}$$

Furthermore, when $\kappa = -\ln(\rho_1)$, and $0 \le \rho_1 \le 1$, Eq. (8) reduces to the classic Markovian ACF of an AR(1) process, given by, $\rho_{\tau}^{AR(1)} = \rho_1^{|\tau|}$. For other parameter values, CAS resembles 284 285 a plethora of alternative autocorrelation structures, that differ from the aforementioned classic 286 models (for further details see, Koutsoyiannis, 2000). The flexibility of CAS is illustrated in 287 Figure 1a where we depict (in a log-log scale) the theoretical ACF of various HK processes, 288 characterized by different values of Hurst coefficient, H, as well as, their approximation with 289 290 CAS. The close agreement of the two theoretical models is further validated in Figure 1b where we plot (also in log-log scale) their climacograms (assuming $\sigma^2 = c_0 = 1$), which are 291 practically indistinguishable. It is noted that for an HK process, which exhibits simple and 292 constant scaling laws, the slope s of the climacogram $\gamma^{(k)}$, i.e., the log-log derivative $s \coloneqq$ 293 $d(\ln(\gamma^{(k)}))/d(\ln(k))$, is related with H parameter by s = 2H - 2. The resemblance of the 294 295 HK and CAS is confirmed by estimating the average mean square error (MSE) of the depicted 296 processes by means of both ACF and climacogram. In terms of ACF, the average MSE value 297 is 0.01 and the corresponding value in terms of climacogram is 0.66.



 $\begin{array}{l} -H = 0.90 \quad -H = 0.80 \quad -H = 0.70 \quad -H = 0.60 \\ \hline \\ \text{Figure 1. a)} \text{ Autocorrelation functions and b) climacograms of HK processes exhibiting different Hurst} \\ 300 \quad \text{coefficients (dashed lines) and their approximation with the CAS (continuous line).} \end{array}$

301 Considering the practical aspects of the auto-dependence structure identification procedure 302 (e.g., estimation of the parameters of CAS or any other theoretical structure, given a sample 303 time series), it is remarked that it is a challenging task, due to the fact that the sample estimates 304 of variance and autocorrelation coefficients (i.e., empirical variance and ACF - calculated from 305 the historical time series) are negatively biased (e.g., Beran, 1994; Koutsoyiannis, 2003, 306 2016, 2017), especially in the presence of LRD (e.g., HK behavior). A thorough treatment on 307 the subject lies beyond the scope of this study, as it has been extensively documented by the 308 aforementioned authors, as well as by Dimitriadis and Koutsoyiannis (2015) who highlighted 309 the advantages of using the climacogram, in comparison with the ACF and power spectrum, 310 for the identification of the auto-dependence structure. The latter authors, via an extended 311 analysis of a wide range of SRD and LRD processes, showed that the climacogram exhibits less uncertainty and bias in its estimation, which can be easily estimated *a priori*, thus providing 312 313 an attractive alternative to the latter classic approaches. Further to this, the latter stochastic tool 314 can be used as a basis for LRD identification algorithms (e.g., Tyralis & Koutsoyiannis, 2011), as well as for the development additional tools (e.g., the climacospectrum) that provide 315 316 further insights regarding the asymptotic behavior of the process (Koutsoyiannis, 2016, 317 2017). It is noted that in this work, the above-mentioned stochastic tools (i.e., ACF and CG) are mainly employed for "diagnostic", and not for identification purposes, i.e., to verify that 318 319 the simulated processes exhibit the desired dependence properties.

320 **3** Methodology

321 **3.1** Theoretical background of the SMARTA model

The central idea of the proposed approach is based on the Nataf's joint distribution model (NDM, Nataf, 1962) which has been originally implemented for the generation of crosscorrelated, yet serially independent, random vectors with arbitrary distributions. One of its key assumptions, which consequently holds for SMARTA or any other Nataf-based method, is that the employed distributions owe to have finite variance. This assumption is implied throughout this work.

- 328 NDM gained popularity after the works of Liu and Der Kiureghian (1986) and Cario and
- 329 Nelson (1997), who also coined the term NORmal To Anything (NORTA) procedure and also

- 330 accounted for combinations of continuous and discrete marginal distributions. Its main concept
- 331 lies in establishing joint relationships with the use of an auxiliary multivariate standard normal
- 332 (i.e., Gaussian) distribution (using an appropriately adjusted correlation matrix); generating
- correlated standard normal variates and then mapping them to the actual domain using their
- ICDF. As noted by Cario and Nelson (1997) and further investigated by Lebrun and Dutfoy
 (2009), NDM is related to the Gaussian copula since the variables' joint distribution is
 established through the multivariate Gaussian distribution.
- 337 An interesting point concerning NDM (see, Tsoukalas et al., 2018a) is that it can be 338 retrospectively associated with several well-known hydrological approaches (e.g., Kelly & 339 Krzysztofowicz, 1997; Klemeš & Borůvka, 1974; Matalas, 1967). Among them, we distinguish the so-called Wilks' type weather generators (Wilks, 1998), which have motivated 340 341 a significant amount of research during the last decades. The latter author, in an effort to 342 simulate cross-correlated random variates, representing either the precipitation occurrence or 343 amount process (neglecting temporal dependence), proposed the simulation of cross-correlated 344 Gaussian variables and their subsequent mapping via their ICDF. Wilks empirically observed 345 that a monotonic relationship exists which links the correlation coefficients of the Gaussian 346 and "real" domain. Hence, the use of inflated correlation coefficients was proposed within the 347 multivariate Gaussian distribution, in order to attain random variates with the required crosscorrelation and distribution. The latter class of models is reviewed in the works of Wilks and 348 349 Wilby (1999) and Ailliot et al., (2015).
- In this study, we employ the concept of NDM, but in a different context, i.e., for the simulation of stationary any-range-dependent stochastic processes. Particularly, the rationale of NDM is combined with an auxiliary Gaussian process in order to capture the stochastic structure (in terms of autocorrelation and cross-correlation coefficients) of the target process and simultaneously preserve the desired marginal distributions after the use of the ICDF.
- Suppose that the goal is to generate a *m*-dimensional discrete-time stationary process $\underline{x}_t = \begin{bmatrix} \underline{x}_t^1, \dots, \underline{x}_t^i, \dots, \underline{x}_t^m \end{bmatrix}^T$, where *t* is the time index and the indices $i, j = 1, \dots, m$ are used to refer to individual process \underline{x}_t^i and \underline{x}_t^j respectively. Also let, $\mathbf{x}_t = \begin{bmatrix} x_t^1, \dots, x_t^i, \dots, x_t^m \end{bmatrix}^T$ denote a realization of it. Furthermore, let us assign a target cumulative distribution function (CDF), denoted by, $F_{\underline{x}^i} \coloneqq P(\underline{x}^i \le x)$ to each individual process \underline{x}_t^i , and let $\rho_{t,t+\tau}^{i,j} \coloneqq \operatorname{Corr}[\underline{x}_t^i, \underline{x}_{t+\tau}^j]$ denote the target Pearson's correlation coefficient between \underline{x}_t^i and \underline{x}_t^j for time lag τ .
- Likewise, and using the same notation as above, let $\underline{z}_t = [\underline{z}_t^1, \dots, \underline{z}_t^i, \dots, \underline{z}_t^m]^T$ be an auxiliary *m*-dimensional stationary standard Gaussian process with zero mean and unit variance. Also,
- let $\tilde{\rho}_{t,t+\tau}^{i,j} \coloneqq \operatorname{Corr}[\underline{z}_t^i, \underline{z}_{t+\tau}^j]$ denote the Pearson's correlation coefficient of the auxiliary process
- between \underline{z}_t^i and \underline{z}_t^j for time lag τ , hereafter, referred to as equivalent correlation coefficient. It
- 365 is noted that throughout the paper the superscripts or subscripts of $\rho_{t,t+\tau}^{i,j}$ or $\tilde{\rho}_{t,t+\tau}^{i,j}$ may be 366 omitted when possible. For brevity, the target autocorrelation of the process \underline{x}_t^i will be denoted 367 ρ_{τ}^i and its lag- τ cross-correlation with \underline{x}_t^j as $\rho_{\tau}^{i,j}$.
- 368 As mentioned earlier, the idea behind SMARTA lies in simulating an auxiliary standard 369 Gaussian process \underline{z}_t using the SMA model with such parameters that after applying the inverse 370 of their distribution function, results in a process \underline{x}_t with the desired correlation structure and 371 marginal distributions. The latter operation can be written as follows,
- 372

$$\underline{x}_{t}^{i} = F_{\underline{x}^{i}}^{-1} \left(\Phi(\underline{z}_{t}^{i}) \right) \tag{10}$$

where $\Phi(\cdot)$ denotes the standard normal CDF and $F_{\underline{x}^i}^{-1}(\cdot)$ stands for the ICDF of process \underline{x}_t^i . An advantage of the above scheme is that since the ICDFs of the target distributions are

- employed (given that they can be analytically or numerically evaluated), the process \underline{x}_t^i will inevitably have the desired marginal properties. On the other hand, the Pearson's correlation coefficient is not invariant under such non-linear monotonic transformations, hence $\rho_{t,t+\tau}^{i,j}$ will differ from $\tilde{\rho}_{t,t+\tau}^{i,j}$. However, as discussed in the literature, they are related (e.g., Biller &
- Nelson, 2003; Cario & Nelson, 1997; Der Kiureghian & Liu, 1986). Since Eq. (10) holds,
 we can write,

$$\rho_{t,t+\tau}^{i,j} = \operatorname{Corr}\left[\underline{x}_{t}^{i}, \underline{x}_{t+\tau}^{j}\right] = \operatorname{Corr}\left[F_{\underline{x}^{i}}^{-1}\left(\Phi(\underline{z}_{t}^{i})\right), F_{\underline{x}^{j}}^{-1}\left(\Phi(\underline{z}_{t+\tau}^{j})\right)\right]$$
(11)

Using the definition of Pearson's correlation coefficient, we can also write (for the sake of simplicity the time index t is omitted when possible due to stationarity),

$$\rho_{t,t+\tau}^{i,j} = \operatorname{Corr}[\underline{x}_{t}^{i}, \underline{x}_{t+\tau}^{j}] = \frac{\operatorname{E}[\underline{x}_{t}^{i} \, \underline{x}_{t+\tau}^{j}] - \operatorname{E}[\underline{x}^{i}] \operatorname{E}[\underline{x}^{j}]}{\sqrt{\operatorname{Var}[\underline{x}^{i}] \operatorname{Var}[\underline{x}^{j}]}}$$
(12)

383 where $E[\underline{x}^i]$, $E[\underline{x}^j]$ and $Var[\underline{x}^i]$, $Var[\underline{x}^j]$ denote the mean and variance of \underline{x}^i and \underline{x}^j 384 respectively; which are known from the corresponding distributions $F_{\underline{x}^i}$ and $F_{\underline{x}^j}$ and have to

be finite. Subsequently, using Eq. (10) and the first cross-product moment of \underline{x}_t^i and $\underline{x}_{t+\tau}^j$ we obtain,

$$E[\underline{x}_{t}^{i} \ \underline{x}_{t+\tau}^{j}] = E\left[F_{\underline{x}^{i}}^{-1}\left(\Phi(\underline{z}_{t}^{i})\right)F_{\underline{x}^{j}}^{-1}\left(\Phi(\underline{z}_{t+\tau}^{j})\right)\right]$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F_{\underline{x}^{i}}^{-1}\left(\Phi(z_{t}^{i})\right)F_{\underline{x}^{j}}^{-1}\left(\Phi(z_{t+\tau}^{j})\right)\varphi_{2}(z_{t}^{i}, z_{t+\tau}^{j}, \tilde{\rho}_{t,t+\tau}^{i,j})dz_{t}^{i}dz_{t+\tau}^{j}$$

$$(13)$$

where $\varphi_2(z_t^i, z_{t+\tau}^j, \tilde{\rho}_{t,t+\tau}^{i,j})$ is the bivariate standard normal probability density function. Hence, by substituting Eq. (13) to Eq. (11) we obtain,

390

$$\rho_{t,t+\tau}^{i,j} = \frac{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F_{\underline{x}^{i}}^{-1} \left(\Phi(z_{t}^{i})\right) F_{\underline{x}^{j}}^{-1} \left(\Phi(z_{t+\tau}^{j})\right) \varphi_{2}(z_{t}^{i}, z_{t-\tau}^{j}, \tilde{\rho}_{t+\tau}^{i,j}) dz_{t}^{i} dz_{t+\tau}^{j} - \mathbb{E}[\underline{x}^{i}] \mathbb{E}[\underline{x}^{j}]}{\sqrt{\operatorname{Var}[\underline{x}^{i}] \operatorname{Var}[\underline{x}^{j}]}}$$
(14)

Inspection of Eq. (14) indicates that $\rho_{t,t+\tau}^{i,j}$ is a function of $\tilde{\rho}_{t,t+\tau}^{i,j}$, since all other quantities are already known from the target (i.e., given) distributions $F_{\underline{x}^i}$ and $F_{\underline{x}^j}$. Therefore, it is compactly written as,

$$\rho_{t,t+\tau}^{i,j} = \mathcal{F}\left(\tilde{\rho}_{t,t+\tau}^{i,j} \middle| F_{\underline{x}^{i}}, F_{\underline{x}^{j}}\right)$$
(15)

394 where $\mathcal{F}(\cdot)$ is an abbreviation of the function defined by Eq. (14).

This relationship implies that prior to the estimation of the auxiliary model's parameters it is essential to identify, and next use within parameter estimation, the equivalent correlations, $\tilde{\rho}_{t,t+\tau}^{i,j}$, that result to the target correlations, $\rho_{t,t+\tau}^{i,j}$, after the subsequent mapping of the auxiliary process to the actual domain. This can be achieved through inversion of Eq. (15), i.e., $\tilde{\rho}_{t,t+\tau}^{i,j} =$ $\mathcal{F}^{-1}\left(\rho_{t,t+\tau}^{i,j} | F_{x^{i}}, F_{x^{j}}\right)$.

400 **3.2** Identification of equivalent correlation coefficients

401 Provided that the identification of equivalent correlation coefficients can be accomplished on 402 a pairwise basis, and for the sake of simplicity, let us define $\underline{x}_{\xi} \coloneqq \underline{x}_{t}^{i}$ and $\underline{x}_{\psi} \coloneqq \underline{x}_{t+\tau}^{j}$, hence

- 403 $\tilde{\rho}_{\xi,\psi}$ and $\rho_{\xi,\psi}$ stand for the equivalent and the target correlation coefficients respectively.
- 404 Furthermore, let $F_{\underline{x}\xi}$ and $F_{\underline{x}\psi}$ denote the corresponding target distributions. It is reminded that
- 405 our ultimate objective is to establish a relationship between $\tilde{\rho}_{\xi,\psi}$ and $\rho_{\xi,\psi}$ and eventually find
- 406 the appropriate value of $\tilde{\rho}_{\xi,\psi}$ that results in the target correlation $\rho_{\xi,\psi}$ after the mapping
- 407 operation of Eq. (10). It is acknowledged that Eq. (15) does not have a general closed-form
- solution, with the exception of few special cases, hence it is typically identified via numerical
 techniques such as crude search, quadrature methods as well as Monte-Carlo procedures (Cario
- 410 & Nelson, 1996, 1997; Chen, 2001; Li & Hammond, 1975; Liu & Der Kiureghian, 1986;
- 411 Xiao, 2014). The abovementioned authors provided a series of Lemmas that can be used in
- 412 order to establish the relationship of Eq. (15). Among them,
- 413 **Lemma 1.** $\rho_{\xi,\psi}$ is a strictly increasing function of $\tilde{\rho}_{\xi,\psi}$.
- 414 Lemma 2. $\tilde{\rho}_{\xi,\psi} = 0$ for $\rho_{\xi,\psi} = 0$ as well as, $\tilde{\rho}_{\xi,\psi} \ge (\le) 0$ if $\rho_{\xi,\psi} \ge (\le) 0$.
- 415 Lemma 3. $|\rho_{\xi,\psi}| \leq |\tilde{\rho}_{\xi,\psi}|.$
- 416 It is remarked that the equality sign in Lemma 3 is valid when $\rho_{\xi,\psi} = 0$ or when both
- 417 marginals are Gaussian. Furthermore, the minimum and maximum attainable values of $\rho_{\xi,\psi}$
- 418 are in accordance with the Fréchet-Hoeffding bounds (Fréchet, 1957; Hoeffding, 1994) and
- 419 are given for $\tilde{\rho}_{\xi,\psi} = -1$ and $\tilde{\rho}_{\xi,\psi} = 1$, respectively. Particularly the following relationship
- 420 holds true, $-1 \leq \mathcal{F}\left(-1 \left| F_{\underline{x}_{\xi}}, F_{\underline{x}_{\psi}} \right) \leq \rho_{\xi,\psi} \leq \mathcal{F}\left(1 \left| F_{\underline{x}_{\xi}}, F_{\underline{x}_{\psi}} \right) \leq 1$. See also the work of Whitt
- 421 (1976) for a comprehensive discussion on the topic. In this paper, unless stated otherwise, in
- 422 order to establish the relationship of Eq. (15) we employ the simple, yet efficient method
- 423 proposed by Tsoukalas et al., (2018a), which in a nutshell, is based on the evaluation of few 424 pairs of $\rho_{\xi,\psi}$ and $\tilde{\rho}_{\xi,\psi}$ using Monte-Carlo simulation and subsequently, the establishment of
- 425 the relationship of Eq. (15) through polynomial interpolation (see also, Appendix A).

426 **3.2.1** An illustrative example

427 To shed some light on the functional form of $\mathcal{F}(\cdot)$ let us consider the case where both variables 428 \underline{x}_{ξ} and \underline{x}_{ψ} are described by the two-parameter Gamma distribution (\mathcal{G}). The probability density 429 function (PDF) of the latter distribution is given by,

$$f_{\mathcal{G}}(x;a,b) = \frac{1}{|b|\Gamma(a)} \left(\frac{x}{b}\right)^{a-1} \exp\left(-\frac{x}{b}\right), \qquad x > 0$$
(16)

430 where $\Gamma(\cdot)$ denotes the gamma function and a > 0 and $b \neq 0$ are shape and scale parameters, 431 respectively. Figure 2a depicts the relationship among $\tilde{\rho}_{\xi,\psi}$ and $\rho_{\xi,\psi}$ (i.e., $\mathcal{F}(\cdot)$; computed via numerical integration) for various values of distribution parameters. Specifically, we assumed 432 433 $a \coloneqq a_{\xi} = a_{\psi}$ and constant $b \coloneqq b_{\xi} = b_{\psi} = 1$. We remind that the theoretical skewness coefficient of a Gamma distributed variable is given by $C_{s_x} = 2/\sqrt{a}$. From the latter figure we 434 observe that the non-linearity of $\mathcal{F}(\cdot)$ increases with low values of a (i.e., high skewness), and 435 that the maximum attainable value of $\rho_{\xi,\psi}$ is equal to 1, due to the fact that $F_{\underline{x}_{\xi}} \equiv F_{\underline{x}_{\psi}}$. In 436 addition, one may observe that the shape parameter a is also related to the minimum attainable 437 438 value of $\rho_{\xi,\psi}$. For example, when a = 0.01 the latter value is practically restricted to zero, something that may be considered a reasonable behavior, attributed to the very high value of 439 positive skewness which does not allow for negative correlations. In a similar vein, in Figure 440 441 2b we set $a_{\xi} = 5$ and vary parameter a_{ψ} from 5 to 0.01 (assuming again that $b := b_{\xi} = b_{\psi} =$ 442 1). In this case, both the minimum and maximum attainable values of $\rho_{\xi,\psi}$ are affected. It is 443 observed that, when a_{ξ} and a_{ψ} exhibit significant differences, the range of feasible values 444 $\rho_{\xi,\psi}$ is getting narrower. This implies that two variables with considerable different shape 445 (expressed through parameter a) cannot be highly correlated. From an engineering point of 446 view, and similar to the previous case (i.e., when $a \coloneqq a_{\xi} = a_{\psi}$), this is barely considered a

447 limitation of the proposed approach, since such behavior is rarely encountered in 448 hydrometeorological processes. For instance, it is not expected, or rational, two processes, one 449 with skewness ~ 0.9 and one with 20 to be highly correlated (positively or negatively). In any 450 case, we stress the importance of checking the range of attainable correlation coefficients when 451 employing the concept of NDM, (see, Demirtas & Hedeker, 2011; Leonov & Qaqish, 2017), 452 especially within the context of stochastic process simulation. For instance, given the non-453 linear and asymmetric nature of $\mathcal{F}(\cdot)$, for some combinations of marginal distributions, a target 454 correlation coefficient may be inadmissible. This constraint, and the fact that the target 455 marginal distributions ought to have finite variance, drove us to add the designation "nearly" 456 when naming the method. However, in the examples employed in this work, such problems did 457 not occur (for a simulation example also involving negative cross-correlations see section 4.2), a fact which by no means overrules the aforementioned need for compatibility verification. 458



459

460 **Figure 2.** Graphical illustration of function $\mathcal{F}(\cdot)$ (see, Eq. (15)) that expresses the relationship between 461 the equivalent, $\tilde{\rho}_{\xi,\psi}$ and target $\rho_{\xi,\psi}$ correlation coefficients assuming that both \underline{x}_{ξ} and \underline{x}_{ψ} are described 462 by the two-parameter Gamma distribution (assuming that $b := b_{\xi} = b_{\psi} = 1$) with a) equal shape 463 parameters (i. e., $a := a_{\xi} = a_{\psi}$) and b) different shape parameters by setting $a_{\xi} = 5$ and varying a_{ψ} 464 from 5 to 0.01.

465 Evidently, the proper and accurate identification of the relationship $\mathcal{F}(\cdot)$ has a crucial role in NDM-based schemes, since its misspecification may lead to simulation errors. Hence, to assess 466 467 the suitability of the algorithm of Appendix A, which is extensively used in this work, we employed the latter and recreated the cases depicted in Figure 2; which concerned the 468 identification of equivalent correlation coefficients of two Gamma-distributed variables for 469 470 various values of shape parameters. After the specification of the relationship $\mathcal{F}(\cdot)$ by the latter algorithm, the target correlations where evaluated for values of $\tilde{\rho}_{\xi,\psi} \in [-1,1]$ sampled by 471 0.01. To provide a quantitative comparison, we estimated the MSE and maximum square error 472 (Max(SE)) between the estimates of the numerical integration method (i.e., Figure 2) and those 473 474 of the aforementioned algorithm. A synopsis of the results is given on Table 1, where the panels (a) and (b) corresponds to those of Figure 2. The latter analysis illustrates the potential 475 of the employed method to resemble the asymmetric and non-linear nature of $\mathcal{F}(\cdot)$ with high 476 477 accuracy.

				_					
a)	$a \coloneqq a_{\xi} = a_{\psi} \ b \coloneqq b_{\xi} = b_{\psi} = 1$				$a_{\xi} = 5 \ b := b_{\xi} = b_{\psi} = 1$				
	Shape (<i>a</i>)	MSE	Max(SE)		Shape (a_{ψ})	MSE	Max(SE)		
	0.01	8.03×10 ⁻⁵	7.75×10 ⁻⁴		0.01	2.12×10 ⁻⁵	3.79×10 ⁻⁴		
	0.05	5.81×10 ⁻⁵	3.08×10 ⁻⁴		0.05	6.46×10 ⁻⁶	2.70×10 ⁻⁵		
	0.1	2.44×10 ⁻⁶	9.89×10 ⁻⁶		0.1	6.26×10 ⁻⁶	4.15×10 ⁻⁵		
	0.5	4.33×10 ⁻⁶	1.59×10 ⁻⁵		0.5	1.51×10 ⁻⁵	9.37×10 ⁻⁵		
	1	3.31×10 ⁻⁶	1.88×10 ⁻⁵		1	2.54×10 ⁻⁶	1.13×10 ⁻⁵		
	2	1.22×10 ⁻⁶	8.47×10 ⁻⁶		2	7.19×10 ⁻⁷	3.20×10 ⁻⁶		
	5	3.70×10 ⁻⁶	1.80×10 ⁻⁵		5	5.24×10 ⁻⁷	1.77×10 ⁻⁶		

478 Table 1. Comparison between numerical integration and the algorithm of Appendix A for the numerical
479 example illustrate in Figure 2. Panels a) and b) correspond to those of Figure 2.

480 **3.2.2** The Log-Normal case

481 As mentioned earlier, there are some exceptions that have a closed-form solution. Among them

482 the Log-Normal case, which is of particular interest from a hydrological perspective. The PDF

483 of the 3-parameter Log-Normal distribution (\mathcal{LN}) is given by,

$$f_{LN}(x;a,b,c) = \frac{1}{(x-c)a\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{\log(x-c)-b}{a}\right)^2\right), \quad x > c \quad (17)$$

484 where $a > 0, b \in \mathbb{R}$, and $c \in \mathbb{R}$ denote the shape, scale and location parameters respectively;

while, when c = 0, the distribution reduces to the 2-parameter Log-Normal distribution. As shown in Mostafa and Mahmoud (1964), yet without direct reference to NDM, for two

486 shown in Mostafa and Mahmoud (1964), yet without direct reference to NDM, for two 487 random variables x_{ξ} and x_{ψ} that are Log-Normally distributed, Eq. (14) simplifies to,

 $\rho_{\xi,\psi} = \frac{\exp(\tilde{\rho}_{\xi,\psi}a_{\xi}a_{\psi}) - 1}{\sqrt{(\exp(a_{\xi}^2) - 1)(\exp(a_{\psi}^2) - 1)}}$ (18)

488 Which can be easily inverted in order to directly provide the equivalent correlation
489 coefficient
$$\tilde{\rho}_{\xi,\psi}$$
, given the target value of $\rho_{\xi,\psi}$, i.e.,

$$\tilde{\rho}_{\xi,\psi} = \frac{\ln\left(1 + \rho_{\xi,\psi}\sqrt{(\exp(a_{\xi}^{2}) - 1)(\exp(a_{\psi}^{2}) - 1)}\right)}{a_{\xi}a_{\psi}}$$
(19)

490 It is worth remarking that Eq. (18) is identical with the one employed in the celebrated 491 multivariate lag-1 Log-Normal model of Matalas (1967), in order to adjust the correlation 492 coefficients, which interestingly can be identified as a Nataf-based approach.

493 **3.2.3** A cautionary note

494 A delicate point worth standing concerns the use of alternative, rank-based dependence 495 measures, such as Spearman's r_s and Kendall's t, for the parameter identification of NDM (or 496 Gaussian copula). Under the assumption that both marginal distributions and copula are 497 Gaussian (or more generally elliptical distributions), there is a one-to-one relationship between 498 the aforementioned dependence measures and Pearson's correlation coefficient (ρ), which can 499 be expressed as (e.g., Embrechts et al., 1999; Esscher, 1924; Kruskal, 1958; Lebrun & 500 Dutfoy, 2009) (notice that the indices have been omitted for the sake of simplicity),

$$\rho = 2\sin\left(\frac{\pi r_s}{6}\right) \leftrightarrow r_s = \left(\frac{6}{\pi}\right)\arcsin\left(\frac{\rho}{2}\right)$$
(20)

$$\rho = \sin\left(\frac{\pi t}{2}\right) \leftrightarrow t = \left(\frac{2}{\pi}\right) \arcsin(\rho)$$
(21)

Both r_s and t are measures of concordance and are invariant to non-linear monotonic transformations (such as those imposed by Eq. (10)). Thus, specifying NDM with estimates of Pearson's correlation based on the conversion of empirical estimates of r_s or t will inevitably preserve the target values of r_s or t after the application of the mapping procedure (due to the property of invariance) but it will lead to misspecification of the underlying model (i.e., NDM) due to Eq. (14), and of course the target values of ρ won't be preserved.

507 3.3 The auxiliary SMA model

Having described the theoretical background of the proposed approach, this section provides a 508 509 brief introduction to the univariate and multivariate Symmetric Moving Average (SMA) model 510 of Koutsoyiannis (2000), which is used within SMARTA as an auxiliary standard Gaussian process. SMA model consists as a special case of the Backward-Forward Moving Average 511 512 (BFMA) model, whose key idea is that a stochastic process \underline{z}_t can be described as a weighted 513 sum of infinite backward and forward random variables. Note that the notation slightly differs 514 from the original one, in order to highlight the fact that the model is employed in the Gaussian 515 domain using the equivalent correlation coefficients $\tilde{\rho}$, instead of the target correlation 516 coefficients, ρ .

517 **3.3.1** Univariate model

518 In practice, the SMA model slightly relaxes the assumptions of BFMA model and assumes that

a stochastic process \underline{z}_t can be described as a weighted sum of a finite number of backward and

520 forward random variables. Particularly, the generating mechanism of the SMA model is given

521 by the following equation,

$$\underline{z}_{t} = \sum_{\zeta = -q}^{\cdot} \tilde{a}_{|\zeta|} \underline{v}_{t+\zeta} = \tilde{a}_{q} \underline{v}_{t-q} + \dots + \tilde{a}_{1} \underline{v}_{t-1} + \tilde{a}_{0} \underline{v}_{t} + \tilde{a}_{1} \underline{v}_{t+1} + \dots + \tilde{a}_{q} \underline{v}_{t+q} \qquad (22)$$

522 where \underline{v}_t are standard normal i.i.d. variables and \tilde{a}_{ζ} are internal model parameters (i.e., weight

523 coefficients) that are assumed to be symmetric, i.e., $\tilde{a}_{\zeta} = \tilde{a}_{-\zeta}$ (for $\zeta = 1, 2, ...$) and approach

524 zero after some value $|\zeta| > q$, where q denotes a large positive integer value. The selection of

q depends on the degree of auto-dependence imposed by the target process (see Eq. (23)) and the desired level of accuracy. Furthermore, q cannot be greater than the length of the time series

to simulate. Particularly, the parameters \tilde{a}_{ζ} are related to the autocorrelation coefficients $\tilde{\rho}_{\tau}$ via a 2q + 1 equation system of the following form, $a = \tau$

$$\tilde{\rho}_{\tau} = \sum_{\zeta = -q}^{r} \tilde{a}_{|\zeta|} \tilde{a}_{|\tau+\zeta|}, \quad \tau = 0, 1, 2, ..., q$$
(23)

$$\tilde{\rho}_{\tau} = \sum_{\zeta = \tau - q}^{q} \tilde{a}_{\zeta} \tilde{a}_{\tau - \zeta}, \qquad \tau = q + 1, \dots, 2q$$
(24)

Evidently, if Eq. (23) is honored, the model resembles the theoretical ACF up to $\tilde{\rho}_a$, while it 530 531 decays to zero after 2q (see Eq. (24)). In order to estimate the parameters \tilde{a}_{ζ} , Koutsoyiannis 532 (2000) proposed two solutions, one closed-form and one based on a formulation of an 533 optimization problem. The interested reader is referred to the latter publication for a thorough 534 and in-depth description of the two methods. In this work we restrict our attention in briefly 535 describing only the first one, since it is a fast and direct method. The aforementioned author 536 showed that the discrete Fourier transformation (DFT) of \tilde{a}_{ζ} , i.e., $S_{\tilde{a}}(\omega)$, is related to the power spectrum of the autocorrelation function, i.e., $S_{\tilde{\rho}}(\omega)$, by, $S_{\tilde{a}}(\omega) = \sqrt{2S_{\tilde{\rho}}(\omega)}$. 537 If the autocorrelation structure $\tilde{\rho}_{\tau}$ is known (or specified), its power spectrum can be calculated 538

using the DFT, hence estimate $S_{\tilde{a}}(\omega)$. Then, by applying the inverse Fourier transformation

one can obtain the parameters \tilde{a}_{ζ} . It is remarked that algorithms that facilitate the latter calculations are nowadays built-in in many high-level programming languages (e.g., R or MATLAB), which in turn allow the straightforward implementation of SMA and SMARTA models in most computational environments. At this point we note that Koutsoyiannis (2002, 2016) proposed an even simpler and straightforward procedure for the estimation of \tilde{a}_{ζ} coefficients, which however is applicable only for HK (i.e., fGn) type autocorrelation structures.

547 **3.3.2** Multivariate model

548 Furthermore, the SMA model can be extended for the multivariate simulation of contemporaneously cross-correlated processes, via the explicit preservation of the lag-0 cross-549 550 correlation coefficients. This assumption, which significantly simplifies the parameter 551 estimation procedure, is often regarded adequate within hydrological domain, and can be found 552 in several other stochastic simulation schemes (e.g., Camacho et al., 1985; Efstratiadis et al., 2014; Koutsoyiannis & Manetas, 1996; Pegram & James, 1972; Tsoukalas et al., 2018a). 553 With this in mind, for simulation of hydrometeorological processes characterized by strongly 554 555 lagged cross-correlations (e.g., rainfall-runoff at fine time scales), it may be advantageous to 556 employ the same modelling strategy as the one proposed herein, using alternative auxiliary Gaussian models that, apart from the lag-0 cross-correlations, are able to directly model 557 558 (preferably, for parsimony and stability, in combination with suitable theoretical auto- and cross-correlation structures; e.g., similar to CAS) the lagged cross-correlation coefficients. 559

Regarding the multivariate SMA model, let $\underline{z}_t = [\underline{z}_t^1, ..., \underline{z}_t^i, ..., \underline{z}_t^m]^T$ be a *m*-dimensional vector, as defined in section 2, and $\tilde{\rho}_{\tau}^{i,j} \coloneqq \operatorname{Corr}[\underline{z}_t^i, \underline{z}_{t+\tau}^j]$ denote the equivalent lag- τ crosscorrelation between processes \underline{z}_t^i and \underline{z}_t^j for time lag τ . Similar to the univariate case, each process \underline{z}_t^i is represented by a weighted sum of random variables \underline{v}_t^i , i.e.,

$$\underline{z}_{t}^{i} = \sum_{\zeta = -q}^{q} \tilde{a}_{|\zeta|}^{i} \underline{v}_{t+\zeta}^{i}$$
(25)

In this case, the random variables \underline{v}_t^i are considered serially independent but contemporaneously cross-correlated. Therefore, the problem lies in generating such variables in a way that they reproduce the equivalent lag-0 cross-correlation coefficients $(\tilde{\rho}_0^{i,j})$. It has been shown that it suffices to generate random variables \underline{v}_t^i with correlation $\tilde{g}^{i,j} :=$ $\operatorname{Corr}[\underline{v}_t^i, \underline{v}_t^j]$ equal to,

$$\tilde{g}^{i,j} = \frac{\tilde{\rho}_0^{i,j}}{\sum_{\zeta = -q}^q \tilde{a}^i_{|\zeta|} \tilde{a}^j_{|\zeta|}}$$
(26)

569 Hence, the $(m \times m)$ correlation matrix \tilde{G} is formulated, with ones in the diagonal and its $i^{\text{th}} \neq$

- 570 j^{th} elements determined by, $\tilde{\boldsymbol{G}}_{[i,j]} = \tilde{g}^{i,j}$. Furthermore, the theoretical lag- τ cross-correlation
- 571 structure (for $\tau = 0, 1, 2, ...$) of the model is given by,

$$\tilde{\rho}_{\tau}^{i,j} = \tilde{\rho}_{0}^{i,j} \frac{\sum_{\zeta=-q}^{q-\tau} \tilde{a}_{|\tau+\zeta|}^{i} \tilde{a}_{|\zeta|}^{j}}{\sum_{\zeta=-q}^{q} \tilde{a}_{|\zeta|}^{i} \tilde{a}_{|\zeta|}^{j}} = \tilde{g}^{i,j} \sum_{\zeta=-q}^{q-\tau} \tilde{a}_{|\tau+\zeta|}^{i} \tilde{a}_{|\zeta|}^{j}$$

$$(27)$$

Regarding simulation, a vector of correlated random variables $\underline{\boldsymbol{v}}_t = [\underline{\boldsymbol{v}}_t^1, \dots, \underline{\boldsymbol{v}}_t^i, \dots, \underline{\boldsymbol{v}}_t^m]^T$ can be generated by, $\underline{\boldsymbol{v}}_t = \widetilde{\boldsymbol{B}}\underline{\boldsymbol{w}}_t$, where $\underline{\boldsymbol{w}}_t = [\underline{\boldsymbol{w}}_t^1, \dots, \underline{\boldsymbol{w}}_t^i, \dots, \underline{\boldsymbol{w}}_t^m]^T$ is a vector of standard normal i.i.d. variables, and $\widetilde{\boldsymbol{B}}$ is a $m \times m$ matrix obtained by finding the so-called square root of matrix $\widetilde{\boldsymbol{G}}$, i.e., Eq. (28). A solution to the latter problem can be obtained by standard decomposition techniques (e.g., Cholesky or singular value decomposition) or via optimization-based methods
(Higham, 2002; Koutsoyiannis, 1999).

578

$$\widetilde{\boldsymbol{B}}\widetilde{\boldsymbol{B}}^{\mathrm{T}} = \widetilde{\boldsymbol{G}} \tag{28}$$

In more detail, it is reminded that if \tilde{G} is positive definite (which indicates that the multivariate 579 580 process is admissible), then Eq. (28) has infinite solutions, hence, both decomposition and optimization-based methods can be employed. On the other hand, when \tilde{G} is non-positive 581 definite (implying that the multivariate process is inadmissible), the decomposition methods 582 583 cannot offer a solution. In this case, optimization-based techniques can provide a potential 584 remedy, by formulating an optimization problem, where the objective is to identify a matrix \widetilde{B}^* which results to a feasible and near-to-optimum matrix $\widetilde{G}^* \coloneqq \widetilde{B}^* \widetilde{B}^{*T}$ which is as closest 585 (typically quantified in terms of some distance measure; e.g., Euclidean norm) as possible to 586 the original matrix \tilde{G} . Of course, in such cases, the target process will not be exactly resembled, 587 while, the difference between \widetilde{G} and \widetilde{G}^* can be regarded as a proxy for the magnitude of 588 approximation introduced to the simulation. Bras and Rodríguez-Iturbe (1985 p. 98), as well 589 590 as Koutsoyiannis (1999) discuss several situations which may lead to a non-positive definite 591 matrix \tilde{G} . Almost all of these situations are related with the estimates of correlation coefficients 592 from the empirical data. In the case of SMARTA, and provided that a feasible autocorrelation 593 structure has been identified for each individual process, a non-positive definite matrix \tilde{G} may 594 arise due to data-based estimates of lag-0 cross-correlation coefficients, imprecise 595 approximation of equivalent correlation coefficients or incompatible combinations of marginal 596 distributions, autocorrelation structures and target cross-correlations (see section 3.2.1). For 597 instance, since the proposed scheme (in multivariate mode) treats each individual process 598 separately of the cross-correlations, the simulation of highly cross-correlated processes with 599 particularly different distributions and autocorrelation structures (e.g., very fast-decaying and 600 very slow-decaying) may be infeasible (see section 4.2 for a simulation example involving both positively and negative cross-correlated LRD and SRD processes), even if the latter are 601 602 individually valid.

603 At this point it is noted that an incidental contribution of SMARTA is the alleviation of a burden 604 related to preservation of the skewness coefficient. As mentioned in the introduction, a broad 605 class of linear stochastic models, in an attempt to preserve the coefficients of skewness of the 606 target process, \underline{x}_t , employ non-Gaussian white noise for the innovation term, \underline{v}_t , typically from Pearson type-III distribution. However, the latter practice may lead to very high coefficients of 607 608 skewness for the innovation term which are hardly attainable (Koutsoyiannis, 1999; Todini, 609 1980). This practice was also adopted by Koutsoyiannis (2000) in the original SMA scheme, 610 where the Pearson type-III distribution has been employed for the generation of skewed white noise. More specifically, regarding the univariate formulation of the latter model (assuming 611 $q = 2^{10}$), in Figure 3a-b we depict (from two distinct points of view) the relationship between 612 the skewness coefficient $(C_{s_{\underline{v}}})$ of innovation term, \underline{v}_t , that is required to attain the target 613 coefficient of skewness $(C_{s_{\underline{x}}})$ of the variable, \underline{x}_{t} , for several hypothetical HK process 614 characterized by different values of H coefficient. See also Eq. (29) in Koutsoyiannis (2000). 615 It is apparent from in Figure 3a-b that the higher the value of H, the higher the required 616 617 skewness of the innovation term, \underline{v}_t . For example, in an HK process with H = 0.8, the skewness coefficient of innovation term v_t has to be set twice as high as than the one of x_t . We remark 618 that this issue is further amplified (not shown herein) when the underlying model is used in 619 multivariate mode (Koutsoyiannis, 1999). On the other hand, SMARTA completely alleviates 620 621 the latter difficulties since the SMA scheme is used as an auxiliary model in the standard

Normal (i.e., Gaussian) domain and the generated data are subsequently mapped to the actual domain using the target ICDFs. Therefore, the target marginal statistics are attained without making any attempts to generate skewed innovation terms, neither in univariate nor in multivariate mode. Moreover, an additional contribution of SMARTA regards the optimization problem that arises when the matrix \tilde{G} is non-positive. Particularly, the latter is simplified in a nearest correlation matrix problem, since the 3rd term of Eq. (28) in Koutsoyiannis (1999), that accounts for skewness, is no longer needed.



629

630 **Figure 3.** Graphical illustration of the relationship between the required skewness coefficient $(C_{s_{\underline{v}}})$ of 631 innovation term \underline{v}_t and a) the skewness $(C_{s_{\underline{x}}})$ of an fGn process \underline{x}_t for various values of *H* and b) the 632 value of *H* of an fGn process \underline{x}_t for various values of skewness of $C_{s_{\underline{x}}}$ (using the SMA model with 633 $q = 2^{10}$).

634 **3.4** Generation procedure of SMARTA

Having described in detail all the key components of SMARTA approach in the previous
sections, it is useful to provide the complete generation procedure, decomposed into the
following six steps:

638 **Step 1.** Define a target distribution $F_{\underline{x}^i}$ for each process \underline{x}_t^i ; i = 1, ..., m. SMARTA, as well 639 as all Nataf-based methods, is flexible in terms of distribution fitting method; hence one can 640 select a fitting method of their preference.

641 **Step 2.** Define a target auto-correlation structure (ρ_{τ}^{i}) for each process \underline{x}_{t}^{i} ; i = 1, ..., m using 642 a theoretical ACF model. For instance, for each process \underline{x}_{t}^{i} identify the parameters of CAS that 643 better fit the observed data. Furthermore, in the multivariate case, identify the target lag-0 644 cross-correlation coefficients $(\rho_{0}^{i,j})$ between processes, \underline{x}_{t}^{i} and \underline{x}_{t}^{j} ; $i \neq j = 1, ..., m$.

645 **Step 3.** Identify the equivalent correlation coefficients $(\tilde{\rho}_{\tau}^{i})$ of each theoretical ACF, up to the 646 maximum specified lag (which depends on the type of the process; LRD or SRD), for each process \underline{x}_{t}^{i} ; i = 1, ..., m. Furthermore, in the multivariate case, estimate the equivalent lag-0 647 cross-correlation coefficient $\tilde{\rho}_0^{i,j}$. Assuming that the algorithm of Appendix A is employed for 648 649 the identification of equivalent correlations, and given the fact that it allows the direct 650 estimation of the equivalent ACF up to any lag, the latter has to be employed m times, one for 651 each process \underline{x}_t^i ; i = 1, ..., m. Furthermore, in order to estimate the lag-0 equivalent crosscorrelation coefficient $\tilde{\rho}_0^{i,j}$, the same procedure should be employed m(m-1)/2 additional 652

- times. For instance, in a 4-dimensional problem (m = 4), the algorithm of Appendix A is executed in total, m(m + 1)/2 times (=10).
- 655 Step 4. Calculate the parameters of the auxiliary SMA model (section 3.3), i.e., the weight 656 coefficients (\tilde{a}_{ζ}^{i}) of each auxiliary process \underline{z}_{t}^{i} ; i = 1, ..., m. Additionally, in the multivariate
- 657 case, calculate the elements of matrices \tilde{G} and \tilde{B} (see also, Eq. (26) and (28)).
- 658 **Step 5.** Employ the auxiliary Gaussian SMA model and generate a realization of the auxiliary 659 univariate (\underline{z}_t) or multivariate process (\underline{z}_t).
- 660 **Step 6.** Attain the actual process \underline{x}_t (or \underline{x}_t), by mapping the auxiliary Gaussian process \underline{z}_t (or 661 \underline{z}_t) to the actual domain using the ICDF, $F_{\underline{x}^i}^{-1}$, of each process \underline{x}_t^i ; i = 1, ..., m, via Eq. (10).
- By now, it should be clear that the basis of the proposed methodology consists an explicit 662 663 simulation method, in terms of reproducing the distribution function (relieved from the limitations and constraints of such schemes; see section 1), that fundamentally differs from the 664 other two typical schemes (implicit and transformation-based; see section 1) used in hydrology, 665 which also employ linear stochastic models. Compared to the implicit approaches, that employ 666 non-Gaussian white noise, Nataf-based schemes (e.g., SMARTA) alleviate several notable 667 668 limitations. Among them, the approximation of the distribution function, the generation of negative values, the bounded dependence patterns and the (often) narrow type of possible 669 670 correlation structures, which can be attributed to the limited number of schemes for which 671 analytical equations can be derived to link the moments of the process with those of the white 672 noise. Additionally, in contrast to transformation-based approaches, that aim to normalize the 673 data, Nataf-based schemes explicitly model them using target marginal distributions. Though, 674 it has to be noted, that in principle, the rationale of transformation-based approaches can be 675 easily aligned with the theoretical background of Nataf's distribution model, by using the 676 concept of equivalent (i.e., adjusted) correlation coefficients. This modification would mitigate their major weakness (i.e., the introduction of bias) but still will not be equivalent with the 677 678 reproduction of certain, pre-specified, distribution functions. On top of this, since the ICDF is 679 employed, a unique advantage of SMARTA (and other Nataf-based approaches) over the 680 aforementioned schemes is that it can be used for the simulation of both univariate and multivariate stationary processes with discrete, continuous and mixed-type distributions. 681 682 Regarding parameterization, the proposed Nataf-based approach exhibit a parsimonious 683 character, as it is evident by the small number of required parameters, which are equal or lower 684 than those required by the aforementioned schemes (for a comparison see section 4.1). Finally, it is noted that, due to the definition and use of Pearson's correlation coefficient (see Eq. (12)), 685 686 none of the latter methods (including SMARTA), can be used for the simulation of processes 687 characterized by distributions functions exhibiting infinite variance. In such situations the use 688 of alternative simulation methods is required (e.g., Samoradnitsky, 2017). Random variables 689 with infinite moments typically arise when heavy-tailed distribution functions with power-type 690 tails are employed. For instance, a Pareto type-I distribution with CDF, $F(x) = 1 - (x/b)^{-a}$, 691 where b > 0 (scale), a > 0 (shape) and $x \ge b$, has finite variance only for a > 2. The literature 692 offers a plethora of studies indicating the suitability of heavy-tailed distributions for both precipitation (e.g., Cavanaugh et al., 2015; Koutsoyiannis & Papalexiou, 2016; Papalexiou 693 et al., 2013; Papalexiou & Koutsoyiannis, 2013, 2016) and streamflow (e.g., Anderson & 694 695 Meerschaert, 1998; Basso et al., 2015; Blum et al., 2017; Bowers et al., 2012) processes, 696 especially regarding the description of their extreme behavior. After reviewing the outcomes 697 of these studies, which involve the analysis of numerous worldwide historical records, we 698 found that the majority of them, agree that the hydrological variables are characterized by

distribution functions (with either exponential or power-type tails) with finite variance. On top of the empirical evidence provided by the aforementioned works, theoretical reasoning (related with entropy and energy production) further supports the finite variance hypothesis for hydrometeorological processes (Koutsoyiannis, 2016, 2017). In this vein, it is regarded that the finite variance assumption poses a practical barrier of limited impact, if any, on the application of latter methods for the simulation of hydrometeorological processes.

705 4 Hypothetical simulation studies

Prior to employing real-world datasets to demonstrate the proposed approach, we decided to 706 707 setup two hypothetical simulation studies. One univariate and one multivariate. The motivation 708 behind this choice was based on conducting experiments where all the assumptions are a priori 709 known, hence allowing the comprehensive evaluation and assessment of the model without the 710 effect of exogenous factors, such as, erroneous or short length historical data. However, it is 711 remarked that the proposed method is generic, and can be directly applied for the simulation of 712 univariate and multivariate stationary processes (e.g., geophysical, hydrometeorological and 713 beyond). In that respect, in section 5 the applicability of SMARTA is demonstrated using two 714 real-world datasets, one that concerns the simulation of annual non-Gaussian streamflow at 715 four stations and another that involves the simulation of intermittent, non-Gaussian, daily 716 rainfall at a single location.

717 **4.1** Simulation of univariate processes

718 The first simulation study constitutes a comparison between the original SMA and the proposed SMARTA models (with $q = 2^{12}$ for both) for the simulation of long (i.e., 2^{20} time steps) 719 720 721 0.8, 0.9 and Pearson type-III marginal distribution (PIII). With this in mind, we identified a total of 4 scenarios, each one characterized by \mathcal{P} III and different H coefficients. It is reminded 722 723 that the original SMA model, in order to approximate the marginal statistics, uses PIII variates 724 for the innovation term (hence hereafter referred to as SMA-PIII), while SMARTA uses the 725 ICDF of the target distribution—in this case PIII. The rationale regarding the selection of this 726 distribution was the intention to conduct a fair and meaningful comparison among the two 727 models, which, in this formulation, have exactly the same number of parameters, i.e., three for 728 the marginal distribution (see, Eq. (29)) and one (i.e., H) for the autocorrelation structure. We 729 point out that, the comparison is not intended to infer which model is the best, but rather used 730 as a benchmark to highlight the merits of the proposed approach. \mathcal{P} III is essentially a Gamma 731 distribution (see, Eq. (16))) with an additional location (else known as threshold or shift) 732 parameter, whose PDF is given by,

$$f_{\mathcal{P}\text{III}}(x;a,b,c) = \frac{1}{|b| \Gamma(a)} \left(\frac{x-c}{b}\right)^{a-1} \exp\left(-\frac{x-c}{b}\right), \begin{cases} \text{if } b > 0 & c \le x < \infty\\ \text{if } b < 0 & -\infty < x \le c \end{cases}$$
(29)

where
$$\Gamma(\cdot)$$
 denotes the gamma function, while, $a > 0$, $b \neq 0$ and $c \in \mathbb{R}$ are shape, scale and

location parameters, respectively; and they are interconnected with the mean $(\mu_{\underline{x}})$, variance $(\sigma_{\underline{x}}^2)$, skewness $(C_{s_{\underline{x}}})$ and kurtosis $(C_{k_{\underline{x}}})$ coefficients of random variable \underline{x} by,

$$\mu_{\underline{x}} = c + ab, \qquad \sigma_{\underline{x}}^2 = ab^2, \qquad C_{s_{\underline{x}}} = \frac{2b}{|b|\sqrt{a}}, \qquad C_{k_{\underline{x}}} = \frac{6}{a} + 3$$
(30)

More specifically, in all scenarios, we employed a \mathcal{P} III distribution with parameters a = 0.75614, b = 11.5 and c = 1.30434, whose theoretical moments are presented in **Table 2**.

738
Table 2. Summary of theoretical and simulated statistics as reproduced by SMA and SMARTA models.

	Theoretical	Simulated (SMA-PIII)				Simulated (SMARTA)				
Scenario	All	H = 0.6	H = 0.7	H = 0.8	H = 0.9	<i>H</i> =0.6	H = 0.7	H = 0.8	H = 0.9	
Mean (μ)	10	9.99	10.08	9.85	10.23	10.00	9.99	9.99	10.00	
Variance (σ^2)	100	100.61	100.78	100.04	99.79	100.03	99.86	100.07	101.65	
Skewness coeff. (C_s)	2.30	2.35	2.34	2.32	2.35	2.30	2.29	2.30	2.35	
Kurtosis coeff. (C_k)	10.93	11.43	11.80	12.62	15.97	10.94	10.85	11.00	11.53	
Hurst coeff. (H)	0.60, 0.70,	0.61	0.70	0.80	0.89	0.60	0.71	0.80	0.90	
*The theoretical moments correspond to PIII distribution ($a = 0.75614$, $b = 11.5$ and $c = 1.30434$)										

Regarding SMARTA and the given marginal distribution, Figure 4a illustrates the relationship 739

740 between the equivalent correlation coefficients $\tilde{\rho}$ and the target ones ρ (the superscripts are omitted for simplicity), while Figure 4b depicts the equivalent autocorrelation coefficients $\tilde{\rho}_{\tau}$

741

742 employed by SMARTA, in order to capture the target autocorrelation structure ρ_{τ} of the target 743



744

745 **Figure 4.** a) The established relationship between equivalent, $\tilde{\rho}$ and target ρ correlation coefficients. b) 746 Comparison between the target and equivalent autocorrelation coefficients employed within the SMARTA model for HK processes with the various values of H. 747

748 Table 2 presents the simulated (by the two approaches) first four moments; which are 749 apparently well-captured by both models. It is noted that, while SMA does not explicitly 750 accounts for the kurtosis coefficient, it is able to reproduce it in a satisfactory degree; especially 751 when one considers the high uncertainty associated with its estimation (cf., Lombardo et al., 752 2014). Nevertheless, it is reminded that the resemblance of the moments does not imply the 753 reproduction of the marginal distribution (Matalas & Wallis, 1976). This is clearly depicted 754 in Figure 5a-d, where we compare the target theoretical cumulative distribution (CDF) with 755 the empirically derived cumulative density functions (ECDFs) of the two models. In this case, 756 only SMARTA was able to reproduce the target distribution, regardless of the value of Hcoefficient (its ECDF is almost indistinguishable from the theoretical one). On the other hand, 757 758 the ECDF of SMA- \mathcal{P} III departs from the theoretical one for high values of H (e.g., see Figure 5d). Furthermore, SMARTA explicitly avoids the generation of negative values; since the 759 target distribution (\mathcal{P} III) is positively bounded at c = 1.30434. A property of high importance 760 in hydrology due to the (often) non-negative nature of such variables (e.g., streamflow and 761 762 precipitation).

Regarding the resemblance of the auto-dependence structure of the processes, it is apparent 763 from Figure 5e-h and Figure 5i-l that, both models were able to reproduce the theoretical HK 764

765 ACFs as well as the corresponding climacograms, even for high values of *H*. The latter graphs 766 also provide an empirical evidence of the theoretical consistency of both approaches. In

addition, the Hurst coefficient of the synthetic realizations (see Table 2) was estimated using 767

- the climacogram-based, least squares variance (LSV) method (Tyralis & Koutsoyiannis, 2011) and are in agreement with the theoretical values.
- Finally, in order to visually assess the form of the established dependencies, for both models
- and each HK process (i.e., scenario), we employ scatter plots of the lagged synthetic data for
- 772 $\tau = 1$ (Figure 5m-p) and $\tau = 10$ (Figure 5q-t). It is observed that, despite the fact that both
- models reproduced the same autocorrelation coefficient for $\tau = 1$ and $\tau = 10$, they establish
- particularly different dependence patterns. This is attributed to the underlying assumption of
- 575 SMARTA regarding the joint behavior of the process which is related to the Gaussian copula
- 776 (expressed through the auxiliary Gaussian model).



777 778 Figure 5. Comparison between theoretical and simulated CDFs (using the Weibull's plotting position) 779 of SMA- \mathcal{P} III and SMARTA models for HK processes with a) H = 0.6, b) H = 0.7, c) H = 0.8, d) 780 H = 0.9. Comparison between theoretical (HK) and empirical ACF of SMA- \mathcal{P} III and SMARTA models 781 for HK processes with e) H = 0.6, f) H = 0.7, g) H = 0.8, h) H = 0.9. Comparison between theoretical 782 (HK) and empirical climacograms of SMA-PIII and SMARTA models models for HK processes with 783 i) H = 0.6, j) H = 0.7, k) H = 0.8, l) H = 0.9. Scatter plots of SMA-PIII and SMARTA models for time 784 lag $\tau = 1$ for simulated HK processes with m) H = 0.6, n) H = 0.7, o) H = 0.8, p) H = 0.9. Scatter plots 785 of SMA-PIII and SMARTA models for time lag $\tau = 10$ for simulated HK processes with q) H = 0.6, r) 786 H = 0.7, s) H = 0.8, t) H = 0.9.

787 **4.2** Simulation of multivariate processes

788 To further elaborate on the SMARTA approach, we setup a multivariate problem that concerns the simultaneous generation of four contemporaneously cross-correlated SRD and LRD 789 790 processes. The latter may be seen as four (4) different processes at the same site, or processes 791 of the same variable at 4 different sites. Hereinafter, we consider the latter for convenience and 792 refer to them as sites A-D, as well as model them in that order, i.e., as 4-dimensional stationary process $\underline{x}_t = [\underline{x}_t^1, \underline{x}_t^2, \underline{x}_t^3, \underline{x}_t^4]^T$, where for instance, i = 3 refers to site C. In this demonstration, 793 794 the target auto-dependence structure of each process is described by the two-parameter CAS 795 (i.e., Eq. (6)). More specifically, sites A and B are characterized by LRD behavior (particularly 796 HK, since we set $\beta > 1$ and $\kappa = \kappa_0$ and slowly-decaying ACF, while sites C and D by SRD 797 (since we set $\beta = 0$) and fast-decaying ACF. In addition, we assigned different target 798 distributions to the sites A-D, i.e., Burr type-XII (Eq. (31)), Pearson Type-III (Eq. (29)), Log-799 Normal (Eq. (17)) and Weibull (Eq. (32)). The PDF of the Burr type-XII distribution is given 800 by,

$$f_{\mathcal{B}rXII}(x;a_1,a_2,b) = \left(\frac{a_1a_2}{b}\right) \left(\frac{x}{b}\right)^{a_1-1} \left(1 + \left(\frac{x}{b}\right)^{a_1}\right)^{-a_2-1}, \quad x > 0$$
(31)

where $a_1, a_2 > 0$ are shape parameters and b > 0 is a scale parameter. It is noted that $\mathcal{Br}XII$ is a power-type distribution and its r^{th} moment exist if and only if $a_1a_2 > r$. Furthermore, the PDF of the Weibull reads as follows,

$$f_{W\mathcal{E}\mathcal{J}}(x;a,b) = \left(\frac{a}{b}\right) \left(\frac{x}{b}\right)^{a-1} \exp\left(-\left(\frac{x}{b}\right)^{a}\right), \qquad x \ge 0$$
(32)

where a > 0 and b > 0 are shape and scale parameters respectively. **Table 3**a provides a synopsis of the latter assumptions, as well as the parameters of CAS and the theoretical moments of the corresponding distributions. Note that, the Kurtosis coefficient of site A is infinite, since $a_1a_2 < 4$. Further to this, the target and equivalent lag-0 cross-correlation coefficients (involving both positive and negative ones) are given in **Table 3**b. It is apparent that this is a peculiar simulation scenario, which was devised in order stress-test the SMARTA method.

811 **Table 3.** a) Synopsis of theoretical distribution models and their moments, as well as, of CAS 812 parameters for each variable of the multivariate simulation study. b) The upper triangle (grey cells) 813 contains the target lag-0 cross-correlation coefficients ($\rho_0^{i,j}$) between sites A-D, while the lower triangle

b) Lag-0 cross-correlation a) Theoretical Site A Site B Site C Site D **Distribution**/ Parameters Site A Site B Site C Site D BrXII \mathcal{P} III WEI Site A -0.700 0.750 0.600 \mathcal{LN} 1 $2.5(a_1)$ Site B -0.940 -0.600 -0.700 3 0.5 1.5 1 а 1 Site C 0.862 -0.749 b 2 10 1 0.650 1 $1.5(a_2)$ 10 -Site D 0.811 -0.923 0.707 С -1 Statistic Theoretical Mean (*u*) 4.76 13 8.37 9.02 Variance (σ^2) 11.42 3 19.91 37.56 Skewness coeff. (C_s) 5.01 1.15 1.75 1.07 <u>Kurtosis</u> coeff. (C_k) 8.89 4.39 8 -CAS parameter, β 1.25 1.66 0 0 CAS parameter, κ 11.32 5 0.5 0.2 Hurst coeff. (H)0.6 0.7 0.5 0.5

814 depicts the corresponding estimated equivalent correlation coefficients ($\tilde{\rho}_{0}^{i,j}$).

*Distribution abbreviations: \mathcal{Br} XII: Burr type-XII (a_1 = shape, a_2 = shape, b = scale), \mathcal{P} III: Pearson type-III (a = shape, b = scale), \mathcal{WEI} : Weibull (a = shape, b = scale), \mathcal{WEI} : Weibull (a = shape, b = scale).

815 In order to provide further insights regarding the theoretical consistency of the model, we generated 100 independent realizations with length 2¹¹ time steps and set the number of 816 SMARTA model's internal weight coefficients equal to $q = 2^{10}$. Figure 6 provides a synopsis 817 of some basic dependence-related statistics in terms of box-plots. Clearly, SMARTA resembled 818 with high precision the lag-1 autocorrelation and lag-0 cross-correlation coefficients (including 819 820 the negative ones), despite the fact that the target processes are characterized by very different 821 auto-dependence structures and distribution functions. Additionally, regarding the Hurst coefficient of the simulated series, it was once again estimated with the LSV method. A small 822 823 discrepancy that concern site D, which is an SRD process (i.e., H = 0.5) is observed. This may 824 be attributed to the associated estimation method and the high lag-1 autocorrelation (~ 0.8) of site D. Furthermore, in Figure 7a-d we compared the empirical distribution of each realization 825 826 of each site A-D, with the corresponding theoretical distribution, in terms of the survival function (SF), also known as complementary CDF or tail function. The latter is denoted by $\overline{F_x}$ and expresses the probability of exceedance, i.e., $\overline{F_x} \coloneqq P(\underline{x} > x) = 1 - F_x$. The latter figure 827 828 highlights the ability of the model to preserve the target distribution functions, even in 829 830 multivariate mode, since the median SF of all 100 realizations for the 4 sites is virtually 831 identical to the associated theoretical model. Furthermore, in Figure 7e-h we depict the 832 relationship between the equivalent, $\tilde{\rho}$ and target ρ correlation coefficients for each site A-D, while the preservation of the theoretical auto-dependence structure can be verified by the 833 simulated ACFs (Figure 7i-l) and climacograms (Figure 7m-p) of the four variables, that 834 closely resemble the corresponding theoretical ones. To further explore the joint behavior of 835 the model and the established dependence patterns, we employ scatter plots. Figure S1 of 836 837 supplementary material (SM) depicts the established dependence patterns among the variables for time lag 0 (SM, Figure S1e, i, j, m, n, o), as well as for each variable for time lag 1 (SM, 838 **Figure S1**a, f, k, p). Finally, the relationship between equivalent, $\tilde{\rho}^{i,j}$ and target $\rho^{i,j}$, correlation 839 coefficients is provided for every combination of sites A-D (SM, Figure S1b, c, d, g, h, l). 840



Figure 6. Comparison between theoretical (red dots, •) and simulated lag-1 autocorrelation and Hurst coefficient for sites A-D. Target (red dots, •) and simulated lag-0 cross-correlation coefficients for all pairs of sites A-D.



845Scale, kScale, kScale, k846Figure 7. (a-d) Theoretical and simulated (SMARTA) distribution functions (using the Weibull's847plotting position) for sites A-D. (e-h) The established relationships between equivalent, $\tilde{\rho}$ and target ρ 848correlation coefficients given the marginal distribution of sites A-D. (i-l) Theoretical and simulated849ACFs for sites A-D. (m-p) Theoretical and simulated climacograms (CGs) for sites A-D. In all cases,850the simulation intervals have been established using all 100 realizations.

851 5 Real-world simulation studies

852 5.1 Generation of multivariate annual streamflow time series

853 The first real-world simulation study concerns the application of SMARTA for the synthesis 854 of annual streamflow time series at 4 stations in New South Wales region, Australia (Australian Government Bureau of Meteorology, 2015). Particularly, we employed historical data (Figure 855 **8**a-d) from the following stations: Maragle Creek at Maragle (ID1: 401009), Goobarragandra 856 857 River at Lacmalac (ID2: 410057), Adelong Creek at Batlow Road (ID3: 410061), Cotter River 858 at Gingera (ID4: 410730). Hereinafter, we refer to them using their station ID, as well as model them in that order, as 4-dimensional stationary process $\underline{x}_t = [\underline{x}_t^1, \underline{x}_t^2, \underline{x}_t^3, \underline{x}_t^4]^{-1}$; (i.e., i = 3 refers 859 to station Adelong Creek at Batlow Road with ID3: 410061). The distribution of historical data 860

861 does not exhibit the typical bell-type shape that is often encountered in annual data, hence we 862 use the Gamma and Weibull distributions to model them. Specifically, using the maximum likelihood estimation method we identified the following distributions, $x_t^1 \sim \mathcal{G}(a = 2.13, b =$ 863 16.95), $\underline{x}_t^2 \sim \mathcal{WEI}(a = 2.30, b = 302.11), \underline{x}_t^3 \sim \mathcal{WEI}(a = 2.40, b = 15.75)$ and $\underline{x}_t^4 \sim \mathcal{G}(a = 2.40, b = 15.75)$ 864 1.95, b = 48.48). In addition, they are characterized by moderate-to-high temporal 865 dependence and high lag-0 cross-correlation coefficients, that range from 0.83 $(\rho_0^{1,4})$ to 0.93 866 $(\rho_0^{2,3})$. Following Koutsoyiannis (2000), the parameters of CAS (i.e., Eq. (6) - given in vector 867 format), $\beta = [0.99, 0.75, 1.13, 0.72]$ and $\kappa = [2.57, 4.41, 6.01, 5.07]$ were identified for each 868 process by minimizing the mean square error (MSE) among the sample and theoretical 869 870 autocorrelation coefficients. In this case study, we simulated one realization of 1 000 years using the SMARTA model (with $q = 2^9$). Figure 8e-h provides, for each station, a visual 871 comparison among the empirical, theoretical and simulated distribution. Furthermore, Figure 872 8i-l depicts, for each process, the relationship between the equivalent and target autocorrelation 873 874 coefficients. The ability of the model to establish the target auto-dependence structures is verified by comparing, the theoretical and simulated ACF (Figure 8m-p) and corresponding 875 climacogram (Figure 8q-t) of each process. Finally, the model reproduced the target lag-0 876 877 cross-coefficients with high accuracy (SM, Figure S2) and established dependence patterns 878 that are in agreement with the observed ones (SM, Figure S2).



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Figure 8. Synopsis of annual streamflow simulation study at 4 stations in New South Wales region. (ad) Historical time series. (e-h) Empirical, simulated and theoretical distribution functions (using the Weibull's plotting position) for stations ID1-4 (i-l) The established relationships between equivalent, $\tilde{\rho}$ and target ρ correlation coefficients given the marginal distribution of stations ID1-4. (m-p) Empirical, simulated and theoretical ACFs for stations ID1-4. (q-t) Empirical, simulated and theoretical climacograms (CGs) for stations ID1-4.

886 5.2 Generation of univariate daily rainfall time series

In the final case study, we employ SMARTA for the stochastic simulation of a univariate daily rainfall process characterized by intermittency. The available data concern an observation period spanning from 1/1/1964 to 31/12/2006 (43 years) from Pavlos rain gauge located at Boeticos Kephisos river basin, Greece (**Figure 9**a). See also Efstratiadis et al. (2014) for further details regarding the dataset. In general, apart from *ad-hoc* techniques to handle 892 intermittency (e.g., truncation to zero of values below a threshold), typical stochastic 893 simulation schemes (e.g., Papalexiou, 2018; Serinaldi, 2009; Serinaldi & Kilsby, 2014) rely on the use of mixed-distributions or employ two-part models, which, in a nutshell, describe 894 895 precipitation processes as the product of two different processes, particularly, that of occurrence (rain or no-rain) and that of intensity (e.g., Ailliot et al., 2015; Breinl et al., 2013; 896 897 Brissette et al., 2007; Khalili et al., 2009; Lee, 2016, 2017; Lombardo et al., 2017; Mhanna 898 & Bauwens, 2012; Thompson et al., 2007; Wilks, 1998; Wilks & Wilby, 1999). Herein, we 899 employ the former approach, that is, mixed-distributions, as it seems a convenient option 900 (Papalexiou, 2018) given the characteristics of SMARTA and particularly its flexibility 901 regarding the selection of the marginal distribution. An alternative option, also compatible with the proposed method (and Nataf-based schemes in general), would be the use of single 902 903 distribution functions that exhibit an atom of probability mass at zero. A characteristic example, 904 which in the past has been used for this purpose (Dunn, 2004; Hasan & Dunn, 2011), is the 905 Tweedie distribution (Jorgensen, 1987; Tweedie, 1984). Nevertheless, in this simulation study, in order to simultaneously account for the effect of seasonality and the stationarity 906 907 assumption of the model, we treat each month as separate stochastic process, by varying the 908 distribution function and autocorrelation structure on a monthly basis. Specifically, regarding 909 the marginal distribution, we employ a discrete-continuous (i.e., mixed or zero-inflated) model 910 whose CDF is given by,

$$F_{\underline{x}}(x) = \begin{cases} p_D, & x \le 0\\ p_D + (1 - p_D)G_{\underline{x}}(x), & x > 0 \end{cases}$$
(33)

911 where, p_D denotes the probability of a dry interval (abbreviated as probability dry), i.e., $p_D \coloneqq$ 912 $P(\underline{x} \le x_D)$ and $G_{\underline{x}}$ stands for the distribution of amounts greater than the threshold x_D , i.e., 913 $G_{\underline{x}} \coloneqq F_{\underline{x}|\underline{x}>x_D} = P(\underline{x}|\underline{x}>x_D)$. Moreover, the corresponding ICDF is given by,

$$F_{\underline{x}}^{-1}(u) = \begin{cases} 0, & 0 \le u \le p_D \\ G_{\underline{x}}^{-1} \left(\frac{(u - p_D)}{(1 - p_D)} \right), & p_D < u \le 1 \end{cases}$$
(34)

914 where $u \in [0, 1]$ denotes probability. In this formulation values less or equal to x_D (that arise 915 with probability p_D) are assumed equal to zero. We remind the reader that the solely 916 requirement of the algorithm of Appendix A, that is used to approximate the relationship $\mathcal{F}(\cdot)$ 917 of Eq. (15), hence the equivalent correlations $\tilde{\rho}_{\tau}$, is the ICDF (thus conveniently accounting 918 for mixed distributions; e.g., Eq. (33)). Nevertheless, after the specification of the threshold x_D , 919 the empirical probability dry, p_D , can be directly obtained from the available data by counting 920 the number of dry occurrences and dividing it with the total number of observed data. 921 Regarding, G_x , it is obtained by selecting and fitting a theoretical distribution to the amount 922 data above threshold x_D . In this demonstration, we set $x_D \coloneqq 0$, and for the description of the 923 positive daily precipitation amounts of all months, we employ the generalized gamma (GG) 924 distribution (Stacy, 1962), which has been proved particularly capable for the task at hand 925 (Chen et al., 2017; Papalexiou, 2018; Papalexiou & Koutsoyiannis, 2016). Of course, depending on the case, the GG could be replaced with other distribution functions. Back in our 926 927 case, the parameters of the GG distribution were identified using a fitting approach based on Lmoments (Hosking, 1990); specifically the one proposed by Papalexiou and Koutsoyiannis 928 929 (2016). The PDF of *GG* distribution is given by,

$$f_{\mathcal{GG}}(x;a_1,a_2,b) = \frac{a_2}{b\Gamma(a_1/a_2)} \left(\frac{x}{b}\right)^{a_1-1} \exp\left(-\left(\frac{x}{b}\right)^{a_2}\right), \qquad x > 0$$
(35)

930 where $\Gamma(\cdot)$ denotes the gamma function, while, $a_1 > 0$, $a_2 > 0$ are parameters that control the

- shape of the distribution and b > 0 is a scale parameter. The interested reader is referred to the
- 932 latter works for further details regarding the \mathcal{GG} distribution and the associated fitting method.

933 For instance, concerning the marginal characteristics of October's daily rainfall, we estimated the probability dry, $p_D = 0.84$, while the parameters of GG were found b = 3.96, $a_1 = 0.851$ 934 and $a_2 = 0.588$. Furthermore, regarding the description of the auto-dependence structure of the 935 process, we employed CAS and estimated its parameters on a monthly basis (e.g., for October 936 it we identified, $\beta = 0$ and $\kappa = 1.36$) by minimizing the MSE among the sample and theoretical 937 autocorrelation coefficients. Finally, we generated 1 000 years (i.e., 365 000 days) of synthetic 938 939 data (Figure 9b depicts a random window of 60 years) and performed a similar analysis with the previous cases studies; which is summarized in Figure 9, where we depict the results of 940 941 three characteristic months, i.e., February, June and October (the results are similar for the 942 other months – see SM, Figure S3-S6). Particularly, panels (c)-(e) illustrate the capability of 943 the model to reproduce the target distributions (in terms of the SF) of positive precipitation amounts (p_D) is explicitly preserved since it is embedded in the employed mixed-distribution 944 945 model), while, panels (f)-(h) depicts the relationship of equivalent, $\tilde{\rho}$ and target ρ correlation 946 coefficients for both GG and mixed-distribution models. It is observed that, the non-linearity of 947 this relationship increases from GG to mixed distribution due to the fact that the latter is zero-948 inflated. Furthermore, panels (i)-(k) depict the accurate resemblance of the target 949 autocorrelation structure (i.e., CAS), while, panels (1)-(n) provide a comparison of empirical 950 and simulated scatter for time lag 1, which seems to be in agreement with the historical pattern. 951 Finally, preliminary analysis (not shown herein) indicated that the model has the potential to 952 approximate some of the empirical statistics (in terms of L-moments) across coarser time 953 scales, even though they are not explicitly modelled by it. This observation should not be 954 interpreted as a general conclusion, rather as a direction for further investigation. We remark 955 that the literature offers several well-established techniques with proven results, specifically 956 designed for this purpose, i.e., to address scaling and intermittency, such as disaggregation 957 (e.g., Kossieris et al., 2016; Lombardo et al., 2017) and multi-fractal methods, based on 958 cascade models (e.g., Deidda et al., 1999; Kantelhardt et al., 2006; Tessier et al., 1996). 959 The latter methods, by design, aim to simultaneously resemble the process at multiple 960 aggregation levels, employing scaling relationships for high order moments (often greater than second). In our view, an interesting topic of future research would be a comparison among the 961 962 latter simulation techniques with Nataf-based methods for the reproduction of the multi-scale 963 behavior that characterizes hydrometeorological processes. Similar works, yet involving 964 alternative simulation schemes, are those of Lombardo et al. (2012) and Pui et al. (2012).



965

Figure 9. Synopsis of daily rainfall simulation at Pavlos' station. a) Historical time series. b) Synthetic 966 967 time series; randomly selected window of 60 years. Empirical, simulated and theoretical distribution 968 function of positive precipitation amounts for c) February, d) June and e) October (using the Weibull's 969 plotting position); the title of each plot provides the parameters of the GG distribution, as well as the 970 historical (p_D) and simulated (\hat{p}_D) values of probability dry. The established relationship between 971 equivalent, $\tilde{\rho}$ and target ρ correlation coefficients for the mixed and GG distribution for f) February, g) 972 June and h) October. Empirical, simulated and theoretical ACF for i) February, j) June and k) October; 973 the title of each plot depicts the parameters of CAS. Empirical and simulated dependence pattern for 974 time lag 1 for l) February, m) June and n) October; the title of each plot depicts the lag-1, target (ρ_1^{CAS}), simulated $(\hat{\rho}_1)$, and equivalent $(\tilde{\rho}_1)$ autocorrelation coefficients. 975

976 Conclusions 6

- 977 This paper introduces a novel and versatile stochastic model, termed SMARTA, with solid theoretical background and proven capability of addressing important hydrometeorological 978 979 simulation problems. A prominent characteristic of the model is its ability to simulate univariate and multivariate stationary processes with any autocorrelation structure and 980 marginal distribution, provided that the former is feasible and the latter have finite variance. 981 982 The central idea of the method relies on the use of an appropriately parameterized (expressed 983 through *equivalent* correlation coefficients) auxiliary Gaussian process which after its mapping to the actual domain results in a process with the desired stochastic structure and marginal 984 985 distribution.
- 986 Briefly, the proposed approach is built upon three major elements: a) The SMA scheme of 987 Koutsoyiannis (2000), which is used as an auxiliary model in the Gaussian domain, b) a 988 generalized autocorrelation structure, that allows the parsimonious description of SRD and LRD processes, and c) the rationale of NDM (Nataf, 1962), and the associated mapping 989 990 procedure, that provide the theoretical basis of the method and in turn allows the identification 991 of the *equivalent* correlation coefficients; hence determine the parameters of the auxiliary 992 model.
- 993 Overall, the proposed methodology maintains the flexible and parsimonious character of the 994 original SMA model and simultaneously exhibit a series of additional virtues, as demonstrated 995 through two hypothetical and two real-world simulation studies. Among them:
- 996 a) The unambiguous advantage of explicitly simulating any-range dependent (SRD or LRD) 997 stationary processes with arbitrary distributions (even from different families, see section 998
 - 4.2), using a single simulation scheme.
- 999 b) Its ability to simulate univariate and multivariate processes that exhibit contemporaneous 1000 cross-correlations. The generation of time series at multiple locations, or of individual 1001 correlated processes, is often the case in hydrological studies, making SMARTA a useful 1002 method for such tasks.
- 1003 c) The possible incorporation of novel advances in statistical science in stochastic simulation; 1004 such as new distributions and robust fitting methods (e.g., L-moments). In addition, 1005 regarding distributions of hydrometeorological processes, SMARTA can take advantage of years of research in statistical analysis of hydrometeorological variables, since it can 1006 incorporate any distribution function whose variance exists. 1007
- 1008 d) The ability of the model to explicitly avoid the generation of negative values, which simultaneously is a shortcoming of many linear stochastic models. This is due to the direct 1009 use of the distribution function(s) within the generation mechanism of the model. If the 1010 1011 latter is defined in the positive real line, then all the generated values will be within those 1012 bounds (i.e., positive).
- Typical, but not limited, applications of SMARTA entail the simulation of stationary processes 1013 1014 at time scales not affected by cyclostationary correlation structures (e.g., monthly scale). For 1015 instance, given the wide range of admissible correlation structures and distributions, it could be applied for the generation of synthetic time series at annual and fine time scales (e.g., daily) 1016 1017 for various hydrometeorological processes, such as, precipitation, streamflow and temperature. The latter time series can be used as input in a variety of water resources risk-related studies 1018 1019 and it is anticipated to improve the quality of their outcomes, due to more accurate 1020 representation of the input processes. Ongoing research aims in an enhanced stochastic simulation scheme that will combine (using disaggregation techniques) both stationary (e.g., 1021 1022 SMARTA) and cyclostationary Nataf-based models (Tsoukalas et al., 2017, 2018a), thus 1023 providing an even more flexible and versatile simulation method for synthetic time series 1024 generation.

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1034 <u>http://www.itia.ntua.gr/en/docinfo/1863/</u>.

1035 Appendix A

1036 Tsoukalas et al. (2018a) proposed a generic, yet simple and efficient method for the 1037 establishment of the relationship of Eq. (15), that concerns the estimation of equivalent 1038 correlation coefficients $\tilde{\rho}_{\xi,\psi}$ required by Nataf-based schemes. The method is essentially a 1039 combination of Monte-Carlo simulation and polynomial approximation and is applicable for 1040 discrete, mixed and continuous-type marginal distributions; since its only requirement is the 1041 ICDF. The basic steps of the algorithm are synopsized below (the indices were omitted for 1042 simplicity):

- 1043 Let \underline{x}_{ξ} and \underline{x}_{ψ} be two random variables while $\tilde{\rho}_{\xi,\psi}$ and $\rho_{\xi,\psi}$ stand for the equivalent (in 1044 Gaussian domain) and the target correlation coefficients respectively. Furthermore, let $F_{\underline{x}_{\xi}}$ 1045 and $F_{x_{ib}}$, denote the corresponding target distributions, whose variance is assumed finite.
- 1046 **Step 1.** Create a Ω -dimensional, equally spaced, vector $\tilde{\boldsymbol{r}} = [\tilde{r}^1, ..., \tilde{r}^i, ..., \tilde{r}^{\Omega}]$ in the interval 1047 $[r_{min}, r_{max}]$. Lemma 2 (see section 3.2) can be employed in order to determine the values of r_{min} 1048 and r_{max} since it provides insights regarding the sign of $\tilde{\rho}_{\xi,\psi}$. For instance, if the target
- 1049 correlation $\rho_{\xi,\psi}$ is positive we restrict our attention on the interval [0, 1].
- 1050 Step 2. For each value of \tilde{r} generate N samples from the bivariate standard normal distribution 1051 with correlation \tilde{r}^i .
- 1052 Step 3. Map the generated values to actual domain using their ICDF (i.e., $F_{\underline{x}_{\xi}}$ and $F_{\underline{x}_{\psi}}$) as in 1053 Eq. (10).
- 1054 Step 4. Calculate and store the resulting correlation r^i in the vector $\mathbf{r} = [r^1, ..., r^i, ..., r^{\alpha}]$.
- 1055 Step 5. Since Eq. (15) is a continuous function, bounded in the interval $[r_{min}, r_{max}]$, according

to Weierstrass approximation theorem it can be approximated by a *p*-order polynomial of the form of Eq. (A.1) between \tilde{r} and r.

$$\rho = \mathcal{F}\left(\tilde{\rho} \left| F_{\underline{\xi}}, F_{\underline{\psi}} \right) \approx r = a_p \tilde{r}^p + a_{p-1} \tilde{r}^{p-1} + \dots + a_1 \tilde{r}^1 + a_0 \tag{A.1}$$

- 1058 Note that the constant term a_0 could be omitted as indicated by Lemma 2. Furthermore, in 1059 order to avoid over-fitting and possible ill-conditions, which could lead to simulation errors, 1060 the order of the polynomial can be determined with the use of cross-validation or Akaike information criterion (AIC). Alternatively, the degrees of freedom of the polynomial can be 1061 restricted (as in Xiao (2014)) by setting $p = \Omega - 1$. The latter author, based on a systematic 1062 1063 analysis of a variety of distributions characterized by wide combinations of skewness and 1064 kurtosis coefficients, argued that the relationship of Eq. (15) can be well approximated by a 1065 polynomial of less than ninth degree (p < 9); hence proposed setting $\Omega = 9$ and p = 8. Moreover, it is noted that instead of a polynomial relationship, other type of functions can be used (e.g., 1066 Papalexiou, 2018; Serinaldi & Lombardo, 2017). 1067
- 1068 Step 6. Given a target correlation $\rho_{\underline{\xi},\underline{\psi}}$, evaluate the equivalent correlation $\tilde{\rho}_{\underline{\xi},\underline{\psi}}$ by inverting the 1069 fitted polynomial of Eq. (A.1).

- 1070 It is remarked that the implementation of the latter algorithm in high-level programming
- 1071 languages (e.g., R or MATLAB) is fairly easy and straightforward, while a single run requires
- 1072 less than 0.5 second (with $N = 150\ 000$ and $\Omega = 9$) on a typical 3.0 GHz Intel Dual-Core i5
- 1073 processor with 4 GB RAM. Finally, it is noted that since it is a Monte-Carlo based method, the
- 1074 three parameters N, Q and p control its accuracy and computational efficiency.

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