### 1 Stochastic synthesis approximating any process dependence and

### 2 distribution

- 3 Panayiotis Dimitriadis\* and Demetris Koutsoyiannis
- 4 Department of Water Resources and Environmental Engineering, School of Civil Engineering,
- 5 National Technical University of Athens, Heroon Polytechneiou 5, 15880 Zographou, Greece
- 6 \*corresponding author, email: pandim@itia.ntua.gr

### 7 Abstract

8 An extension of the symmetric-moving-average (SMA) scheme is presented for stochastic synthesis of a stationary process by approximating any dependence structure and marginal 9 distribution. The extended SMA model can exactly preserve an arbitrary second-order structure 10 as well as the high order moments of a process, thus enabling a better approximation of any type 11 of dependence (through the second-order statistics) and marginal distribution function (through 12 statistical moments), respectively. Interestingly, by explicitly preserving the coefficient of 13 kurtosis, it can also simulate certain aspects of intermittency, often characterizing the 14 geophysical processes. Several applications with alternative hypothetical marginal distributions, 15 as well as with real world processes, such as precipitation, wind speed and grid-turbulence, 16 highlight the scheme's wide range of applicability in stochastic generation and Monte-Carlo 17 analysis. Particular emphasis is given on turbulence, in an attempt to simulate in a simple way 18 several of its characteristics regarded as puzzles. 19

Keywords: stochastic modelling; grid-turbulence; hourly surface wind speed; daily
 precipitation; intermittency; Kumaraswamy distribution; normal-inverse-Gaussian distribution

### 22 **1. Introduction**

The scientific interest on stochastic dynamics has increased over the last decades as an 23 alternative approach of deterministic or chaotic models to simulate the so-called random (i.e. 24 unexplained or unpredictable) fluctuations recorded in non-linear physical processes. 25 Koutsoyiannis (2010) argues that distinguishing deterministic from random is a false 26 dichotomy. Randomness can emerge even in a fully deterministic system with non-linear 27 dynamics. The dice throw, regarded as the emblem of randomness, is such an example 28 (Dimitriadis et al., 2016b). The line distinguishing whether determinism (i.e. predictability) or 29 randomness (i.e. unpredictability) dominates is related to the scale (or length)  $l(\varepsilon)$  of the time-30 31 window within which the future state deviates from a deterministic prediction by an error 32 threshold  $\varepsilon$ . For errors smaller than  $\varepsilon$ , we assume that the system is predictable within a time-33 window  $l(\varepsilon)$  and for larger errors unpredictable. Therefore, by applying stochastic analysis we identify the observed unpredictable fluctuations of the system under investigation with the 34 35 variability of a devised stochastic process. This stochastic process enables generation of an 36 ensemble of realizations, while observation of the given natural system can only produce a 37 single observed time series (or multiple ones in repeatable experiments). The simplest and yet 38 powerful technique to reveal and analyze entirely the system's variability, is the Monte-Carlo approach. However, this technique requires a generation algorithm capable of modelling any 39

selected marginal probability distribution and second-order dependence structure of the
stochastic processes, appropriate for the investigated natural system.

Although there are several methods for simulating arbitrary stochastic process, they all have 42 43 limitations and advantages (Lavergnat, 2016 and references therein). For example, the nonlinear method for the preservation of the distribution function (i.e., a Gaussian distributed 44 process with the desired dependence structure is produced and then transformed to the desired 45 distribution through a non-linear transformation or the inverse distribution function) is often 46 applied for synthesis of long-term (cyclostationary) processes (e.g., Koutsoyiannis et al., 2008), 47 but it has a disadvantage of e.g., distorting the dependence structure (because of the 48 transformation), while, in addition, the transformation cannot be invariant with respect to the 49 time scale (Lombardo et al. 2012). A generalization of this implicit scheme is the so-called copula 50 in which the joint distribution function is approximated, albeit through numerical methods. The 51 latter implicit approaches, whose detailed overview is beyond the scope of this paper (the 52 interested reader is referred to Hoeffding, 1940; Frechet, 1951; Sklar, 1959; as well as to more 53 recent publications, e.g. by Nelsen, 2006 and references therein). Typically they apply non-linear 54 transformations to the processes, often based on the autocovariance function (see Appendix D). 55 However, it is widely known that despite the high flexibility of copulas, the fractal and Hurst-56 Kolmogorov behaviour (i.e. strong correlation structures at zero scale and long-term persistence 57 at infinite scale, respectively) cannot be easily handled (e.g. Lavergnat, 2016; Ibragimov and 58 Lentzas, 2017). The reason for this, is that the process structure is invariant at these scales (as 59 they tend to zero and infinity) and thus, the structure of the originally generated process is 60 61 preserved rather than the back-transformed one (see also Appendix D for an example).

Another category of existing methods concern the preservation of the dependence structure 62 through autoregressive models such as the SAR model (Sum of many AR(1) or ARMA(1,1) 63 64 models; Koutsoyiannis, 2002; Dimitriadis and Koutsoyiannis, 2015a, supplementary material 65 sect. 3). Although these models can simulate a variety of dependence structures, they have a 66 disadvantage if preservation of high order moments is of interest (see also sect. 3.3.1 in 67 Dimitriadis, 2017). A rigorous and general method is the symmetric-moving-average (SMA) scheme introduced by Koutsoyiannis (2000), further advanced by Koutsoyiannis (2016) and 68 implemented within the Castalia computer package (Efstratiadis et al., 2014). This method can 69 70 fully preserve in an exact way any second-order structure of a process and, simultaneously, the 71 complete multivariate distribution function if it is Gaussian (because of the preservation of the 72 Gaussian attribute within linear transformations). Koutsoyiannis (2000) also studied the application of the same scheme to non-Gaussian processes by preserving the skewness of the 73 74 marginal distribution. Here, we extend the SMA scheme so that it preserves exactly four (or, if necessary, more) central moments of the distribution, while simultaneously preserving in an 75 exact way any type of second-order dependence structure, such as short-range (e.g., Markov) or 76 long-range (e.g., Hurst-Kolmogorov, abbreviated as HK). Note that the term 'HK behaviour' 77 78 corresponds to the behaviour of process at large scales while the process itself could not be 79 necessarily an HK process or follow a Gaussian distribution. For example, both the fractional Gaussian noise (fGn) and the generalized-HK (GHK; see below) process are processes exhibiting 80 an HK behaviour, but while the former's autocorrelation function is a power-law type at the 81 whole range of scales, the latter's autocorrelation function is a power-law type only at large 82 scales (at small scales behaves like a Markov process) and its distribution function is not 83 necessarily Gaussian. 84

To our knowledge there is no other method that can preserve explicitly (i.e. fully analytical 85 calculations) four (or more) marginal moments of a process for any type of dependence 86 structure. In most problems preservation of four moments suffices for a very good 87 approximation of the distribution function. In particular, the fourth moment has been regarded 88 of great importance in some problems, e.g., in the characterization of intermittency in turbulence 89 (Batchelor and Townsend, 1949). Therefore, turbulence is an ideal field for application of the 90 proposed framework. This study has given particular emphasis on turbulence, which is included 91 as the final and most detailed of the case studies presented, in an attempt to show that several 92 93 aspects of turbulence that are regarded as puzzles can be easily reproduced by a simple model 94 without a major effort. While all applications presented below handle moments up to fourth, the methodology proposed can handle explicitly even higher moments (see Appendix A) and thus 95 even approximate the joint (univariate, multivariate) structures that extend beyond the second-96 97 order statistics. Specifically, higher order moments for different time scales can also be adequately approximated, since this scheme can explicitly preserve the high-order moments of 98 the lowest scale, as well as those of the largest scales (which by virtue of the Central Limit 99 100 Theorem are expected to be close to the Gaussian distribution and thus, can be precisely represented by the second-order dependence structure; for an example see section 4.4). The 101 only limitation of this methodology is that the marginal distribution is approximated to a desired 102 103 degree, rather than precisely preserved (particularly in non-divisible distributions). This 104 limitation may create difficulties in variables with upper or lower bounds, since these can be 105 only treated in an ad-hoc manner (see Section 4.2). However, this limitation rarely concern 106 practical applications to geophysical processes.

107 In section 2, we present in detail the computational scheme for preserving in an exact way the dependence structure. We also explain why the preservation of solely the second-order joint 108 109 statistics can be adequate for capturing the most important attributes of a physical process and 110 suggest that often it is impractical to estimate high-order statistics from observations. In section 3, we present the generation algorithm for simultaneously preserving an approximation of the 111 marginal probability function (through cautiously selected distributions as described in 112 Appendices A and B), a task that we deal with when the actual process distribution departs from 113 normality, along with the dependence structure of the process. Finally, in section 4 we apply the 114 generation scheme to various examples in order to highlight not only its robustness but also its 115 use as a statistical tool to investigate the stochastic nature of complex geophysical processes 116 such as surface wind speed, daily precipitation and turbulent phenomena dominated by 117 intermittent behaviour. 118

### **119 2.** Generation scheme for preserving the dependence structure of a process

In this section, we discuss the practical limitations of using popular multi-parameter stochastic models for geophysical processes. In contrast, the SMA generation scheme (Koutsoyiannis, 2000; 2016) is very convenient in preserving the stochastic structure of a process based only on a parsimonious representation of the second-order statistics. Important advantages of this scheme are the parsimony of parameters and the fact that it can deal with non-Gaussian distribution, as will be detailed in the next session.

### 126 2.1. Background and notation on stochastic processes

As introduced by Kolmogorov (1931, 1933), a stochastic process  $\underline{x}(t)$  is a family of infinitely 127 many random variables, commonly (but not exclusively) indexed by time t, here assumed to be 128 continuous. A random variable  $\underline{x}$  is an abstract mathematical object that can take on all of its 129 possible values according to a (marginal) distribution function F(x). In addition to the marginal 130 distribution, a stochastic process is also characterized by its dependence structure. Note that in 131 the above notation we are using the Dutch convention, where an underlined symbol denotes a 132 random variable. A random variable  $\underline{x}$  should not be confused by its realizations (e.g., 133 observations) x and a stochastic process  $\underline{x}(t)$  should not be confused with its realizations 134 (sample functions or time series) x(t). A realization is usually known (e.g. by observation) only 135 in discrete time, at time intervals of length D, either by taking observations (sampling, with 136 137 approximately zero response time) at equidistant times iD (i = 1, 2, ...) or by averaging the process at each interval D (see more details in Koutsoyiannis, 2016). In the former case, the 138 sampling operation at equidistant times evokes to introduce the discrete-time stochastic process 139 140  $\underline{x}_i := \underline{x}(iD)$ . In the latter case, the observations are not of the process  $\underline{x}(t)$  per se, but of the time-141 averaged process:

$$\underline{x}_{i}^{(D)} = \frac{1}{D} \int_{(i-1)D}^{iD} \underline{x}(\xi) \mathrm{d}\xi \tag{1}$$

where *i* denotes discrete time. While in the definition of the discrete-time process *i* takes on 142 infinite values ( $i \in \mathbb{N}$ ), in an observed time series it obviously has an upper limit, the total 143 number of observations n, determined from the observation period  $T \ge D$ , i.e.  $n = \lfloor T/D \rfloor$ . In the 144 analysis below, to avoid confusion, we will omit the superscript (D) in the notation of the 145 process and we will use x<sub>i</sub> regardless of the manner the discrete-time process is constructed 146 from the continuous-time one. We also assume that  $\underline{x}(t)$  is a stationary and ergodic process (and 147 hence  $\underline{x}_i$  too). Note that the proposed SMA model can be used for simulation of both stationary 148 and non-stationary processes (by extracting the deterministic model and transform the original 149 150 non-stationary process to stationary) following the methodology described in Appendix C. The marginal characteristics of the process are estimated through the classical central moments and 151 the dependence structure of the process is estimated through  $\gamma(k)$ , i.e. the variance of the 152 averaged process  $\underline{x}_i^{(k)}$  vs. scale k, here called climacogram (also, hastily, referred to as aggregate 153 variance), where  $k = \kappa D$  is the continuous-time scale in time units and  $\kappa$  the dimensionless 154 discrete one, assuming that D is a time unit that is used for discretization (see Eqn. 1). The 155 climacogram is directly linked to the autocovariance c(h) by  $c(h) = 1/2d^2(h^2\gamma(h))/dh^2$  (e.g. 156 Koutsoyiannis, 2016), where h is the continuous-time lag (in time units). Also, the 157 autocovariance is linked to the power spectrum by  $s(w) = 4 \int_0^\infty c(h) \cos(2\pi wh) dh$ , where *w* is 158 the frequency (in inverse time units). Thus, each of these three stochastic tools contains exactly 159 the same information. However, it has been shown that the climacogram provides better 160 estimates than the other two (Dimitriadis and Koutsoyiannis, 2015a) and therefore, all 161 applications here are based on that. 162

### **163** 2.2. The impracticality of stochastic modelling with many parameters

Several families of autoregressive models are typically used in stochastic modelling with the 164 most popular in literature being model families so-named AR, ARMA, ARIMA, FARIMA. These 165 models are easy to handle and fast in stochastic generation once their parameters are known 166 and not too many. However, whenever the process exhibits long-range dependence these 167 models require a large number of parameters (except only in the FARIMA(0,d,0) special case) to 168 preserve in an exact way up to a large number of autocorrelation estimates. Conversely, the 169 typically available observation records can support the estimation of only a few parameters 170 (Lombardo et al. 2014; Koutsoyiannis, 2016). Interestingly, most geophysical processes exhibit 171 such long-term behaviours, as expected considering the maximization of entropy 172 (Koutsoyiannis, 2011) and as verified in several geophysical processes (O'Connell et al., 2016) 173 and specifically in key hydrometeorological processes such as: solar radiation and wind speed 174 (Tsekouras and Koutsoyiannis, 2014; Koutsoyiannis, et al., 2018); precipitation (Iliopoulou et al., 175 2016); paleoclimatic temperature reconstructions (Markonis and Koutsoyiannis, 2013); and 176 177 temperature, dew point, wind, precipitation and pressure processes classified by the Köppen-178 Geiger scheme (Dimitriadis et al., 2017). Additionally, the more complicated dependence structures and similarities identified e.g. among the microscale of turbulent, wind and 179 precipitation processes (Dimitriadis et al., 2016a and references therein) increase the need for 180 parsimonious stochastic approaches. 181

An additional difficulty may arise when estimating the prediction intervals of a long-range 182 process (Papoulis, 1990, pp. 240-242; Tyralis et al., 2013). Even if the model parameters are 183 184 calculated with adequate accuracy, this does not guarantee an adequate approximation of the 185 prediction intervals (e.g., see sect. 3.3.1 in Dimitriadis, 2017). Finally, the above model families may confront difficulties even in case of short-range processes but with a non-Gaussian marginal 186 distribution. Only in case of the AR(1) model can non-Gaussian distributions and/or seasonality 187 be simulated simultaneously (e.g., the PGAR model of Fernandez and Salas, 1986) while in 188 higher order autoregressive models this is not possible. For example, consider the simplest 189 model of the ARMA family, which is the ARMA(1,1) model: 190

$$\underline{x}_i = a\underline{x}_{i-1} + \underline{v}_i + b\underline{v}_{i-1} \tag{2}$$

191 where  $\underline{v}_i$  is a white noise process and *a*, *b* are parameters. This model can simulate well shortrange dependence, e.g., a Markov process in continuous time discretized by averaging in time 192 steps D > 0 (Dimitriadis and Koutsoyiannis, 2015a), but it cannot handle explicitly marginal 193 moments beyond the second moment (Koutsoyiannis, 2016). If simulation of moments higher 194 than the second order is needed, then in the parameter estimation equations mixed joint 195 moments of the form  $E[\underline{x}_{i-1}^p \underline{v}_{i-1}^q]$  will emerge (with p, q > 0, p + q > 2), which are not possible to 196 directly estimate from observed data (since <u>v</u> is artificial white noise) or handle (because  $x_{i-1}$  is 197 not independent from  $v_{i-1}$ ). A good alternative could be not to use such models but rather a sum 198 of multiple AR(1) models (SAR), to approximate the correlation structure up to the desired lag 199 by the sum of many independent AR(1) models, with their coefficients theoretically derived 200 rather than arbitrarily calculated. This was introduced and applied for 3 AR(1) models by 201 Koutsoyiannis (2002) and further developed for an arbitrary large number of components by 202

Dimitriadis and Koutsoyiannis (2015a). However, all of these models (AR, ARMA, SAR etc.) still have several limitations, as for example, it is impossible for them to preserve some important stochastic properties as scale tends to zero in continuous time (see section 4). Interestingly, the SMA model overcomes all the aforementioned limitations as also shown in the next sections and in the applications of this paper.

### 208 2.3. Derivation of the SMA coefficients

In the SMA scheme, the simulated process is expressed through the sum of products of coefficients (not parameters)  $a_i$  and white noise terms  $\underline{v}_i$ , i.e. (Koutsoyiannis, 2000):

$$\underline{x}_i = \sum_{j=-l}^l a_{|j|} \underline{v}_{i+j} \tag{3}$$

where l theoretically equals infinity but a finite number can be used for preserving the 211 dependence structure up to lag *l* (Koutsoyiannis, 2016). Also, for simplicity and without loss of 212 generality we assume that E[x] = E[v] = 0 and  $E[v^2] = Var[v] = 1$ . This scheme can be used for 213 stochastic generation of any type of second-order process structure represented by functions 214 such as the climacogram, the autocovariance function, the power spectrum or the variogram. It 215 exhibits several advantages over widely used backward moving average (BMA) schemes, the 216 most important being that it allows closed expressions for the coefficients  $a_i$ , based on any of the 217 above functions (Koutsoyiannis, 2000). 218

As an example, let us consider the HK process, whose climacogram in continuous time is:

$$\gamma(\kappa) = \frac{\gamma(D)}{\kappa^{2-2H}} \tag{4}$$

where  $\kappa = k/D$  denotes discrete time scale,  $\gamma(D)$  is the variance at the unit time scale *D*, and *H* is the Hurst parameter (0 < *H* < 1).

For an HK process with H > 0.5 the SMA coefficients can be estimated analytically (Koutsoyiannis, 2016):

$$a_{j} = C\left(\frac{|j+1|^{H+\frac{1}{2}} + |j-1|^{H+\frac{1}{2}}}{2} - |j|^{H+\frac{1}{2}}\right)$$
(5)

224 where

$$C = \sqrt{\frac{2\Gamma(2H+1)\sin(\pi H)\gamma(D)}{\Gamma^2(H+1/2)(1+\sin(\pi H))}}$$
(6)

#### whereas $\Gamma(x)$ is the gamma function.

Another example that will be used below is the so-called Hybrid Hurst-Kolmogorov (HHK)
 process (Koutsoyiannis 2016), whose climacogram is:

$$\gamma(k) = \frac{\lambda}{(1 + (k/q)^{2M})^{\frac{1-H}{M}}}$$
(7)

where  $\lambda$  is the variance of the continuous-time process  $\underline{x}(t)$ , *M* is a fractal parameter (see also Gneiting 2000; Gneiting and Schlather 2004; Gneiting et al. 2012; Dimitriadis 2017 and references therein), *H* is the Hurst parameter and *q* is a characteristic time parameter. A particular case of the HHK, which will be later used and referred to as GHK, is when  $M = \frac{1}{2}$ , i.e.:

$$\gamma(k) = \frac{\lambda}{(1+k/q)^{2-2H}} \tag{8}$$

An explicit expression for the coefficients  $a_j$  for the HHK or the GHK may not be easy to derive. However, they can be numerically calculated through the Fourier transform of the discrete power spectrum of the coefficients which is directly linked to the discrete power spectrum of the process (Koutsoyiannis, 2000):

$$s_{\rm d}^a(\omega) = \sqrt{2s_{\rm d}(\omega)} \tag{9}$$

where  $s_d^a(\omega)$  and  $s_d(\omega)$  are the power spectra of the SMA coefficients and of the discrete time process, respectively, and  $\omega = D/k$  is the dimensionless frequency.

## 3. Generation scheme for approximate preservation of the marginal distribution of a process

In this section, we first discuss the natural and statistical intrinsic limitations of fitting multi-240 parameter probability functions to geophysical processes, while we emphasize the need to fit 241 and reproduce non-Gaussian distributions, which very often appear in geophysical variables. A 242 non-Gaussian distribution can still be parsimonious in terms of parameters (e.g., two-parameter 243 244 marginal distributions are often used). While fitting low-parametric marginal distributions to a certain variable is easy, stochastic generation schemes can hardly deal with non-Gaussian 245 distributions and can hardly handle moments higher than second-order. Here, we introduce an 246 extension of the SMA generation scheme for approximating the marginal probability function of 247 a process by exactly preserving its first four central moments which is found to be adequate for 248 249 various distributions commonly applied in geophysical processes, while in Appendix A we extend the method for even higher moments. We emphasize that these moments that are to be 250 preserved are not necessarily estimated from data. On the contrary, in typical sizes their 251 estimation from data is strongly discouraged as explained below. Rather, the values of these 252 moments should be obtained theoretically, once a specific distribution function is fitted. 253

# 3.1. The impracticality of estimating high-order moments in geophysical processes

Non-Gaussian distributions are very common in Nature. It has been shown (Lombardo et al., 256 2014) that the estimation of high order raw moments is highly uncertain and, thus, it is 257 inefficient to use the schemes described in the previous section to preserve high moments for 258 259 natural processes with limited sample sizes, as is the case for typical geophysical records. In the case of a continuous HK process the variance of the mean estimator is  $\gamma(D)/n^{2-2H}$  (e.g. 260 Koutsoyiannis, 2003), where *n* is the sample size. Consequently, for estimating the population 261 mean  $\mu$  of a process with a standard error  $\pm \varepsilon$ , we would require a time series of length at least 262  $(\sigma/\varepsilon)^{1/(1-H)}$ , where  $\sigma = \sqrt{\gamma(D)}$  is the standard deviation at scale *D* (Fig. 1). For example, for an 263 HK process with H = 0.8, to estimate the mean of the process with an error  $\varepsilon \approx \pm 10\%\sigma$ , we 264 need a time series of length  $n = 10^5$ . Such lengths are hardly available in observations of 265 geophysical processes, which are not only characterized by HK behaviour (a conclusion based on 266 the maximization of entropy as derived in Koutsoyiannis, 2011) but also include sub-daily and 267 seasonal periodicities (e.g., Dimitriadis and Koutsoyiannis, 2015b) that complicate the 268 estimation further. 269



270

Figure 1: Standard deviation of the mean estimator of an HK process standardized by  $\sigma$  vs. the sample size (*n*) for various Hurst parameters.

To give another example, we perform a Monte Carlo experiment for an HK process with H = 0.8that follows a standard Gaussian distribution (i.e.  $\mu = 0$  and  $\sigma = 1$ ) and the results are shown in Fig. 2. For each synthetic time series we estimate the mean, standard deviation as well as skewness and kurtosis coefficients for six different lengths, i.e.,  $n = 10, 10^2,..., 10^6$ . This experiment shows that for  $n = 10^6$  the uncertainty (measured in terms of the standard deviation of sample estimates of each property) is below 10% for all these moments. Therefore, to adequately estimate these moments from data we would need time series with at least similar lengths.



Figure 2: Standard deviation of the sample estimates of the mean ( $\mu$ ), standard deviation ( $\sigma$ ), skewness coefficient ( $C_s$ ) and kurtosis coefficient ( $C_k$ ) of an HK process with H = 0.8 and N(0,1) distribution vs. the simulation length.

### **3.2.** Derivation of the SMA distribution parameters

The SMA method can explicitly preserve high order marginal moments. However, as already 286 mentioned above, high-order moments cannot be estimated reliably from data while non-287 Gaussianity can be easily verified empirically but also derived by theoretical reasoning 288 (Koutsoyiannis 2005; 2014). A simple way to simulate non-Gaussian distributions is to calculate 289 theoretically (not from the data but rather from the distribution model) their moments and then 290 explicitly preserve these moments in simulation. Koutsoyiannis (2000) estimated the first three 291 moments of the marginal distribution of the white noise process  $\underline{v}_i$ , required to reproduce those 292 293 of the actual process  $\underline{x}_{i}$ , using the SMA scheme. With the conventions used in this paper (see above), the mean and variance of  $\underline{v}_i$  are 0 and 1, respectively, while the third moment, which is 294 equal to the coefficient of skewness, is: 295

$$C_{s,\nu} = \frac{\left(\sum_{j=-l}^{l} a_{[j]}^{2}\right)^{3/2}}{\sum_{j=-l}^{l} a_{[j]}^{3}} C_{s,x}$$
(10)

296 where  $C_{s,x}$  is the coefficient of skewness of  $\underline{x}_i$ .

Although preservation of three central moments usually provides acceptable approximations to
the theoretical distributions, a non-Gaussian distribution cannot be precisely preserved. Here,
we expand the calculations to include the coefficient of kurtosis of the white noise (see Appendix
A for proof):

$$C_{\mathbf{k},\nu} = \frac{\left(\sum_{j=-l}^{l} a_{|j|}^{2}\right)^{2}}{\sum_{j=-l}^{l} a_{|j|}^{4}} C_{\mathbf{k},x} - 6 \frac{\sum_{j=-l}^{l-1} \sum_{k=j+1}^{l} a_{|j|}^{2} a_{|k|}^{2}}{\sum_{j=-l}^{l} a_{|j|}^{4}}$$
(11)

where  $C_{k,\underline{x}}$  is the coefficient of kurtosis of  $\underline{x}_i$ . Note that the constant term in the right-hand side depends only on the SMA coefficients and not on the marginal distribution of the process. Also, note that the kurtosis of the white noise is not proportional to the kurtosis of the process, as is in the case of the skewness (Eqn. 10).

For the generation of the auxiliary variable  $\underline{v}$  we need distributions that: (a) contain at least four 305 parameters, creating in such way a large variety of combinations between the first four 306 moments; (b) have closed analytical expressions for the first four central moments; and (c) can 307 easily and quickly generate random numbers. Here, we propose the four-parameter 308 309 Kumaraswamy (1980) distribution, which is mostly appropriate for generating thin-tailed 310 distributions, and the four-parameter normal inverse Gaussian distribution (e.g., Barndorff-Nielsen, 1978) for generating heavy-tailed distributions. The details of the distributions are 311 contained in Appendix B. 312

### 313 4. Applications

314 In this section, we present several applications of the extended SMA scheme, first to non-315 Gaussian white noise process with several two-parameter marginal distributions used extensively in geophysics and we show that even complicated distributions can be well 316 approximated by their first four central moments. We then apply the scheme to a 130-year daily 317 precipitation time series, by fitting an HK model along with a three-parameter marginal 318 distribution. Also, we apply the scheme to multiple hourly wind speed time series recorded over 319 a wide area, by fitting a GHK model along with a three-parameter marginal distribution. Finally, 320 we apply the scheme into a massive database of experimental time series of turbulent velocities 321 recorded at high frequency, by fitting an HHK process and by approximating the unknown 322 marginal distribution with the first four empirical moments. 323

# 4.1. Application to white noise processes with various two-parameterdistributions

In the examples below, we apply the extended generation scheme to Weibull, gamma, Pareto and lognormal distributions and we illustrate that the preservation up to the fourth moment is adequate for capturing the main body of the distribution as well as a part of the tail (see Fig. 3, which also displays the parameter sets of the specified distributions). As all these variables used in our examples are non negative, any generated negative values are set to zero. This does not cause any distortion worth discussing, as the approximation of the probability density function

- by the four moments is satisfactory (see Fig. 3 and other figures below), and since this density is
- typically zero in negative values, the number of generated negative values is negligibly small.
- We expect that using the approximation based on the first four moments, the distribution which
- we actually simulate is the maximized entropy (ME) distribution produced by constraining these
- moments. The ME resulting distribution, i.e.  $f(x; \lambda') := e^{\lambda_0' + \lambda_1' x + \lambda_2' x^2 + \lambda_3' x^3 + \lambda_4' x^4}$  (Jaynes, 1957),
- can also be written as:

$$f(x; \lambda) := \frac{1}{\lambda_0} e^{-\left(\frac{x}{\lambda_1} + \operatorname{sign}(\lambda_2)\left(\frac{x}{\lambda_2}\right)^2 + \left(\frac{x}{\lambda_3}\right)^3 + \left(\frac{x}{\lambda_4}\right)^4\right)}$$
(12)

where  $\lambda = [\lambda_0, \lambda_1, \lambda_2, \lambda_3, \lambda_4]$ , with  $\lambda_0, \lambda_1, \lambda_2, \lambda_3, \lambda_4$  (with  $\lambda_4 \ge 0$ ) having same units as x and with constraints:

$$\int_{-\infty}^{\infty} x^r f(x; \lambda) dx = \mathbf{E}[\underline{x}^r], \text{ for } r = 0, ..., 4$$
(13)

The solution to the above system of equations for  $\lambda$  can be achieved through optimization or other numerical algorithms (cf. Balestrino et al., 2009). Parameter  $\lambda_0 > 0$  equals  $1/f(0; \lambda)$ (where the denominator is the value of the ME probability density at x = 0). For the estimation of the ME distribution parameters we minimize the error  $\varepsilon_f$  defined in Eqn. (14), which is based on the absolute value of the difference between the main body of the empirical and modelled distribution along with their left and right tails:

$$\varepsilon_{f} = \sum_{i} \left| 1 - \frac{f_{\rm m}(x_{i})}{f_{\rm e}(x_{i})} \right| \sum_{i} |f_{\rm e}(x_{i}) - f_{\rm m}(x_{i})| \sum_{i} \left| 1 - \frac{f_{\rm e}(x_{i})}{f_{\rm m}(x_{i})} \right|$$
(14)

where  $f_{\rm m}$  and  $f_{\rm e}$  are the model and empirical distribution functions, respectively.

The quantities  $1/\lambda_1$ ,  $1/\lambda_2$ ,  $1/\lambda_3$ ,  $1/\lambda_4$  can be also regarded as weighting factors representing the 347 dependence of the distribution on each raw moment. Interestingly, after standardizing these 348 four parameters based on the sum of their absolute values,  $1/\lambda_1$  contributes to the Weibull, 349 gamma, lognormal and Pareto distributions of Fig. 3, approximately 65%, 66%, 69% and 93%, 350 respectively. Similarly, the contribution of  $1/\lambda_2$  is approximately 20%, 20%, 18% and 4%, the 351 contribution of  $1/\lambda_3$ , 11%, 10%, 9% and 2% and the contribution of  $1/\lambda_4$ , 4%, 4%, 4% and 1%, 352 respectively. Therefore, we may use the ME probability density to approximately determine the 353 weight for each statistical moment. As a rough indicator of the goodness of fit, the correlation 354 coefficient between the theoretical values of these four distributions and the simulated ones is 355 estimated as 99.57%, 99.38%, 99.26%, and 99.84%, respectively. 356



Figure 3: Various two-parameter distributions along with the fitted ME probability density function and the empirical probability density from one single simulation with  $n = 10^5$  using the proposed generation scheme.

# 4.2. Application to daily precipitation; an HK process with a three parameter distribution

In this application, we analyse one of the longest daily precipitation time series recorded for over 100 years at the site of Hohenpeißenberg in Germany (latitude 47.801°N, longitude 11.011°E; data from www.gkd.bayern.de/). We apply an HK process (Eqn. 4) with a single continuous-state Pareto II marginal distribution (a special case of the Pareto-Burr-Fuller—PBF distribution, i.e.  $F(x) = 1 - (1 + (x/a - h)^b)^{-c}$ ; Koutsoyiannis et al., 2018), introduced for use in precipitation by Koutsoyiannis (2004a) and theoretically justified by Koutsoyiannis (2004b):

$$F(r) = 1 - \left(1 + \left(\frac{r}{a} - h\right)\right)^{-c} \tag{15}$$

where r > ah is precipitation; a > 0 is a dimensionless scale parameter; c > 0 is a dimensionless parameter characterizing the right tail (extreme events) of the distribution and his a dimensionless parameter representing a threshold value and characterizing the left tail (dry events) of the distribution.

Theoretically h = 0, but values slightly different from zero not only highly improve fitting (Fig. 4), but also preserve the left tail of the distribution (i.e. probability dry), by simulating the

probability dry through  $F(0) := P(\underline{r} \le 0)$ . An h different from 0 is also physically justified since 376 precipitation measurements are usually corrupted with significant uncertainties (Krajewski et 377 al., 1998; Villarini et al., 2008) causing losses mostly due to wind effects (Nespor and Sevruk, 378 1998) and so, a slightly larger amount of precipitation is expected to be lost before measured. 379 After the generation we can set to zero any negative values of the synthetic time series in order 380 to emulate the observed distribution function. This approach of mixing wet and dry events 381 within a single distribution function is rather simple but can sometimes provide good results 382 (Fig. 4; see also Dimitriadis , 2017, sect. 6, where a more generalized distribution performs an 383 even better fit). For a more accurate approach, in terms of the simulation of the wet/dry 384 probability, one could separate these events and model their joint distribution instead 385 (Lombardo et al., 2017, and references therein). 386

To account for the seasonal periodicity of precipitation (Langousis and Koutsoyiannis, 2006) we 387 apply a non-linear transformation based on the known marginal distribution of the process 388 which is also preserved. Note that here, the process exhibits weak seasonality that only causes a 389 small increase in the dependence structure, as depicted in the intermediate area of the 390 climacogram in Fig. 4. Therefore, for the simulation of the seasonality we may then use the 391 392 inverse non-linear transformation (i.e. concept of homogenization, Dimitriadis, 2017, sect. 2.1) or apply a cyclostationary model, where each cycle is treated separately but with the same white 393 noise process, thus, additionally preserving the cross-correlations values (Dimitriadis, 2017, 394 sect. 3.3.3). 395

To account for estimation bias, since we have a single time series, we apply the innovative 396 method of estimating the parameters of the dependence structure of the process through the 397 mode second-order measure (e.g. climacogram, autocovariance, power spectrum etc.) rather 398 than the expected one (see also Dimitriadis et al., 2016c). For this, we apply a Monte-Carlo 399 analysis by generating one thousand daily time series of 130 years following the fitted marginal 400 distribution and an HK process. From the Monte-Carlo ensemble, we calculate the mode for each 401 scale with an acceptable accuracy and construct the mode climacogram for the specified process. 402 403 For the estimation of the parameters of the marginal distribution we minimize the same norm as 404 in Eqn. (14) and for the parameters of the dependence structure we use a similar one:

$$\varepsilon_{\gamma} = \sum_{\kappa} \left| 1 - \frac{\gamma_{\rm m}(\kappa)}{\gamma_{\rm e}(\kappa)} \right| \sum_{i} |\gamma_{\rm e}(\kappa) - \gamma_{\rm m}(\kappa)| \sum_{i} \left| 1 - \frac{\gamma_{\rm e}(\kappa)}{\gamma_{\rm m}(\kappa)} \right|$$
(16)

where  $\gamma_{\rm m}$  is the model (i.e., the mode for this application) climacogram and  $\gamma_{\rm e}$  is the empirical climacogram estimated from the classical estimator:

$$\underline{\hat{\gamma}}(\kappa D) = \frac{1}{\lfloor n/\kappa \rfloor - 1} \sum_{i=1}^{\lfloor n/\kappa \rfloor} \left( \underline{\overline{x}_i} - \underline{\overline{x}} \right)^2$$
(17)

where  $\lfloor n/\kappa \rfloor$  is the integer part of  $n/\kappa$ ,  $\bar{x}_{\kappa} = \left(\sum_{l=\kappa(i-1)+1}^{\kappa i} \underline{x}_l\right)/\kappa$  is the sample average of the time-407 averaged process  $\underline{x}_{\kappa}$  at scale  $\kappa = k/D$  as defined in Eqn. (1) and  $\overline{\underline{x}} = \sum_{l=1}^{n} \underline{x}_{l}/n$  is the sample 408 average at scale  $\kappa = 1$ . 409

The parameters of the process are estimated as a = 42.25 mm, c = 7.7, h = -0.1,  $\gamma(D) = r_s^2$ , 410 with  $r_s = 6.5$  mm the standard deviation of the process, and H = 0.6. Through a single synthetic 411 412 time series of equivalent length and after setting negative values to zero, the modelled marginal characteristics are estimated as:  $\mu = 3.3$  (3.1) mm,  $\sigma = 6.5$  (6.5) mm,  $C_s = 4.5$  (4.3),  $C_k = 36.4$ 413 (30.2) and probability dry 44% (48%), where inside parentheses are the values of the 414 observations, which are relatively well preserved. For illustration purposes, in Fig. 4 we plot a 415 3000 days window of the observed vs. the simulated precipitation. Note that here, the explicit 416 preservation up to the fourth moment is adequate, since preservation of additional moments 417 slightly improve the distribution simulation (specifically, the  $R^2$  coefficient is estimated for 418 preservation of the 1st, 2nd, 3rd, 4th, 5th, and 6th moment as 0.953, 0.985, 0.985, 0.9861, 0.9863 and 419 0.9864, respectively). 420



*Figure 4*: [upper left] Empirical (original and transformed to approximately remove seasonality), 423 modelled and simulated marginal distributions (corresponding weights for the ME distribution: 424 73%, 15%, 7% and 5%); [upper right] climacograms for the standardized precipitation process; 425 [lower left] the mode and several other essential statistical measures of the standardized 426 climacograms estimated from  $10^3$  synthetic time series (in the figure we depict only 50 427 empirical climacograms); [lower right] a 3000 days window of the observed precipitation record 428 along with a simulated one. 429

# 430 4.3. Application to hourly surface wind; a GHK process with a three-431 parameter distribution

For the hourly wind process we adopt the GHK process (Eqn. 8) for the dependence structure. 432 For the distribution function we apply a special case of the PBF distribution which approximates 433 the Weibull distribution for small hourly velocities and the Pareto distribution for larger ones 434 (e.g., Aksoy et al., 2004; Lo Brano et al., 2011). The dependence structure, marginal distribution 435 and standardization scheme of wind are based on the preliminary analysis from thousands of 436 stations around the globe, performed by Dimitriadis and Koutsoyiannis (2016). A more 437 438 thorough analysis justifying the above choices for the wind process can be seen in Koutsoyiannis et al. (2018) and references therein. The three-parameter GHK process and selected PBF 439 marginal probability function can be written as: 440

$$\gamma(k) = \frac{\lambda}{(1+k/q)^{2-2H}}$$
(18)

$$F(v) = 1 - \left(1 + \left(\frac{v}{\alpha v_{\rm s}}\right)^b\right)^{-c/b}$$
<sup>(19)</sup>

where v > 0 is the wind process;  $k = \kappa D$  is the continuous time scale with D = 1 h the sampling 441 time interval and  $\kappa$  the discrete time scale; *q* is the scale parameter of the process;  $\lambda$  is the true 442 variance of the instantaneous (continuous-time) process; H is the Hurst parameter;  $v_s$  is the 443 standard deviation of the discretized process that should equal the expected value of the square 444 root of the climacogram for scale  $\kappa = 1$ , i.e.  $v_s = \sqrt{\gamma(D)} = (1 + D/q)^{H-1}\sqrt{\lambda}$ ; in addition,  $\alpha$  is the 445 scale parameter and b and c are the shape parameters of the marginal distribution, all 446 dimensionless. Interestingly, here the survival function and the dependence structure have 447 identical expressions (Koutsoyiannis, et al., 2018). Note that by assuming stationarity and 448 ergodicity, we are able to standardize the wind process (Fig. 5), in order to homogenize all time 449 series recorded at different locations, altitude and climatic conditions (this should not be 450 confused with normalization through a non-linear transformation). 451

We choose to apply the above stochastic model to the longest nine hourly wind time series of different lengths located in Greece (Table 1). The expression for the bias of the classical estimator of the climacogram is derived in Tyralis and Koutsoyiannis (2011) for an HK process and generalized for all processes in Koutsoyiannis (2011). Here, we use the general expression and, since the time series have different lengths *n*, we apply an estimator of the climacogram adjusted for *n*:

$$\underline{\hat{\gamma}}(\kappa D) = \frac{1}{\lfloor n/\kappa \rfloor} \sum_{i=1}^{\lfloor n/\kappa \rfloor} \left( \overline{\underline{x}_{l}} - \overline{\underline{x}} \right)^{2} + \gamma(\lfloor n/\kappa \rfloor \kappa D)$$
(20)

458 where  $\hat{\gamma}(\kappa D)$  is an unbiased estimator of the climacogram  $\gamma(kD)$ , since  $\mathbb{E}\left[\hat{\gamma}(\kappa D)\right] = \gamma(\kappa D)$ .

*Table* 1: General information of the meteorological stations and statistical characteristics of thehourly wind time series (downloaded from ftp.ncdc.noaa.gov).

hourly wind station	longitude (deg)	latitude (deg)	elevation above sea level (m)	no. of years	mean (m/s)	st. deviation (m/s)	missing values (%)	zero values (%)
Heraĸleio	25.183	35.333	39	39	4.583	2.918	8.8	6.3
N. Aghialos	22.8	39.217	15	17	3.258	2.331	28	19
Karpathos	35.417	27.15	20	17	7.506	4.074	30.4	3.9
Santorini	36.4	25.483	38	24	5.701	3.229	29.5	7.5
Kos	36.8	27.083	125	33	4.805	2.7	15	7
El. Venizelos	37.93	23.93	96	11	3.954	2.995	0.6	1.9
Limnos	39.917	25.233	5	38	4.458	3.546	23	17.5
Paros	37.02	25.13	36	11	5.567	3.265	46.8	6.5
Meganissi	38.95	20.767	4	40	3.571	2.746	36.3	19.4

461 The parameters related to the dependence structure via the climacogram are estimated as: 462  $\lambda = 1.3$ , q = 5 h and H = 0.75, whereas for the marginal distribution as: a = 6, b = 1.9 and c = 14.8, corresponding to  $\mu = 1.9$ ,  $\sigma = 1.1$  ( $\approx \sqrt{\lambda}$ ),  $C_s = 1.2$  and  $C_k = 4.8$  (all estimations are based 463 on the fitting norms in Eqns. 14 and 16). Again, the explicit preservation up to the fourth 464 moment is adequate, since preservation of additional moments slightly improve the distribution 465 simulation (specifically, the R<sup>2</sup> coefficient is estimated for preservation of the 1<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup>, 4<sup>th</sup>, 5<sup>th</sup>, 466 and 6<sup>th</sup> moment as 0.936, 0.949, 0.977, 0.983, 0.984, and 0.984, respectively). To emulate the 467 observed wind time series one could set to zero any values of the synthetic time series that are 468 below the corresponding recording threshold of a typical anemometer, which is around 0.5 m/s 469 470 depending on the type of the anemometer (e.g. Conradsen et al., 1984). For illustration purposes, 471 in Fig. 5 we plot a 1000-day window of the observed vs. the simulated wind speed at Kos Island. The empirical and modelled probability of standardized wind speed less than or equal to 1 are 472 473 both around 50%. Note that  $\sigma$  and  $\lambda$  should approximate unity but they are slightly larger due to 474 the double cyclostationary effects of the daily and seasonal periodicities of the wind process (Deligiannis et al., 2016). These effects cause the small increase of climacogram around daily and 475 annual scales (Fig. 5) but here, for simplicity, we apply a stationary rather than a cyclostationary 476 model through the non-linear transformation of the probability function of Deligiannis et al. 477 (2016). Again, due to the weak periodicities of the examined process the double 478 cyclostationarity can be generated through the inverse transformation. 479





# 488 4.4. Application to turbulence; an HHK process with an unknown 489 distribution

As already mentioned, high-order moments cannot be reliably estimated from typically short 490 time series of geophysical processes. However, in laboratory experiments with high sampling 491 rates, very large time series of observations can be formed, which allow direct estimation of high 492 order moments from data. Here, we use a grid-turbulence massive database provided by the 493 Johns Hopkins University (www.me.jhu.edu/meneveau/datasets/datamap.html). This dataset 494 includes 40 time series, each with  $n = 36 \times 10^6$  data points of longitudinal wind velocity along the 495 flow direction, all measured by X-wire probes placed downstream of the grid and with a 496 sampling time interval of 25 µs (Kang et al., 2003). Due to the laboratory nature of the 497 experiment we may apply the Taylor's hypothesis of frozen turbulence (Taylor, 1938) and shift 498 499 from the spatial to the temporal domain (Castro et al., 2011). We then use a standardization scheme illustrated in Fig. 6 to homogenize all series (Dimitriadis et al., 2016a) and, by setting the 500 501 empirical mean to zero, we calculate the standardized empirical variance as  $E[\hat{\gamma}(D)] \approx 1$ . By the standardization, we are able to form a sample of  $40 \times 36 \times 10^6 = 1.44 \times 10^9$  values for the 502 estimation of the marginal characteristics of the process and an ensemble of 40 series, each with 503 36 ×10<sup>6</sup> values for the estimation of the dependence structure characteristics. 504

- 505 It can be observed that the time series are not Gaussian but rather nearly-Gaussian as shown in Fig. 7. This is also verified by the skewness and kurtosis estimates of 0.2 and 3.1, respectively. If 506 those values were estimated from a small sample, for example n = 100, then the probability 507 density function of the process would be regarded Gaussian and the divergence from normality 508 would be attributed to statistical error, since for n = 100 the uncertainty measured through the 509 standard deviation of the skewness and kurtosis, is as high as 30% and 50%, respectively (Fig. 510 2). However, for  $n \approx 1.5 \times 10^9$  the uncertainty of the mean will drop below 1% for H = 0.8 and 511 therefore, based on extrapolation of curves in Fig. 2, it is seen that the uncertainty of skewness 512 and kurtosis will be low too. Moreover, there are theoretical arguments justifying the divergence 513 of fully developed turbulent processes from normality (Wilczek et al., 2011). 514
- 515 In contrast to the earlier application, where the value of the fourth moment was inferred from 516 the fitted theoretical distribution, here we directly estimate it from the data since the estimation 517 error is very low due to the huge number of data points as well as due to the high quality of the 518 measurements.

For the stochastic structure, we apply a stochastic model (modified HHK process) and fit it by incorporating both discretization and bias effects (Fig. 8). This model combines both fractal and HK dynamics using four parameters and it attributes the grid-turbulent process to an HHK process (Eqn. 8) and the independent effect of the boundaries of the experiment, which cause a drop of variance at intermediate scales, to a Markov process:





*Figure* 6: Standardization scheme for grid-turbulence data, where  $\mu$  and  $\sigma$  are the mean and standard deviation, *r* is the distance from the grid, with the first 16 time series corresponding to transverse points abstaining *r* = 20*L* from the source, the second 4 to *r* = 30*L*, the third 4 to 40*L* and the last 16 to 48*L*, with *L* = 0.152 m the size of the grid.



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Figure 7: Empirical probability density function of the overall standardized time series (observed) along with that from a single synthetic time series produced by the SMA scheme to preserve the first four moments (simulation); for comparison the theoretical distributions N(0,1), sum of two Gaussian distributions (double Gaussian), and ME constrained on the four moments (corresponding weights for the ME distribution are estimated as 15%, 51%, 21% and 13%.

Again here, the explicit preservation up to the fourth moment is adequate, since preservation of additional moments slightly improve the distribution simulation (specifically, the  $R^2$  coefficient is estimated for preservation of the 1<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup>, 4<sup>th</sup>, 5<sup>th</sup>, and 6<sup>th</sup> moment as 0.0372, 0.990, 0.991, 0.998, 0.999, and 0.999, respectively).

For the estimation of the climacogram we use the estimator of Eqn. (17) and we apply the 540 methodology by fitting the expected model to the mean climacogram calculated from the 36 time 541 series of identical length. However, to improve the fitting of the model, we include in the analysis 542 the climacogram-based structure function (abbreviated CBF) and the climacogram-based 543 spectrum (abbreviated CBS), as introduced in Koutsoyiannis (2016). The climacogram is more 544 representative of the large and intermediate scales, the CBF of the small and intermediate scales 545 546 and the CBS of small and large scales and thus, by combining all three of them we can achieve a 547 better fitting of the model (Dimitriadis et al., 2016a). The CBF and CBS are defined through the 548 climacogram respectively, as:

$$\xi(k) := \gamma(0) - \gamma(k) \tag{22}$$

$$\psi(w) := \frac{2}{w\gamma(0)} \gamma(1/w)\xi(1/w) = \frac{2\gamma(1/w)}{w} \left(1 - \frac{\gamma(1/w)}{\gamma(0)}\right)$$
(23)

549 where  $\gamma(0) = \lambda$  for the specified mode; and w = 1/k is the frequency for a continuous-time 550 process (in inverse time units).

The model parameters are estimated as:  $\lambda = 1$ , M = 1/3, H = 5/6 and q = 14 ms, through the 551 fitting norm of Eqn. 16. Here a large number of parameters could be justified due the large data 552 size but the above model is quite parsimonious (it has two parameters less than that used by 553 Dimitriadis et al., 2016a, for modelling the same process). Also, the applied extended HHK model 554 is theoretically justified through the maximization of entropy (Koutsoyiannis, 2011) and 555 therefore, each parameter has a physically-based interpretation. Moreover, we observe from Fig. 556 8 that this model comes also in agreement with the work on the turbulent power spectrum by 557 von Karman (1948) for the large scale range, by Kolmogorov (1941a-c; K41 model) for the 558 intermediate range and by Kraichnan (1959) for the dissipation range (cf. Pope 2000, pp. 232-559 233), while here we also simulate the Hurst-Kolmogorov behaviour that clearly appears in the 560 very small frequencies (very large scales) of the power spectrum and in the other stochastic 561 tools in Fig. 8. Additionally, certain aspects exhibited in the power spectrum such as the 562 563 bottleneck effect (Kang et al., 2003) and the spike at large frequencies (which is often ignored and attributed to instrumental noise; Cerutti and Meneveau, 2000) are also well represented. 564 Finally, the preservation of kurtosis of the velocity increments enables to even simulate the 565 effect that the intermittent behaviour of the process has on the marginal probability 566 distribution, first discovered in turbulence by Batchelor and Townsend (1949). 567

It is interesting to further investigate the latter issue through the behaviour of a generalized 568 structure function  $V_p(h) := \mathbb{E}[|\underline{x}_i - \underline{x}_{i+h}|^p]$  and in particular the power-law behaviour for the 569 intermediate range of lags, i.e.  $V_n(h) \approx h^{\zeta_p}$ . Such behaviours have been attributed to 570 intermittency (Frisch, 2006, sect. 8.3) which initiated the need for exploring models different 571 572 from the K41 such as the multifractal ones (Frisch, 2006, sect. 8.5 to 8.9). As shown in Fig. 9 to 12, the drop of skewness (Fig. 9) and the drop of kurtosis (Fig. 10) of the velocity increments for 573 a wide range of lag (h) or the regular velocity vs scale (high order climacogram; Fig. 11) are 574 impressively well preserved by the proposed model. It is important to notice in Figs. 9 and 10 575 that, if preservation up to third (rather than fourth) marginal moment was made, then the 576 lagged skewness and kurtosis would not be preserved adequately. In addition, the increase of 577 the exponent  $\zeta_p$  is equally well preserved by the proposed model for a wide range of the p 578 exponent (Fig. 12). This is achieved with no particular effort or provision (e.g., without using 579 extra assumptions, parameters or models) but merely by simultaneously simulating the first 580 four moments (with focus on the coefficient of kurtosis) and the stochastic structure of the 581 process. To further highlight this finding, we illustrate in Fig. 12 that the HHK model alone 582 cannot simulate the observed behaviour of the high order structure function but rather 583 approaches the structure function as simulated by the K41 self-similarity model and reproduced 584 by Frisch (2006, Fig. 8.8). Similar results are obtained in case a Markov dependence structure is 585 adopted but by simultaneously preserving the empirical non-Gaussian marginal distribution. 586 Interestingly, if both the proposed dependence structure and marginal distribution are 587 588 combined, then the observed behaviour of the high order structure function is approximated

- and, as a consequence, the intermittent behaviour of turbulence. For comparison, in Fig. 12 we
- plot the She-Leveque model (1994) that behaves also exceptionally well and originates from the

<sup>591</sup> alternative assumption of independent identically distributed log-Poisson multiplicative factors



592 (Frisch, 2006, sect. 8.6.4, 8.6.5).

*Figure* 8: The empirical, true and expected values of the climacogram [upper left], CBF [upper right], CBS [lower left] and power spectrum [lower right] along with some important logarithmic slopes; and with a correlation coefficient (as a rough indicator of the goodness of fit) between the modelled and simulated values estimated as 99.99%, 99.99%, 99.56%, and 94.08%, for each metric, respectively.



*Figure* 9: Empirical and simulated skewness coefficient of the first order structure function vs.lag.







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*Figure* 11: High-order climacograms: coefficients of skewness ( $\gamma_3$ ) and kurtosis ( $\gamma_4$ ) vs. scale (empirical vs. simulated).



*Figure* 12: Empirical and simulated (through the She-Leveque model, the SMA scheme, a
Gaussian HHK model and a Markov model with the ME distribution) structure function for
various orders of the velocity increments vs. lag.

### 612 **5.** Conclusions

We present an extension of the SMA framework to include representation of high-order 613 moments and in particular the simulation of the kurtosis coefficient of the process. In this way, 614 the probability density function of any process is approximated by its first four central moments, 615 thus, according to the maximum entropy approach, yielding a probability density function that is 616 an exponentiated fourth order polynomial. In the generation phase, the approximation is 617 performed using convenient four-parameter distributions (a standardized Kumaraswamy 618 distribution for thin-tailed distributions, or a standardized Normal-Inverse-Gaussian 619 distribution for heavy-tailed ones). Application to non-Gaussian white noise with various 620 customary distributions shows that the approximation achieved is very satisfactory. 621

The presented scheme is very useful for stochastic generation as well as Monte-Carlo 622 experiments (for sensitivity analyses, for the derivation of confidence intervals etc.), especially 623 when numerous measurements exist (e.g. in laboratory experiments), while a theoretical 624 distribution cannot be easily identified but several statistical moments can be estimated. The 625 limitation of this methodology is that the marginal distribution is approximated to a desired 626 degree, rather than precisely preserved (particularly in non-divisible distributions). This 627 limitation may create difficulties in variables with upper or lower bounds, since these can be 628 only treated in an ad-hoc manner. However, this limitation rarely concern practical applications 629 630 to geophysical processes.

In this work, we apply the methodology to a long daily precipitation record, to various record
lengths of hourly surface wind time series, and to a grid-turbulence massive database. In all
applications the extended SMA scheme performs exceptionally well, additionally preserving
other important statistical characteristics of the processes such as the intermittent behaviour.
Particular emphasis has been given on turbulence, in an attempt to show that several aspects of
turbulence regarded as puzzles can be easily reproduced by a simple unpuzzling model without
a particular effort.

Additional contributions of this paper are the estimators of the dependence structure of a process, accounting for the statistical bias, in the case of the analysis of a single time series (as in the application of precipitation) and of several time series of the same process with different lengths (as in the application of wind) and identical lengths (as in the application of gridturbulence). Also, we note the very good fit of special cases of the PBF distribution to the marginal distribution of the precipitation and wind processes.

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### 650 **Code availability**

The SMA model used in this paper as well as a fast code for estimation of the climacogram for long time series, both implemented in Matlab can be downloaded from www.itia.ntua.gr/1656/. In this link, we also provide scripts for various stochastic models, such as the HK, GHK and HHK as well as the applied models in section 4 for the precipitation, wind speed and grid-turbulence processes.

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### 853 Appendix A

Here, we describe how the SMA scheme can preserve an approximation of the marginal distribution of a process through the preservation of high-order moments. Although this scheme can preserve any number of moments, here we specify the analytical solution for the preservation up to the fourth moment corresponding to kurtosis and to the fifth raw moment (for illustration). Assuming  $E[\underline{x}_i] = E[\underline{v}] = 0$ , raw moments are identical to the corresponding central moments; the  $p^{\text{th}}$  moment can be expressed through the SMA scheme as:

$$\mathbf{E}[\underline{x}_{i}^{p}] = \mathbf{E}\left[\left(\sum_{j=-l}^{l} a_{|j|} \underline{v}_{i+j}\right)^{p}\right]$$
(A-1)

Therefore, assuming also that  $E[\underline{v}^2] = 1$ , the second and third raw moments can be expressed as (Koutsoyiannis, 2000):

$$E[\underline{x}^{2}] = (a_{0}^{2} + 2\sum_{j=1}^{l} a_{j}^{2})$$
(A-2)

$$\mathbf{E}[\underline{x}^3] = (a_0^3 + 2\sum_{j=1}^l a_j^3)\mathbf{E}[\underline{v}^3]$$
(A-3)

#### 862 For a raw moment of order *p* we use the multinomial theorem:

$$\mathbf{E}[\underline{x}_{i}^{p}] = \mathbf{E}\left[\left(\sum_{j=-l}^{l} a_{|j|}\underline{v}_{i+j}\right)^{p}\right] = \sum_{k_{-l}+k_{1-l}+\dots+k_{l}=p} {p \choose k_{-l}, k_{1-l}, \dots, k_{l}} \mathbf{E}\left[\prod_{-l \leq j \leq l} {a_{|j|}\underline{v}_{i+j}}^{k_{j}}\right] \quad (A-4)$$

- 863 where  $\binom{p}{k_{-l}, k_{1-l}, \dots, k_l} = \frac{p!}{k_{-l}!k_{1-l}!\dots k_l!}$  is a multinomial coefficient.
- We notice that all combinations with  $k_j = 1$  are zero and thus, after algebraic manipulations we obtain for p = 4:

$$E[\underline{x}^{4}] = E[\underline{v}^{4}] \sum_{j=-l}^{l} a_{|j|}^{4} + 6 \sum_{j=-l}^{l-1} \sum_{k=j+1}^{l} a_{|j|}^{2} a_{|k|}^{2}$$
(A-5)

After typical manipulations we derive the expressions for the coefficients of skewness and kurtosis shown in Eqns. (10) and (11), respectively. Also, Eqn. 11 can be further simplified for faster calculations to:

$$C_{k,\nu} = \frac{C_{k,x} (a_0^2 + 2\sum_{j=1}^l a_j^2)^2 - 6\sum_{j=1}^l a_j^4 - 12a_0^2\sum_{j=1}^l a_j^2 - 24\sum_{j=1}^{l-1} (a_j^2\sum_{k=j+1}^l a_k^2)}{(a_0^4 + 2\sum_{j=1}^l a_j^4)}$$
(A-6)

with l > 1, while for l = 1 the last term of the double sum is zero.

870 For illustration, we also present the 5<sup>th</sup> raw moment as estimated from Eqn. A-1 and A-4 (above

that moment the computation requirements highly increase due to multiplication of more than

two coefficients):

$$E[\underline{x}^{5}] = E[\underline{v}^{5}] \sum_{j=-l}^{l} a_{|j|}^{5} + 10 \sum_{j=-l}^{l} \sum_{k=-l; k \neq j}^{l} a_{|j|}^{2} a_{|k|}^{3}$$
(A-7)

However, the extension to higher than the fourth moment is not required for the applications of
this paper, since as illustrated in sect. 4 through the estimation of the ME distribution, the
contribution of the fourth moment is small and even more so will be that of even higher
moments.

### 877 Appendix B

Here, we describe how we can use selected distributions as a means to preserve the desirable
statistical central moments through the SMA model. For random number generation from thintailed distributions we adopt an extended standardized version of the Kumaraswamy (1980)
distribution (abbreviated as ESK) with probability distribution function:

$$F(x; \boldsymbol{p}) := 1 - \left(1 - \left(\frac{x-c}{d}\right)^a\right)^b \tag{B-1}$$

where  $x \in [c, c + d]$ , p = [a, b, c, d], the parameters of the distribution (see also Table B-1 and B-2), with  $c, d \in \mathbb{R}$  (location and scale parameters, respectively, with units same as in x) and a, b > 0 (dimensionless shape parameters).

885 Below, we estimate several statistical characteristics of the ESK distribution such as the mean, variance, and coefficients of skewness and kurtosis, as well as the minimum and maximum 886 kurtosis as a function of skewness. A detailed analysis on the general expansion of the 887 Kumaraswamy distribution can be found in Cordeiro and Castro (2011), and Khan et al. (2016). 888 The ESK distribution has simple, analytical and closed expressions for its statistical central 889 moments. Notably, we find through numerical investigation that ESK has a low kurtosis 890 boundary based on its skewness and approximately expressed by  $C_k \ge C_s^2 + 1$ , which is also the 891 mathematical boundary for the sample skewness and kurtosis (Pearson, 1930). 892

893 The central moments of the ESK distribution can be expressed as:

$$\operatorname{E}\left[\left(\underline{x}-\mu\right)^{p}\right] = d^{p} \sum_{\xi=1}^{p+1} \left((-1)^{p+1-\xi} {p \choose \xi-1} B_{1}^{p+1-\xi} B_{\xi-1}\right)$$
(B-2)

for p > 1 and where  $\mu = c + dB_1$ ,  $\binom{p}{\xi-1}$  the binomial coefficient and  $B_{\xi} = bB(1 + \xi/a, b)$ , with B the beta function.

896 Thus, the variation, skewness and kurtosis coefficients can be expressed as:

$$C_{\rm v} = \frac{B_2 - B_1^2}{(B_1 + c/d)^2}, C_{\rm s} = \frac{2B_1^3 - 3B_1B_2 + B_3}{(B_2 - B_1^2)^{3/2}}, C_{\rm k} = \frac{-3B_1^4 + 6B_1^2B_2 - 4B_1B_3 + B_4}{(B_2 - B_1^2)^2}$$
(B-3)

respectively. After the numerical estimation of a and b, the parameters c and d can be analytically calculated as:

$$d = \sigma / \sqrt{bB\left(1 + \frac{2}{a}, b\right) - b^2 B^2\left(1 + \frac{1}{a}, b\right)}, \ c = \mu - bdB\left(1 + \frac{1}{a}, b\right)$$
(B-4)

Therefore, we can use the ESK distribution to approximate a variety of thin-tailed distributions based on the estimation of *a*, *b*, *c* and *d* parameters from data. Note that if we wish to extend the SMA model to preserve additional moments, we could similarly expand the ESK distribution to simulate two (or more) additional moments, i.e.,  $F(x; \mathbf{p}) = 1 - (1 - F(x; \mathbf{p})^{a'})^{b'}$ , with *a*' and *b*' two extra parameters.

For heavy-tailed distributions we use the standardized version of the Normal-Inverse-Gaussian
(abbreviated as NIG) distribution with probability density function (cf., Barndorff-Nielsen,
1978):

$$f(x; \mathbf{p}) \coloneqq \frac{\sqrt{a^2 + b^2} e^{b + \frac{a(x-c)}{d}}}{\pi d \sqrt{1 + \left(\frac{(x-c)}{d}\right)^2}} K_1\left(\sqrt{a^2 + b^2} \sqrt{1 + \left((x-c)/d\right)^2}\right)$$
(B-5)

where 
$$x \in \mathbb{R}$$
,  $p = [a, b, c, d]$ , the parameters of the distribution with  $c \in \mathbb{R}$ ,  $a \neq 0$  and  $b, d > 0$   
(see also Table B-1 and B-2); again  $c, d$  are location and scale parameters, respectively, with  
units same as in  $x$ , and  $a, b > 0$  are dimensionless shape parameters.

910 The NIG distribution has similar advantages to the ESK, such as closed expressions for the first 911 four central moments. Also, it enables a large variety of skewness-kurtosis combinations and its 912 random numbers can be generated almost as fast as the ESK ones through the normal variance-913 mean mixture:

$$x = c + \frac{a}{d}z + \sqrt{z}g \tag{B-6}$$

914 where

$$g \sim N(0,1), z \sim f(y; b, d) = d/\sqrt{2\pi y^3} e^{-\frac{b^2(y/d-d/b)^2}{2y}}$$
 (B-7)

915 The latter distribution is the inverse Gaussian distribution which can be easily and fast916 generated (e.g. Chhikara and Folks, 1989, section 4.5).

Below, we estimate the statistical characteristics of the NIG and we justify the use of the NIG
distribution as a heavy-tailed distribution. Note that the central moments of the NIG function
cannot be expressed as closed and analytical forms and thus, we can estimate them through the
NIG characteristic function (cf. Barndorff-Nielsen, 1978):

$$\varphi_X(t) = \mathbf{E}[\mathbf{e}^{itX}] = \mathbf{e}^{ict+b-\sqrt{b^2-i2adt+d^2t^2}}$$
(B-8)

921 where the  $p^{\text{th}}$  raw moment corresponds to:

$$\mathbf{E}[X^p] = (-i)^p \lim_{t \to 0} \left( \frac{\mathrm{d}^p \varphi_X(t)}{\mathrm{d}t^p} \right). \tag{B-9}$$

#### 922 Particularly, the first moment and the sequent three central moments are given by:

$$\mu = c + ad/b \tag{B-10}$$

$$E\left[\left(\underline{x} - \mu\right)^{2}\right] = (a^{2} + b^{2})d^{2}/b^{3}$$
(B-11)

$$E\left[\left(\underline{x}-\mu\right)^{3}\right] = \frac{3a\left((a^{2}+b^{2})d^{2}/b^{3}\right)^{3/2}}{\sqrt{b(a^{2}+b^{2})}}$$
(B-12)

$$E\left[\left(\underline{x}-\mu\right)^{4}\right] = \frac{3\left((a^{2}+b^{2})d^{2}/b^{3}\right)^{2}}{b}\left(1+\frac{4}{1+(b/a)^{2}}\right) + 3\left((a^{2}+b^{2})d^{2}/b^{3}\right)^{2}$$
(B-13)

923 After algebraic manipulations the coefficients of variation, skewness and kurtosis can be924 expressed as:

$$C_{\rm v} = \frac{a^2 + b^2}{b(a + bc/d)^2}, C_{\rm s} = \frac{3a}{\sqrt{b(a^2 + b^2)}}, C_{\rm k} = \frac{3}{b} \left( 1 + \frac{4}{1 + (b/a)^2} \right) + 3$$
(B-14)

#### 925 respectively. The NIG parameters can then be calculated from these equations as:

$$d = \frac{3\sigma\sqrt{3c_{k} - 5c_{s}^{2} - 9}}{3c_{k} - 4c_{s}^{2} - 9}, b = \frac{d}{\sigma}\sqrt{\frac{3}{c_{k} - \frac{5}{3}c_{s}^{2} - 3}}, a = \frac{b^{2}c_{s}\sigma}{3d}, c = \mu - ad/b$$
(B-15)

Also, we can derive theoretically the minimum kurtosis of NIG for a given skewness:

$$C_{\rm k} \ge \frac{5}{3} C_{\rm s}^2 + 3$$
 (B-16)

927 with the equality holding only for the limit where the NIG tends to the normal distribution.

For the classification of tails we use the test based on the functions proposed by Klugman (1998,
sect. 3.4.3; see also Halliwell, 2013) and here defined as:

$$\tau_{\mathbf{r}} \coloneqq -\lim_{x \to \infty} \left( \frac{\mathrm{d}f(x; p)}{f(x; p) \mathrm{d}x} \right), \tau_{\mathbf{l}} \coloneqq \lim_{x \to -\infty} \left( \frac{\mathrm{d}f(x; p)}{f(x; p) \mathrm{d}x} \right)$$
(B-17)

930 After calculations we get:

$$\tau_{\rm r} = \sqrt{a^2 + b^2}/d - a/d \ge 0, \tau_{\rm l} = \sqrt{a^2 + b^2}/d + a/d \ge 0 \tag{B-18}$$

and hence, the NIG is expected to represent a large variety of heavy-tailed distributions.

Note that again, if we wish to extend the SMA model to preserve additional moments through
the NIG distribution, we could similarly expand the normal variance-mean mixture to simulate
two additional moments, i.e.:

$$x = c + \frac{a}{d}z' + a'\sqrt{z'}g \tag{B-19}$$

with a' an extra parameter and z' the so-called generalized inverse Gaussian distribution.

In Fig. B-1 and B-2, we observe that the smaller possible kurtosis of the ESK distribution for a 936 given skewness coincides with the theoretical limit defined by Pearson (1930). Also, the larger 937 kurtosis of the ESK includes a variety of sub-Gaussian and thin-tailed distributions. On the 938 contrary, the smaller kurtosis of the NIG distribution is very close to the larger one of the ESK 939 and thus, it can include (as shown above) a variety of heavy-tailed distributions. Note that these 940 two distributions are chosen to simulate unbounded processes (NIG) and bounded between two 941 real values (ESK). We could easily find similar distributions for upper (or lower) bounded 942 processes as, for example, the generalized Kumaraswamy or hypergeometric ones. 943



#### 

*Figure* B-1: Combinations of skewness and kurtosis coefficients for various two-parameter
(Weibull, GEV, lognormal, generalized normal I, skew-exponential-power —SEP— and gamma),
three-parameter (generalized normal II and skew normal) and the four-parameter Pareto-BurrFuller (PBF, further described in section 4) distribution functions along with the thin-heavy
tailed separation based on the ESK and NIG functions, respectively.





954	able B-1: Mean, variance, and coefficients of skewness and kurtosis for the ESK and N	IIG
955	istributions. Note that $B_i = bB(1 + i/a, b)$ , where $B(x, y)$ is the beta function and <i>i</i> an integer.	

	ESK	NIG
μ	$c + dB_1$	c + ad/b
$\sigma^2$	$d^2(B_2-B_1^2)$	$\frac{(a^2+b^2)d^2}{b^3}$
Cs	$\frac{2B_1^{3} - 3B_1B_2 + B_3}{\left(B_2 - B_1^{2}\right)^{3/2}}$	$\frac{3a}{\sqrt{b(a^2+b^2)}}$
C <sub>k</sub>	$\frac{-3B_1^4 + 6B_1^2 B_2 - 4B_1 B_3 + B_4}{\left(B_2 - B_1^2\right)^2}$	$\frac{3}{b}\left(1+\frac{4}{1+(b/a)^2}\right) + 3$
min C <sub>k</sub>	$\approx C_{\rm s}^{2} + 1$	$=\frac{5}{3}C_{s}^{2}+3$
$\max C_k$	$\approx \frac{5}{3}C_{s}^{2} + 3^{*}$	+∞

\* This is a fair approximation only for  $C_s \le -2$ . A more exact but empirical approximation for  $-10 \le C_s \le 10$ , can be given by:  $0.039C_s^3 + 1.724C_s^3 + 0.032C_s^3 + 2.7$ . Note that the maximum kurtosis for the ESK for a given skewness approximately coincides with the kurtosis of the Weibull distribution (Fig. B-1).

960

961 *Table* B-2: Parameters of the ESK and NIG distributions in terms of the mean, standard deviation,962 and coefficients of skewness and kurtosis (see also Fig. B-2).

distribution	ESK	NIG
а	non- analytical *	$\frac{b^2 C_{\rm s} \sigma}{3d}$
b	non- analytical *	$\frac{d\sqrt{3}}{\sigma\sqrt{C_{\rm k}-\frac{5}{3}C_{\rm s}^2-3}}$
С	$\mu - dB_1$	$\mu - ad/b$
d	$\frac{\sigma}{\sqrt{\left(B_2-{B_1}^2\right)}}$	$\frac{3\sigma\sqrt{3C_{\rm k}-5{C_{\rm s}}^2-9}}{3C_{\rm k}-4{C_{\rm s}}^2-9}$

\*The two parameters of the ESK distribution *a* and *b* can be estimated by solving numerically the two following equations:  $C_s = (2B_1^3 - 3B_1B_2 + B_3)/(B_2 - B_1^2)^{3/2}$  and  $C_k = (-3B_1^4 + 6B_1^2B_2 - 4B_1B_3 + B_4)/(B_2 - B_1^2)^2$ .

In case additional moments need to be preserved, a more generalized methodology includes theuse of the ME distribution, which can be applied for any type of distribution (see Eqn. 12-13):

$$f(x; \boldsymbol{\lambda}) := \frac{1}{\lambda_0} e^{-\left(\frac{x}{\lambda_1} + \operatorname{sign}(\lambda_2)\left(\frac{x}{\lambda_2}\right)^2 + \left(\frac{x}{\lambda_3}\right)^3 + \operatorname{sign}(\lambda_4)\left(\frac{x}{\lambda_4}\right)^4 + \left(\frac{x}{\lambda_3}\right)^5 + \operatorname{sign}(\lambda_6)\left(\frac{x}{\lambda_6}\right)^6 + \dots + \left(\frac{x}{\lambda_m}\right)^m}\right)$$
(B-20)

968 where  $\lambda = [\lambda_0, \lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \lambda_6, ..., \lambda_m]$ , (where *m* even) with  $\lambda_0, \lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \lambda_6, ..., \lambda_m$ 969 having same units as *x* and with *m* + 1 constraints, where *m* is the number of moments we wish 970 to preserve:

$$\int_{-\infty}^{\infty} x^r f(x; \lambda) dx = \mathbf{E}[\underline{x}^r], \text{ for } r = 0, ..., m$$
(B-21)

For the generation scheme of the above distribution, we may use the random number generator described in the next steps. After we estimate the  $\lambda$  parameters of the MED we can rewrite the above equation as:

$$f'(x; \lambda') := \lambda'_{0} e^{-((\lambda'_{1}x + \lambda'_{2})^{2} + (\lambda'_{3}x + \lambda'_{4})^{4} + (\lambda'_{5}x + \lambda'_{6})^{6} + \cdots)}$$
(B-22)

with exactly the same number of unknown parameters (note that an exact solution for  $\lambda'$  always exists).

976 After we estimate the new parameters  $\lambda'$  we can approximate the above distributions with an 977 auxiliary distribution function for an even *m*:

$$g(x; \boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}, \boldsymbol{d}) = \begin{cases} c_1 e^{-(a_1 x + b_1)^2}, d_1 < x < d_2 \\ c_2 e^{-(a_2 x + b_2)^4}, d_3 < x \le d_1, d_2 \le x < d_4 \\ c_3 e^{-(a_3 x + b_3)^6}, d_5 < x \le d_3, d_4 \le x < d_6 \\ \cdots \end{cases}$$
(B-23)

where  $a = [a_1, a_2, a_3, ...]$ ,  $b = [b_1, b_2, b_3, ...]$ ,  $c = [c_1, c_2, c_3, ...]$  and  $d = [d_1, d_2, d_3, ...]$  with the last two *d* parameters to be  $-\infty$  and  $+\infty$ , respectively. The above distribution is subjected to the constraint  $\int_{-\infty}^{\infty} g(x; a, b, c, d) dx = 1$ , and continuity in all its branches.

After the estimation of all the parameters through optimization techniques (so as g to be as close as possible to f') we can use the rejection method (Papoulis, 1990, pp. 261-263) to generate random number for the MED. Note that for the generation of each branch function of the gdistribution, we can use the random number generator of the powered-exponential distribution function through the generation of the gamma distribution function (the latter can be also generated using the rejection method as described in Koutsoyiannis and Manetas, 1996).

### 987 Appendix C

Here we describe how the SMA model can be used to cope with non-stationary processes. The general idea is to convert non-stationary processes to stationary ones, so that eventually the

simulation is made for a stationary process (Dimitriadis, 2017). This conversion is achieved by 990 appropriate transformations or by separating them into segments, as for example in the case of 991 cyclostationary processes. While in the recent literature there is no shortage of publications 992 seeking or assuming non-stationarity, this may just reflect incomplete understanding of what 993 stationarity is (Koutsoyiannis and Montanari, 2015). A common confusion is that non-994 stationarity is regarded as a property of the natural process, while in fact it is a property of a 995 mathematical (stochastic) process. In non-stationary processes some of the statistical properties 996 change in time in a deterministic manner. The deterministic function describing the change in 997 the statistical properties is rarely known in advance and, in studies claiming non-stationarity, is 998 typically inferred from the data. However, it is impractical or even impossible to properly fit a 999 non-stationary mathematical process to time series, as in nature only one time series of 1000 observations of a certain process is possible, while the definition of stationarity or non-1001 1002 stationarity relies on the notion of an ensemble of time series.

A simple example of how we can deal with a non-stationary process through a stationary one 1003 follows. We consider an HK process (denoted as <u>x</u>) with  $H = 0.8 \mu = 0$  and  $\sigma = 1$  and by 1004 aggregation we also take the cumulative process (denoted as  $\underline{y}_i$  i.e.  $\underline{y}_i = \underline{y}_{i-1} + \underline{x}_i$ ). Figure C-1 1005 shows a time series generated from <u>x</u> and the corresponding time series from <u>y</u>. Clearly, <u>x</u> is 1006 stationary and  $\underline{v}$  is non-stationary (the so-called fractional Brownian noise). If we have the 1007 1008 information about the theoretical basis of the two processes, then it is trivial to correctly model 1009 them (Koutsoyiannis, 2016). In particular, we will know that the mean of the process  $\underline{v}$  is constant (zero, not a function of time) while its variance is an increasing function of time (a 1010 1011 power-law function of *i*). Otherwise, if the only available information is the time series of *y*, then 1012 we may be tempted to assume a linear trend for the mean of  $\underline{y}$  and express the mean of the 1013 process as a linear function of time,  $\underline{\mu}_i = a \underline{i} + b$  (with *a* and *b* the parameters of the slope and intercept of a regression line on the time series). This, however, would be plain wrong as in fact 1014 1015 (by construction) the mean of  $\underline{y}$  is zero for any time *i*. In addition, the introduction of the two extra parameters (i.e.,  $\underline{a}$  and b) has negative implications in terms of the overall uncertainty of 1016 the model, which would cease to be parsimonious. But again, even with this wrong assumption, 1017 the next step would be to construct a stationary model, i.e.,  $\underline{z}_i = \underline{y}_i - a\underline{i} - b$  and use that model in 1018 simulations. The correct approach for this case would be to construct the time series of  $\underline{x}$  by 1019 differentiation of <u>y</u> (i.e.,  $\underline{x}_i = \underline{y}_i - \underline{y}_{i-1}$ ), which is stationary, and use the stationary process <u>x</u> for 1020 stochastic simulation; then a synthetic time series of the non-stationary process  $\underline{y}$  will be 1021 1022 constructed from a time series of x. Thus, in all cases, whether with correct or incorrect assumptions, the stochastic simulation is always done for a stationary process. 1023





### 1026 Appendix D

1024

The first applied generic schemes for a stochastic synthesis are the implicit ones, i.e. those 1027 approximating the distribution and dependence structure of a process through non-linear 1028 1029 transformations. These non-linear transformations (or else known as copula, Hoeffding, 1940; 1030 Frechet, 1951; Sklar, 1959; Nelsen, 2006, and references therein) are often based on the 1031 autocovariance function for any distribution function, where the uniform is usually preferred for reasons of simplicity, whereas for reasons of flexibility the Gaussian distribution (the so-called 1032 Gaussian-copula; Lebrun and Dutfoy, 2009) can be also used (for the bivariate Gaussian copula 1033 1034 see Nataf, 1962; Serinaldi and Lombardo, 2017a, Tsoukalas et al., 2018; Papadopoulos and Giovanis, 2018; and references therein). This scheme is also known as Nataf transformation, but 1035 here we propose to use the name Hoeffding-Frechet-Sklar-Nataf (HFSN) transformation, since 1036 1037 Nataf wrote a half-page conference paper (presented by Frechet) just mentioning (without further analyzing it) a specific case of the general methodology earlier discussed by Hoeffding, 1038 Frechet and Sklar. The general HFSN transformation can be written as: 1039

$$\rho_{x_i x_j} \sigma^2 + \mu^2 = \mathbb{E}[\underline{x_i x_j}] = \mathbb{E}\left[T\left(\underline{y_i}\right)T\left(\underline{y_j}\right)\right]$$
$$= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} T(y_i)T(y_j)f\left(y_i, y_j; \rho_{y_i y_j}\right) dy_i dy_j$$
(D-1)

1040 where  $\rho_{x_i x_j}$  and  $\rho_{y_i y_j}$  are the cross-correlations between  $x_i$  and  $x_j$  as well as  $y_i$  and  $y_j$ , 1041 respectively;  $\mu$  and  $\sigma$  are the process mean and standard deviation;  $f(y_i, y_j; \rho_{y_i y_j})$  is the joint 1042 distribution between  $y_i$  and  $y_j$ ;  $T(y_i)$  and  $T(y_j)$  are the transformations of the original known 1043 distribution of  $x_i$  and  $x_j$  to the selected distribution of  $y_i$  and  $y_j$ , respectively (see below for an example of such transformations). In case that  $\underline{y}$  is for example N(0,1) distributed, the bivariate

1045 N(0,1) is used, i.e. 
$$f(y_i, y_j; \rho_{y_i y_j}) = e^{-1/2(y_i^2 + y_j^2 - 2y_i y_j \rho_{y_i y_j})/(1 - \rho_{y_i y_j}^2)} / (2\pi (1 - \rho_{y_i y_j}^2)^{1/2})$$

Similar implicit schemes are developed based on the power spectrum (Cugar, 1968; Lavergnat,
2016 and references therein). This implicit scheme can be also introduced through the
climacogram, i.e.:

$$\gamma_{x}(k) + \mu^{2} = \mathbb{E}\left[\left(\underline{x}^{(k)}\right)^{2}\right] = \mathbb{E}\left[\left(T\left(\underline{y}\right)^{(k)}\right)^{2}\right]$$
$$= \frac{1}{k^{2}} \int_{-\infty}^{+\infty} \left(\int_{0}^{k} T(y(t)) dt\right)^{2} f^{(k)}\left(y; \gamma_{y}(k)\right) dy$$
(D-2)

1049 where  $\underline{x}^{(k)} \coloneqq \frac{1}{k} \int_0^k \underline{x}(t) dt$  is the averaged process of the continuous-time process  $\underline{x}(t)$ ,  $\mu$  is the 1050 process mean, and  $T(\underline{y})$  is a transformation function of the original process  $\underline{y}$  (with the selected 1051 uniform, Gaussian etc. distribution function and with an unknown  $\gamma_y$  dependence structure) to 1052 the desired one  $\underline{x}$  (with known density distribution f(x) and dependence structure  $\gamma_x$  adjusted 1053 for bias). For example, a  $\underline{y} \sim N(0,1)$  can be easily transformed to a  $\underline{x} \sim F(x) = 1 - (a/x)^b$  by 1054  $\underline{x}(t) = T(\underline{y}(t)) = a/(1 - (1/2(1 + \operatorname{erf}(\underline{y}(t)/\sqrt{2})))^{1/b}).$ 

The climacogram-implicit scheme has been applied to several (stationary and single/double 1055 cyclostationary) processes ch as solar radiation (Koudouris et al., 2017), wave height and 1056 wind process for renewable energy production (Moschos et al., 2017), as well as for the wind 1057 1058 speed using a special case of the PBF distribution (Deligiannis et al., 2016) but also a generalized 1059 non-linear transformation (equivalent to a distribution function) based on the maximization of entropy when the distribution function is unknown (Dimitriadis and Koutsoyiannis, 2015b). 1060 Note that in all the above applications same dependence structure is used for the original 1061 and the transformed process, since a small deviation between is noticed and therefore, 1062 additional trials considered not necessary. 1063

A difficulty with the implicit schemes is that they involve non-linear transformations and double 1064 integration (both of which may highly increase the numerical burden, even though fast 1065 algorithms have been discussed by Serinaldi and Lombardo, 2017b). Several exact solutions of 1066 1067 the implicit scheme may exist even though an exact solution may not be possible for some processes (especially in very strong correlation structure as is the case in the small scales 1068 related to the fractal behaviour). Furthermore, there is no guarantee that the resulting 1069 autocorrelation structure of the transformed process will be symmetric positive definite 1070 (Lebrun and Dutfoy, 2009). In addition to the above, the transformation cannot be invariant with 1071 respect to the time lag or time scale, while the fractal and HK behaviour cannot be easily handled 1072 since the transformation is invariant with respect to the zero and infinite time scale. Some of 1073 these limitations can be dealt with through cautiously constructed binary scheme, a 1074 multivariate Gaussian (or with other distribution such as the uniform one) copula scheme, a 1075 Monte-Carlo approach to identify the unknown dependence structure, or a properly handled 1076 disaggregation scheme for generating events of the process or more generally, by adjusting any 1077 desired stochastic properties (dependence structure and distribution function) to each scale 1078 (Lombardo et al., 2017). 1079

However, three of these problems concerning the implicit schemes can be easily dealt by the 1080 proposed explicit scheme. Namely, these are (a) the inability of simulating the effect of the 1081 fractal behaviour of a process at small scales, in which the correlation structure is very strong, 1082 (b) the difficulties in preserving long-term persistence, and in particular its variability (see 1083 below) and (c) the effect of the statistical bias (Dimitriadis, 2017, sect. 2.4.5). In the first two 1084 problems the implicit schemes simulate the fractal and HK behaviour and bias of the non-linear 1085 transformation process  $T(\underline{y})$ , i.e.  $f(T(y_i), T(y_j); \rho_{T(y_i)T(y_j)})$ , which due to discretization and 1086 finite length are not equal to the ones of the infinite length size continuous-time process, i.e. 1087  $f(y_i, y_j; \rho_{y_i y_j})$ . Because of the theoretical origins of these two limitations the implicit schemes 1088 are only theoretically valid for processes with short-term persistence and no fractal behaviour 1089 1090 (i.e., H = M = 0.5), and can be used for long-term processes with fractal behaviour only as a rough 1091 approximation.

1092 For illustration, we present a simple example to highlight the above problems related to the implicit schemes such as the simplest case of the HFSN transformation. Particularly, we generate 1093 1094 (through the SMA scheme) data from a N(0,1) distribution with an HHK dependence structure (q 1095 = 10, M = 1/3, H = 5/6) and we transform them to a Pareto II distribution (a = b = 10) through its 1096 inverse distribution function. Subsequently, we estimate (through Monte-Carlo techniques) the expected climacogram of the transformed process and we perform separately a sensitivity 1097 analysis (as in Dimitriadis et al., 2016a) for the original (Gaussian-HHK) and transformed 1098 Pareto-HHK (q = 6.538, M = 0.431, H = 0.832) processes (Figure D-1). Furthermore, we simulate 1099 the same transformed process but now using the explicit scheme proposed in this paper with 1100 just four moments (Figure D-1). Finally, we compare the differences between the two methods 1101 in the simulation of the fractal and HK behaviour as well as of the distribution function. We 1102 observe that the variances of the sample variance of the two schemes are very different 1103 (although their mean values coincide) and that the implicit scheme overestimates it (by a factor 1104 of 10). Note that the true variance of the sample variance corresponds to that of the explicit 1105 scheme, since it explicitly preserves both the climacogram and the coefficient of kurtosis and 1106 thus, can approximate all the arising moments through the SMA scheme, such as regular 1107 moments (i.e.  $E[X], E[X^2]$  and  $E[X^4]$ ) but also joint moments (i.e.  $E[X_iX_i^2]$  and  $E[X_i^2X_i^2]$ ), which are 1108 all function of a combination of the SMA weight coefficients and the marginal moments of the 1109 white noise process (that are both exactly preserved through the explicit scheme). We believe 1110 that the reason why this is not identified in some of the recent literature is probably because all 1111 1112 applications of the second-order implicit schemes are based solely on the preservation of the expected (mean) value of the dependence structure and not additionally on its variance (or its 1113 distribution in general) for each scale. This can be dealt by higher-order (more than two) copula 1114 schemes (or by selecting other distributions, such as the uniform one, for the transformation) 1115 but some difficulties may still remain (see above for three major ones). 1116



Figure D-1: Mean, 5%, 95% [left] and variance [righr] of the sample climacogram for the implicit and explicit (preserving four moments) scheme of a Pareto II (a = b = 10) and HHK (q = 6.538, M= 0.431, H = 0.832) process.

1121