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Innovative Digital Stochastic Methods for Multidimensional Sensitivity Analysis in Air Pollution Modelling

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Abstract: Nowadays, much of the world has a regional air pollution strategy to limit and decrease the pollution levels across governmental borders and control their impact on human health and ecological systems. Environmental protection is among the leading priorities worldwide. Many challenges in this research area exist since it is a painful subject for society and a fundamental topic for the healthcare system. Sensitivity analysis has a fundamental role during the process of validating a large-scale air pollution computational models to ensure their accuracy and reliability. We apply the best available stochastic algorithms for multidimensional sensitivity analysis of the UNI-DEM model, which plays a key role in the management of the many self-governed systems and data that form the basis for forecasting and analyzing the consequences of possible climate change. We develop two new highly convergent digital sequences with special generating matrices, which show significant improvement over the best available existing stochastic methods for measuring the sensitivity indices of the digital ecosystem. The results obtained through sensitivity analysis will play an extremely important multi-sided role.



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1. Introduction

Mathematical models [1,2] are utilized in many areas as compelling instruments for studying composite processes, but our understanding is generally restricted by uncertainties: inexact data, imperfect understanding, and subjective estimates, etc. Because of that, tools are necessary to estimate how uncertainties [3] in the input affect certain output model results.

The goal of our work is in the field of environmental security [4–6]. To establish itself as a reliable simulation tool, modern mathematical models of remote transport of air pollutants should involve lots of chemical and photochemical reactions [7]. Monte Carlo algorithms [8–11] are the best apparatus for multidimensional air pollution modeling [6].

By definition, Sensitivity analysis (SA) [12–15] is the study of how much the uncertainty in the input data of a model (because of inaccurate evaluations, estimations, and data compression, etc.) is reflected in the accuracy of the output results.

SA is a powerful procedure that verifies and improves the mathematical models [16,17]. It specifies the key role of SA when mathematical modeling is frequently the only strategy to investigate a complicated phenomenon. Furthermore, the authentic explanation of SA calculations relies on the effectiveness of methods supplying SA.

The input data for SA has been derived during runs of a large-scale model of long-range transport of pollutants in the air—Unified Danish Eulerian Model (UNI-DEM) [18–21]),

which includes a large geographical region (4800 × 4800 km) covering the whole Mediterranean, Europe, and parts of Asia and Africa.

The main physical, chemical and photochemical processes between the investigating species, contaminations, and rapidly changing meteorological conditions are taken into account by UNI-DEM. The reason for selecting it is because, in UNI-DEM, the chemical processes are taken into account in a very precise way. UNI-DEM is described mathematically [19,21] by the following system of partial differential equations:

$$\begin{aligned} \frac{\partial c_s}{\partial t} = & -\frac{\partial(uc_s)}{\partial x} - \frac{\partial(vc_s)}{\partial y} - \frac{\partial(wc_s)}{\partial z} \\ & + \frac{\partial}{\partial x} \left(K_x \frac{\partial c_s}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial c_s}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial c_s}{\partial z} \right) \\ & + E_s + Q_s(c_1, c_2, \dots, c_q) - (k_{1s} + k_{2s})c_s, \quad s = 1, 2, \dots, q, \end{aligned}$$

where

c_s —pollutant concentrations,

u, v, w —wind components along the coordinate axes,

K_x, K_y, K_z —diffusion coefficients,

E_s —space emissions,

k_{1s}, k_{2s} —dry and wet deposit coefficients, ($s = 1, \dots, q$),

$Q_s(c_1, c_2, \dots, c_q)$ —nonlinear functions expressed the reactions between pollutants.

A fundamental role in UNI-DEM is played by the chemical reactions, and they connect the equations in the model in the system precisely. The presence of chemical processes determines the nonlinearity and the ‘stiffness’ property of the system of equations (see [7]). The model’s chemical scheme is the condensed CBM-IV (Carbon Bond Mechanism) proposed in [1] and improved in [19]. UNI-DEM involves 35 pollutants and 116 chemical reactions—69 are time-dependent and 47 are time-independent.

Let us assume that the model can be introduced by a model function [22]:

$$u = f(x), \quad x = (x_1, x_2, \dots, x_d) \in U^d \equiv [0; 1]^d.$$

The concept of the Sobol approach is given by the following representation of $f(x)$ and a constant f_0 [22]:

$$f(x) = f_0 + \sum_{v=1}^d \sum_{l_1 < \dots < l_v} f_{l_1 \dots l_v}(x_{l_1}, x_{l_2}, \dots, x_{l_v}). \tag{1}$$

The description (1) is noted to as the ANOVA-representation of $f(x)$ if [22]:

$$\int_0^1 f_{l_1 \dots l_v}(x_{l_1}, x_{l_2}, \dots, x_{l_v}) dx_{l_k} = 0, \quad 1 \leq k \leq v, \quad v = 1, \dots, d.$$

It guarantees that the right-hand side functions of (1) are determined in a distinctive way, where $f_0 = \int_{U^d} f(x) dx$. The quantities

$$D = \int_{U^d} f^2(x) dx - f_0^2, \quad D_{l_1 \dots l_v} = \int f_{l_1 \dots l_v}^2 dx_{l_1} \dots dx_{l_v}$$

are called total and partial variances [22]. An analogical decomposition is fulfilled for the total variance:

$$D = \sum_{v=1}^d \sum_{l_1 < \dots < l_v} D_{l_1 \dots l_v}.$$

Sobol global sensitivity indices [22,23] are determined by:

$$S_{l_1 \dots l_v} = \frac{D_{l_1 \dots l_v}}{D}, \quad v \in \{1, \dots, d\}.$$

Then the total sensitivity index (TSI) of input parameter $x_i, i \in \{1, \dots, d\}$ is determined by [24]:

$$TSI(x_i) = S_i + \sum_{l_1 \neq i} S_{il_1} + \sum_{l_1, l_2 \neq i, l_1 < l_2} S_{il_1 l_2} + \dots + S_{il_1 \dots l_{d-1}},$$

where $S_{il_1 \dots l_{j-1}}$ is the j -th order SI for $x_i (2 \leq j \leq d)$.

By definition [13], if $j = 1$, then the quantity S_i is named *the main effect* of x_i ; if $j = 2$, then S_{ij} are named *two-way interactions (second-order SIs)*; if $j = 3$, then S_{ijk} are the *three-way interactions (third-order SIs)* and so on. The set of input parameters is categorized with respect to their TSI [13]: very important if $0.8 < TSI$; important if $0.5 < TSI < 0.8$; unimportant if $0.3 < TSI < 0.5$ and irrelevant if $TSI < 0.3$.

To introduce the *total* sensitivity of the output variance to an input parameter $x_i, i \in \{1, \dots, d\}$ one can exhibited its TSI: $S_{T_i} = S_i + \sum_{j \neq i} S_{ij} + \sum_{j \neq i, k \neq i, j < k} S_{ijk} + \dots$ (see [2]).

Therefore, performance SA using Sobol’s approach is turned into a problem for high-dimensional numerical integration [25].

2. Algorithms and Methods

Let us examine the following high-dimensional problem:

$$S(f) := I = \int_{U^s} f(x) dx, \tag{2}$$

$x \equiv (x_1, \dots, x_d) \in U^s \subset \mathbb{R}^s$ and $f \in C(U^s)$.

Let $0 \leq t \leq m$ be two integers. By definition [26,27], an elementary s -interval in base b as a subset of U^s of the form $E^s = \prod_{j=1}^s \left[\frac{a_j}{b^{d_j}}, \frac{a_j+1}{b^{d_j}} \right], a_j, d_j \geq 0, a_j < b^{d_j}$ for all $j \in \{1, \dots, s\}$. A (t, m, s) -net in base b is a sequence $x^{(i)}$ of b^m points of U^s such that $Card E \cap \{x^{(1)}, \dots, x^{(b^m)}\} = b^t$ of $\lambda(E) = b^{t-m}$. A (t, s) -sequence in base b is an infinite points sequence $x^{(i)}$ in such a way that for all $k \geq 0, m \geq t$, the sequence $\{x^{(kb^m)}, \dots, x^{((k+1)b^m-1)}\}$ is a (t, m, s) -net in base b .

I. M. Sobol [26] determines the Π_τ -meshes and $\Lambda\Pi_\tau$ sequences, which are (t, m, s) -nets and (t, s) -sequences in base 2, introduced in 1988 by H. Niederreiter [27].

Now let us introduce the first algorithm that we are going to use; the well-known Sobol sequence (SOBOL-SEQ) [28,29]. To generate its j -th component, we will choose a polynomial: $P_j = x^{s_j} + a_{1,j}x^{s_j-1} + a_{2,j}x^{s_j-2} + \dots + a_{s_j-1,j}x + 1$, and $a_{1,j}, \dots, a_{s_j-1,j}$ are either 0 or 1. The sequence $\{m_{1,j}, m_{2,j}, \dots\}$ is defined by

$$m_{k,j} = 2a_{1,j}m_{k-1,j} \oplus 2^2a_{2,j}m_{k-2,j} \oplus \dots \oplus 2^{s_j}m_{k-s_j,j} \oplus m_{k-s_j,j}$$

\oplus is the bit-by-bit *exclusive-or* operator. For the merits $m_{1,j}, \dots, m_{s_j,j}$ is fulfilled in that every $m_{k,j}2^k, 1 \leq k \leq s_j$ is odd. The direction numbers $\{v_{1,j}, v_{2,j}, \dots\}$ are determined with $v_{k,j} = \frac{m_{k,j}}{2^k}$. Then the j -th component of the i -th point in a SOBOL-SEQ, is determined with $x_{i,j} = i_1v_{1,j} \oplus i_2v_{2,j} \oplus \dots$, where i_k is the k -th binary digit of $i = (\dots i_3i_2i_1)_2$. For generating the SOBOL-SEQ, the algorithm with Gray code implementation [30] and SIMD-oriented Fast Mersenne Twister (SFMT) [31] has been used.

We now briefly describe the three algorithms based on modified Sobol sequences. They produced the best results for the problem under consideration up to now [32]. We use the shortcut **MCA-MSS** for the Monte Carlo algorithms based on Modified Sobol Sequences.

In the first algorithm **MCA-MSS-1** [32], we choose a Sobol point (SP) x and a pseudo-random point (p.p.) $\xi \in U^s$ uniformly distributed (u.d.) over the sphere. The sphere has a centrum x and a radius $\rho < 1$. If the i -th SP is

$$x_i = (x_{i,1}, x_{i,2} \dots x_{i,d}) \in \mathbf{E}_i^s, \quad i = 1, \dots, n,$$

then $\xi_i(\rho)$ with a p.d.f. $p(x)$ is determined in the following way

$$\xi_i(\rho) = x_i + \rho\omega_i,$$

where ω_i is a unique u.d. vector in U^s and ρ is the *shaking* radius.

It is assumed that $n = m^s, m \geq 1$. The unit cube U^s is divided into m^s disjoint sub-domains:

$$U^s = \bigcup_{j=1}^{m^s} K_j, \quad \text{where } K_j = \prod_{i=1}^s [a_i^{(j)}, b_i^{(j)}],$$

with $b_i^{(j)} - a_i^{(j)} = \frac{1}{m}$ for all $i = 1, \dots, s$.

Now in every s -dimensional sub-domain K_j exactly one $\Lambda\Pi_\tau$ point $x^{(j)}$ is taken and $\xi^{(j)}(\rho) = x^{(j)} + \rho\omega^{(j)} \in K_j$. Then **MCA-MSS-1** gives the following approximate value of (2):

$$I(f) \approx \frac{1}{m^s} \sum_{j=1}^n f(\xi^{(j)}).$$

For the second algorithm **MCA-MSS-2** [33], two SP $\xi^{(j)}$ and $\xi^{(j)'}$ are taken so that $\xi^{(j)}$ is chosen in the same way as used in **MCA-MSS-1**. The $\xi^{(j)'}$ is selected to be symmetric to $\xi^{(j)}$ in correspondence with the central point $s^{(j)}$ in K_j . Now there are exactly $2m^d$ points. Now, we evaluate all $f(\xi^{(j)})$ and $f(\xi^{(j)'})$, for $j = 1, \dots, m^d$, and **MCA-MSS-2** gives the following approximate value of (2):

$$I(f) \approx \frac{1}{2m^s} \sum_{j=1}^{2n} [f(\xi^{(j)}) + f(\xi^{(j)'})].$$

For **MCA-MSS-1** and **MCA-MSS-2**, the Box–Muller transform is applied for the s -dimensional vector y [34]: if s is even, then

$$y_{2i-1} = \sqrt{-2 \ln \gamma_{2i-1}} \cos (2 \pi \gamma_{2i}), \quad y_{2i} = \sqrt{-2 \ln \gamma_{2i-1}} \sin (2 \pi \gamma_{2i}), \quad i = 1, \dots, s/2,$$

and γ is a random point in $(0, 1)^s$. Therefore, a random point ξ over the s -dimensional sphere is determined by $\xi = x + \rho y / |y|$.

In the third algorithm **MCA-MSS-2-S** [35], the original domain of integration is divided into m^s disjoint subdomains with equal volumes $\mathbf{K}_i^s, i = 1, \dots, m^s$. Now, the first p.p. ξ_i is generated u.d. inside the subdomain \mathbf{K}_i^s . The second point ξ_i' is computed to be symmetric to ξ_i in correspondence with the central point s_i in \mathbf{K}_i^s . This is similar to **MCA-MSS-2** as the *shaking* is with different radiuses ρ in each subdomain. This algorithm is similar to the stratified symmetrized Monte Carlo [26], which is why we use the notation **MCA-MSS-2-S**. The value of (2) obtained approximately with **MCA-MSS-2-S** is given by:

$$I(f) \approx \frac{1}{2m^s} \sum_{i=1}^{m^s} [f(\xi_i) + f(\xi_i')].$$

The algorithms **MCA-MSS-2** and **MCA-MSS-2-S** have an optimal rate of convergence $(n^{-\frac{1}{2} - \frac{2}{s}})$ for the class of continuous functions with continuous first derivatives and bounded second derivatives [35].

Now to introduce lattice rules, let $\mathbf{z} \in N^s$, and N is a natural number. By definition [36], the point set $P = \mathbf{x}_1, \dots, \mathbf{x}_N$ in U^s with $\mathbf{x}_k = k\mathbf{z}/N$ for all $1 \leq k \leq N$ is named a lattice point set and \mathbf{z} is named its generating vector. The algorithm that uses a lattice point set is named a lattice sequence [37].

We will use this rank-1 lattice sequence [38]:

$$\mathbf{x}_k = \left\{ \frac{k}{N} \mathbf{z} \right\}, k = 1, \dots, N,$$

where $N \geq 2$ is an integer, $\mathbf{z} = (z_1, z_2, \dots, z_s)$ is the generating vector and $\{z\}$ denotes the fractional part of z .

There exists an optimal choice of \mathbf{z} according to [39]:

$$\left| \frac{1}{N} \sum_{k=1}^N f\left(\left\{ \frac{k}{N} \mathbf{z} \right\}\right) - \int_{[0,1]^s} f(u) du \right| \leq cd(s, \alpha) \frac{(\log N)^{\beta(s, \alpha)}}{N^\alpha},$$

for the function $f \in E_s^\alpha(c)$ [39], $\alpha > 1$ and $d(s, \alpha), \beta(s, \alpha)$ do not depend on N .

When $s = 2$, the following optimal construction exists [40].

Consider the following generating vector [38]:

$$\mathbf{z} = (1, F_n^{(s)}(2), \dots, F_n^{(s)}(s)), \tag{3}$$

using $F_n^{(s)}(j) := F_{n+j-1}^{(s)} - \sum_{i=0}^{j-2} F_{n+i}^{(s)}$ and $F_{n+l}^{(s)}$ ($l = 0, \dots, j - 1, j$ is an integer, $2 \leq j \leq s$) is the corresponding number of the generalized Fibonacci series [38]. Then

$$F_n^{(s)}(2) = F_{n+1}^{(s)} - F_n^{(s)} = (F_n^{(s)} + F_{n-1}^{(s)} + \dots + F_{n-s+1}^{(s)}) - F_n^{(s)} = F_{n-1}^{(s)} + \dots + F_{n-s+1}^{(s)}.$$

Our generating vector (3) is transformed into [40]:

$$\mathbf{z} = (1, F_{n-1}^{(s)} + F_{n-2}^{(s)} + \dots + F_{n-s+1}^{(s)}, \dots, F_{n-1}^{(s)} + F_{n-2}^{(s)}, F_{n-1}^{(s)}). \tag{4}$$

We construct a special lattice sequence with the generating vector (4), namely **LATTICE-FIBO**.

Now we will improve the convergence of the lattice sequence using the recently developed component and the Component Fast Construction method (CBC) [41–43]. Now we construct a special lattice sequence **LATTICE-CBC** with an optimal generating vector following the idea in [44,45]. At the first step of LATTICE-CBC, $\mathbf{z} = (z_1, z_2, \dots, z_s)$ is generated by the CBC. After that, the points of LATTICE-CBC are obtained by the formula

$$\mathbf{x}_k = \left\{ \frac{k}{N} \mathbf{z} \right\}, k = 1, \dots, N.$$

The approximate value I_N of (2) is evaluated in the following way:

$$I_N = \frac{1}{N} \sum_{k=1}^N f\left(\left\{ \frac{k}{N} \mathbf{z} \right\}\right).$$

Let F_b be the finite field with b elements for a prime power b (when b is a prime, F_b is the residue class ring modulo b) [46]. Using F_b and a bijection $\phi : 0, \dots, b - 1 \rightarrow F_b$

with $\phi(0) = \bar{0}$, we generate a digital (t, s) -sequence over F_b . Now we take $N \times N$ matrices C_1, \dots, C_s over F_b . The matrices are of the form

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & \dots \\ c_{21} & c_{22} & c_{23} & \dots \\ c_{31} & c_{32} & c_{33} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \in F_b^{N \times N}.$$

To now generate one of the points $x_n = (x_{n,1}, \dots, x_{n,s})$, of the (t, s) -sequence, we record n in its b -adic (i.e., base b) expansion

$$n = \sum_{i=0}^{\infty} a_i b^i$$

with $a_i \in 0, \dots, b - 1$ and $a_i = 0$ for all i large enough. Now we choose the column vector

$$\begin{pmatrix} \phi(a_0) \\ \phi(a_1) \\ \phi(a_2) \\ \dots \end{pmatrix} \in (F_b^N)^\top$$

To generate the point $x_n = (x_{n,1}, \dots, x_{n,s})$, for the i -th coordinate $x_{n,i}$, the value of $x_{n,i}$ is derived by multiplying the i -th matrix C_i by \mathbf{n} in F_b^m , which derives a column vector over F_b :

$$C_i \mathbf{n} \begin{pmatrix} \bar{y}_{n,i,1} \\ \bar{y}_{n,i,2} \\ \dots \end{pmatrix} \in (F_b^N)^\top$$

The elements $\phi^{-1} \bar{y}_{n,i,j} \in 0, \dots, b - 1$, for $j \in N$, are now the b -adic digits of $x_{n,i}$, i.e.

$$x_{n,i} = \frac{\phi^{-1} \bar{y}_{n,i,1}}{b} + \frac{\phi^{-1} \bar{y}_{n,i,2}}{b^2} + \dots$$

Now the sequence derived in this way $(\mathbf{x}_0, \mathbf{x}_1, \dots)$ defines a digital sequence by generating matrices C_1, \dots, C_s [47].

Now we will consider two possible choices for the generating matrices. The first digital sequence is generating matrices based on an implementation of the Sobol sequence from [48] with 21201 dimensions, and we called it **DIGITAL-SOBOL**. The second digital sequence uses the construction of Xing and Niederreiter [49]. This sequence was implemented by Pirsic [50] and can be considered as the currently optimal low-discrepancy sequences with a rate of convergence $O(s \log_b s)$. We will call this sequence **DIGITAL-XINGN**.

3. Calculations and Results

The efficient stochastic algorithms, namely **SOBOI-SEQ**, **MCA-MSS-1**, **MCA-MSS-2**, **MCA-MSS-2-S**, **LATTICE-FIBO**, **LATTICE-CBC**, **DIGITAL-SOBOL** and **DIGITAL-XINGN**, have been applied to sensitivity studies with respect to emission levels and some chemical reactions rates of the concentration variations of UNI-DEM pollutants. The estimated quantity is denoted by EQ and its reference value by RV. The relative error is denoted by RE and the approximate evaluation by AE.

In the case of the **sensitivity studies with respect to emission levels**, we will study the sensitivity of the model output (in terms of mean monthly concentrations of several important pollutants—in our case, this is ammonia in Milan) with respect to a variation

of input emissions from the anthropogenic pollutants, which consists of four different components $E = (E^A, E^N, E^S, E^C)$ as follows:

- E^A – ammonia (NH_3);
- E^N – nitrogen oxides ($NO + NO_2$);
- E^S – sulphur dioxide (SO_2);
- E^C – anthropogenic hydrocarbons.

The output of the model is the mean monthly concentration of the following three pollutants:

- s_1 —ozone (O_3);
- s_2 —ammonia (NH_3);
- s_3 —ammonium sulfate and ammonium nitrate ($NH_4SO_4 + NH_4NO_3$).

In the case of the **sensitivity studies with respect to emission levels**, the results for REs for the AE of the f_0, D, S_i and S_i^{tot} , using **SOBOL-SEQ, MCA-MSS-1, MCA-MSS-2, MCA-MSS-2-S, LATTICE-FIBO, LATTICE-CBC, DIGITAL-SOBOL and DIGITAL-XINGN** are shown in Tables 1–5, respectively. The quantity f_0 is represented by a four-dimensional integral, whereas the rest are represented by eight-dimensional integrals.

Table 1. RE for AE of $f_0 \approx 0.048$.

n	DIGITAL-SOBOL	LATTICE-CBC	LATTICE-FIBO	DIGITAL-XINGN
	Rel. Error	Rel. Error	Rel. Error	Rel. Error
2^{10}	3e-04	4e-04	2e-04	2e-06
2^{14}	1e-05	2e-05	2e-05	1e-06
2^{16}	4e-06	4e-06	9e-06	3e-10

Table 2. RE for AE of $f_0 \approx 0.048$.

# of Points n	SOBOL-SEQ	MCA-MSS-1	MCA-MSS-2	MCA-MSS-2-S
	Rel. Error	ρ	ρ	Rel. Error
2^8	2e-03	2e-02	5e-04	
2×2^8			8e-05	3e-03
2^{10}	4e-04	7e-04	3e-05	1e-05
2×2^{10}			7e-04	1e-04
2^{14}	3e-05	1e-04	3e-06	4e-06
2×2^{14}			1e-05	4e-05
2^{16}	7e-06	1e-04	6e-07	2e-07
2×2^{16}			9e-05	8e-04

Table 3. RE for AE of $D \approx 0.0002$.

# of Points n	SOBOL-SEQ	MCA-MSS-1	MCA-MSS-2	MCA-MSS-2-S
	Rel. Error	ρ	ρ	Rel. Error
2^{10}	4e-03	7e-04	9e-03	
(2×2^{10})			7e-04	3e-04
2^{14}	4e-04	1e-04	3e-04	3e-04
(2×2^{14})			1e-05	2e-04
2^{16}	4e-05	1e-04	2e-05	2e-05
(2×2^{16})			9e-05	7e-04

Table 4. RE for AE of $D \approx 0.0002$.

n	DIGITAL-SOBOL	LATTICE-CBC	LATTICE-FIBO	DIGITAL-XINGN
	Rel. Error	Rel. Error	Rel. Error	Rel. Error
2^{10}	3e-04	8e-03	2e-01	1e-04
2^{14}	1e-05	6e-04	3e-03	9e-07
2^{16}	2e-06	4e-05	3e-04	1e-06

Table 5. RE for AE of SIs ($n = 2^{16}$).

EQ	RV	SOBOL-SEQ	MCA-MSS-1	MCA-MSS-2	MCA-MSS-2-S	DIGIT-SOBOL	LAT-CBC	LAT-FIBO	DIGIT-XINGN
S_1	9e-01	8e-05	8e-05	6e-06	5e-04	4e-07	6e-05	4e-04	1e-06
S_2	2e-04	3e-02	3e-02	4e-03	7e-02	4e-06	4e-02	2e-01	6e-03
S_3	1e-01	8e-04	8e-04	7e-05	1e-02	2e-06	3e-05	3e-03	1e-05
S_4	4e-05	7e-02	7e-02	1e-02	6e-01	2e-04	8e-03	5e-01	1e-05
S_1^{tot}	9e-01	8e-05	8e-05	1e-05	1e-03	3e-07	2e-05	5e-04	1e-06
S_2^{tot}	2e-04	5e-03	2e-03	1e-03	3e-03	1e-05	5e-02	3e-01	3e-04
S_3^{tot}	1e-01	7e-04	7e-04	4e-05	4e-03	3e-06	6e-04	2e-03	2e-06
S_4^{tot}	5e-05	6e-02	6e-02	1e-02	1e-01	4e-04	3e-02	5e-01	1e-06

In the case of the **sensitivity studies with respect to chemical reactions rates**, we will study the ozone concentration in Genova according to the rate variation of these chemical reactions: ## 1, 3, 7, 22 (time-dependent) and 27, 28 (time-independent) of the CBM-IV scheme ([19]) given as follows:



Here, “ $h\nu$ ” represents the sunlight in the photochemical reactions and indicates that a photon is proportional to its frequency by Plank’s constant.

In the case of the **sensitivity studies with respect to chemical reactions rates**, the results for REs for the AE of the f_0, D, S_i, S_{ij} and S_i^{tot} , using **SOBOL-SEQ, MCA-MSS-1, MCA-MSS-2, MCA-MSS-2-S, LATTICE-FIBO, LATTICE-CBC, DIGITAL-SOBOL and DIGITAL-XINGN**, are shown in Tables 6–10, respectively. As in the first case study, the quantity f_0 is represented by a six-dimensional integral, whereas the rest are represented by twelve-dimensional integrals.

Table 6. RE for AE of $f_0 \approx 0.27$.

n	DIGITAL-SOBOL	LATTICE-CBC	LATTICE-FIBO	DIGITAL-XINGN
	Rel. Error	Rel. Error	Rel. Error	Rel. Error
2^{12}	1e-05	3e-04	1e-04	3e-08
2^{14}	5e-06	3e-05	4e-04	7e-11
2^{16}	1e-06	3e-06	3e-04	6e-11

Table 7. RE for AE of $f_0 \approx 0.27$.

# of points n	SOBOL-SEQ	MCA-MSS-1		MCA-MSS-2		MCA-MSS-2-S
	Rel. Error	ρ	Rel. Error	ρ	Rel. Error	Rel. Error
2^{12}	5e-05	3e-02	6e-06			
2×2^{12}				4e-04	7e-05	3e-06
2^{14}	2e-05	2e-04	1e-05			
2×2^{14}				2e-04	9e-06	9e-08
2^{16}	2e-06	2e-04	2e-07			
2×2^{16}				2e-05	4e-06	5e-07

Table 8. RE for AE of $D \approx 0.0025$.

# of Points n	SOBOL-SEQ	MCA-MSS-1		MCA-MSS-2		MCA-MSS-2-S
	Rel. Error	ρ	Rel. Error	ρ	Rel. Error	Rel. Error
2^6	1e-02	7e-04	1e-02			
(2×2^6)				7e-03	9e-03	8e-03
2^{12}	6e-04	4e-03	3e-05			
(2×2^{12})				4e-04	4e-04	5e-04
2^{14}	1e-04	2e-04	1e-04			
(2×2^{14})				2e-04	2e-04	6e-06
2^{16}	2e-05	2e-04	7e-05			
(2×2^{16})				2e-05	2e-05	1e-04

Table 9. RE for AE of $D \approx 0.0025$.

n	DIGITAL-SOBOL	LATTICE-CBC	LATTICE-FIBO	DIGITAL-XINGN
	Rel. Error	Rel. Error	Rel. Error	Rel. Error
2^{12}	3e-04	8e-03	5e-01	2e-03
2^{14}	6e-05	3e-03	1e-01	4e-05
2^{16}	1e-05	2e-04	2e-03	2e-05

Table 10. RE for AE of SIs ($n = 2^{16}$).

EQ	RV	SOBOL-SEQ	MCA-MSS-1	MCA-MSS-2	MCA-MSS-2-S	DIGIT-SOBOL	LAT-CBC	LAT-FIBO	DIGIT-XINGN
S_1	4e-01	1e-04	4e-04	2e-04	2e-02	5e-06	1e-03	4e-02	2e-05
S_2	3e-01	3e-05	2e-04	3e-04	6e-02	6e-06	4e-04	1e-02	2e-05
S_3	5e-02	2e-04	2e-03	9e-04	8e-02	1e-04	1e-03	5e-01	1e-05
S_4	3e-01	3e-04	2e-05	2e-04	4e-03	1e-05	5e-04	1e-02	1e-05
S_5	4e-07	3e-01	7e+00	7e-02	2e+02	7e-02	3e+01	3e+03	4e-01
S_6	2e-02	3e-04	1e-03	3e-04	4e-02	4e-06	1e-02	1e+00	3e-05
S_1^{tot}	4e-01	1e-04	4e-05	2e-04	5e-02	8e-07	8e-04	8e-02	4e-05
S_2^{tot}	3e-01	4e-05	5e-04	2e-04	3e-02	3e-06	1e-03	3e-02	3e-05
S_3^{tot}	5e-02	3e-04	2e-03	8e-04	4e-02	1e-04	2e-03	1e+00	3e-05
S_4^{tot}	3e-01	2e-04	5e-04	2e-04	4e-02	2e-05	1e-03	4e-01	2e-05
S_5^{tot}	2e-04	7e-03	1e-02	4e-03	1e+00	9e-03	1e-01	9e+01	6e-03
S_6^{tot}	2e-02	4e-04	1e-03	3e-04	4e-02	1e-05	1e-02	2e+00	7e-06
S_{12}	6e-03	2e-04	5e-03	1e-03	7e-01	1e-04	4e-02	3e+00	3e-04
S_{14}	5e-03	2e-03	2e-02	2e-03	1e+00	2e-05	9e-02	8e+00	6e-04
S_{24}	3e-03	1e-03	2e-02	6e-03	1e+00	2e-04	6e-03	1e+01	1e-03
S_{45}	1e-05	4e-02	1e-01	2e-02	4e+00	1e-02	9e-01	4e+01	2e-02

4. Discussion of the Results

In the case of the **sensitivity studies with respect to emission levels**, a detailed discussion has been made with the previous best available approaches described in [51–53].

For the number of samples $n = 2^{16}$ for the model function f_0 , the best algorithm is the DIGITAL-XINGN, followed by MCA-MSS-2-S and MCA-MSS-1—see the results in Tables 1 and 2 for the maximum number of samples. A big improvement over the older best available result is obtained—the new result is $3e-10$ vs. $2e-08$ [32,35]. For a number of samples $n = 2^{16}$ for the total variance D , the best algorithm is the DIGITAL-XINGN, followed by MCA-MSS-2-S and DIGITAL-SOBOL—see the results in Tables 3 and 4 for the maximum number of samples [32,35].

Our discussion here includes a detailed comparison with the previous results in the field in [54,55]. For the total and first-order sensitivity indices in Table 5, it can be seen that the two digital sequences improve the results produced by the best available approaches up to now [32,33]. The DIGITAL-SOBOL gives the best results for S_1, S_2, S_3, S_1^{tot} and S_2^{tot} , while the DIGITAL-XING gives the best results for S_4, S_3^{tot} and S_4^{tot} . The general conclusion is that our methods significantly improved the accuracy of the sensitivity indices described in [56]. According to [33,54,56], the best available approaches up to now were the SOBOL-SEQUENCE and MCA-MSS-1 for S_4, S_1^{tot} (these two give exactly the same result for all quantities except S_2^{tot}), and MCA-MSS-2 was the best available algorithm for $S_1, S_2, S_3, S_2^{tot}, S_3^{tot}, S_4^{tot}$. From Table 5, one can conclude that between the two lattice sequences, LATTICE-CBC is more accurate by at least 1. Furthermore, we can observe that the worst are MCA-MSS-2-S and LATTICE-FIBO, and the last method gives unsatisfactory relative errors. According to [32,54,56], the best improvements for the sensitivity indexes are obtained for S_2 , the new result is $4e-06$ vs. $4e-03$; for S_4 , the new result is $1e-05$ vs. $1e-02$. For all total sensitivity indices, there are serious improvements over the existing best available results. For S_1^{tot} , the new result is $3e-07$ vs. $1e-05$; for S_2^{tot} , $1e-05$ vs. $1e-03$; for S_3^{tot} , $2e-06$ vs. $4e-05$; and for S_4^{tot} , $1e-06$ vs. $1e-02$. In [24], it is mentioned that having the smallest possible sensitivity indices is the most important aspect of the model. In our case, these are S_4 and S_4^{tot} , and the improvement is with three and four orders, respectively, which will be crucial for taking into account the reliability of the results of the model.

The performance of the algorithms can be generalized in such a way: the two digital sequences proposed by the authors yield the smallest relative errors for all sensitivity indices; algorithm MCA-MSS-2 is after that, followed by SOBOL-SEQUENCE, MCA-MSS-1 and LATTICE-CBC. The worst results are produced by the MCA-MSS-2-S and LATTICE-FIBO. Comparing our results with the results obtained in [32,35,54,56] the main advantages of our methods include the significant improvement in the accuracy and lower computational complexity.

In the case of **sensitivity studies with respect to chemical reaction rates**, a precise discussion has been made with the previous best available approaches from [4,57,58].

For the number of samples $n = 2^{16}$ for the model function f_0 , the best algorithm is the DIGITAL-XINGN, followed by MCA-MSS-2-S and MCA-MSS-1—see the results in Tables 6 and 7 for the maximum number of samples. There is a huge improvement according to the sensitivity studies in [32,35]—the new result is $6e-11$ vs. $2e-07$. For the number of samples $n = 2^{16}$ for the total variance D , the best algorithm is the DIGITAL-SOBOL, followed by DIGITAL-XINGN, MCA-MSS-2 and SOBOL-SEQUENCE—see the results in Tables 8 and 9 for the maximum number of samples [4].

The discussion in this case includes a comparison between our obtained results with other studies and other papers already published [32,59,60]. For all sensitivity indices in Table 10, it can be seen that the two digital sequences improve the results produced by the best available approaches except for the sensitivity index S_5^{tot} obtained in [32,33]. The DIGITAL-SOBOL gives the best results for $S_1, S_2, S_4, S_5, S_6, S_1^{tot}, S_1^{tot}, S_2^{tot}, S_4^{tot}, S_{12}, S_{14}, S_{24}$ and S_{45} , while the DIGITAL-XING gives the best results for $S_3, S_4, S_3^{tot}, S_4^{tot}$ and S_6^{tot} . The general conclusion is that our methods show a significant improvement in the accuracy vs. the other calculations in this field [61]. According to [4,33,59], the best available approaches

up to now were the SOBOL-SEQUNCE for $S_1, S_2, S_6, S_2^{tot}, S_3^{tot}, S_4^{tot}, S_{12}, S_{14}, S_{24}$, MCA-MSS-1 was the best for S_4 and S_1^{tot} , and MCA-MSS-2 was the most accurate for $S_5, S_6, S_4^{tot}, S_5^{tot}, S_6^{tot}, S_{14}, S_{45}$. According to [35,59,60], the best improvement for the relative error is that for the sensitivity index S_6 , the new result is $4e-06$ vs. $3e-04$; for S_1^{tot} , the new is $8e-07$ vs. $4e-05$; and for S_{14} , the new result is $2e-05$ vs. $2e-03$. From Table 10, focusing on the relative errors, one can conclude that between the two lattice sequences, LATTICE-CBC is more accurate by at least two orders. Furthermore, we can observe that MCA-MSS-2-S is one order better than LATTICE-FIBO and one order worse than the LATTICE-CBC.

We can conclude that the two digital sequences proposed by the authors yield the smallest relative errors for all sensitivity indices except S_5^{tot} , and DIGITAL-SOBOL has the edge; the algorithm MCA-MSS-2 is closely behind them, followed by SOBOL-SEQUENCE, MCA-MSS-1, LATTICE-CBC and MCA-MSS-2-S. The lattice sequence LATTICE-FIBO gives unsatisfactory relative errors for most of the quantities.

Based on the described comparison with other sensitivity studies and other papers already published in the field [16,17,62,63], the general conclusion from our discussion is that the main advantages of the proposed methods **LATTICE-FIBO**, **LATTICE-CBC**, **DIGITAL-SOBOL** and **DIGITAL-XINGN** for the very important large-scale air pollution model UNI-DEM are the much higher accuracy and lower computational complexity.

5. Conclusions

The present study is in a very important area of environmental safety. High levels of pollution can damage ecosystems and harm plants, animals and humans, and it is of great importance to study the levels of pollution precisely. That is why it is of great importance to recognize whether the pollution levels are below some critical values and, if so, to establish a well-founded control system to retain the pollution levels within these limits. These problems can be accomplished successfully by the proposed highly efficient stochastic approaches for studying the sensitivity of various pollution-related processes.

The computational efficiency in terms of relative error of one of the best available stochastic methods for high-dimensional integration has been performed for the sensitivity of the UNI-DEM model output to find the variation of rate constants of chosen chemical reactions and the variation of selected input emissions of the anthropogenic pollutants.

The two proposed digital sequences based on Sobol and Xing-Niederreiter matrices show an essential improvement over the existing best available results produced by the modified Sobol sequences. The proposed approaches by the authors LATTICE-CBC, DIGITAL-SOBOL and DIGITAL-XNING are established as the new best available stochastic methods for this particular very important large-scale air pollution model UNI-DEM.

The obtained results will help test and improve the mathematical models and enable a well-founded explanation by the relevant specialists. By recognizing the main chemical reactions that influence the performance of the system, physicists and chemists will be able to gather important information to improve the model, which will increase the reliability and sustainability of forecasts. Therefore, through our sensitivity results, the mathematical model will contribute to a more accurate evaluation of losses in agriculture and, most importantly, enable an estimation of the effects of harmful emissions on human health.

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