# Extending the applicability of the RVT technique for the randomized radioactive decay chain model 

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Received: date / Revised version: date


#### Abstract

In this paper, we improve the existing analysis on the randomized radioactive decay chain model based on Bateman master equations, by Hussein and Selim (2020). For a decay chain of three species of radionuclides, the authors derived the probability density function for the concentrations, by using the random variable transformation (RVT) technique. We extend this application to the general solution of Bateman equations. The density function is expressed as an expectation, which has important implications for parametric density estimation. This may improve the classical kernel estimation when the random dimensionality is not low. Numerical examples are included, where the decay parameters and the initial concentrations are assigned different probability distributions.


## 1 Introduction

Recently, paper [1] investigated the process of radioactive decay in time subject to randomness. The radioactive decay chain (RDC) model was described through Bateman master equations, which set differential-difference equations for the number of radionuclides of the species. The decay parameters and the initial concentrations were assumed to be random variables. Under this setting, the sample-path solution to the model becomes a stochastic process (a random variable that evolves with time) [2], and its uncertainty must be quantified [3]. An important feature of Bateman equations is that the stochastic solution is given in closed form. Given three species of radionuclides with zero concentrations for the daughters at time zero, the authors derived the probability density function (PDF) of the solution via the random variable transformation (RVT) technique [4-7]. This technique expresses the PDF of the output in terms of the joint PDF of the input random coefficients, when the deterministic input-output relation is available in closed form and satisfies certain assumptions (continuous differentiability, one-to-one, and non-vanishing Jacobian, on the whole domain or over a partition of it). This is an effective and direct method for uncertainty quantification. It is analogous to Liouville's equation [8-11], though simpler when the Jacobian computation is straightforward.

In this paper, the aim is to extend the application of the RVT method done by [1] to the general stochastic solution of the RDC model. Namely, for an arbitrary number of species, the expression for the PDF of the solution is obtained. This expression, as usual, is semi-implicit, since it depends on integrations. When the number of integrations is low, as in [1], quadrature methods are applicable (many software perform these multidimensional integrations via built-in commands). For moderate or high integrations, the PDF is alternatively expressed as an expectation. This permits estimating the PDF parametrically and improving the classical kernel methods in a lot of situations [12].

The structure of this paper is the following. In Sect. 2, the solution to the RDC model is reviewed. In Sect. 3, the RVT method and its alternative formulation are described and discussed. In Sect. 4, the PDF of the stochastic solution is obtained, in a general framework. In Sect. 5, we treat the topic of input-uncertainty estimation, by maximizing entropy. In Sect. 6, some numerical computations are presented. Finally, Sect. 7 draws the main conclusions.

## 2 The RDC model

As described in [1], the RDC model formulated through the Bateman equations is

$$
\frac{\mathrm{d} N_{1}(t)}{\mathrm{d} t}=-\lambda_{1} N_{1}(t)
$$

$$
\begin{gathered}
\frac{\mathrm{d} N_{j}(t)}{\mathrm{d} t}=-\lambda_{j} N_{j}(t)+\lambda_{j-1} N_{j-1}(t), \quad j=2, \ldots, n-1 \\
\frac{\mathrm{~d} N_{n}(t)}{\mathrm{d} t}=\lambda_{n-1} N_{n-1}(t)
\end{gathered}
$$

There is a serial decay chain of $n$ nuclear species $X_{1} \rightarrow X_{2} \rightarrow \cdots \rightarrow X_{n}$, where $\lambda_{j}$ is the rate of decay of the radionuclides from the species $X_{j}$ into the species $X_{j+1}$. Transition rates from $j+1$ to $j$ are not allowed. The parameter $\lambda_{n}$ is 0 because the nuclides of species $X_{n}$ are stable. The number of radionuclides of species $X_{j}$ at time $t$ is $N_{j}(t), j=1, \ldots, n$. The analytical solution is [13]

$$
\begin{equation*}
N_{m}(t)=\sum_{i=1}^{m}\left[N_{i}(0)\left(\prod_{j=i}^{m-1} \lambda_{j}\right) \sum_{j=i}^{m} \frac{\mathrm{e}^{-\lambda_{j} t}}{\prod_{p=i, p \neq j}^{m}\left(\lambda_{p}-\lambda_{j}\right)}\right] \tag{1}
\end{equation*}
$$

for $m=1, \ldots, n$.
When $\lambda_{j}$ and $N_{j}(0), j=1, \ldots, n$, are random variables, the solution $N_{m}(t)$ is a stochastic process, $m=1, \ldots, n$. It is assumed that the decay coefficients are different almost surely. The main goal is to compute the PDF of $N_{m}(t)$ at each time $t$, denoted as $f_{N_{m}}\left(x_{m} ; t\right)$ (evaluated at $x_{m} \in \mathbb{R}$ ). In [1], the authors restricted to $n=3$ (parameters $\lambda_{1}$ and $\lambda_{2}$, with $\left.\lambda_{3}=0\right), N_{1}(0)=N_{1,0} \neq 0, N_{2}(0)=0$ and $N_{3}(0)=0$. In this paper, the PDF will be computed for arbitrary $n, m$, decay parameters and initial abundances.

## 3 The RVT technique

### 3.1 Classical formulation

The RVT technique, also called change of variables technique, is used to find the relation between the PDFs in a closed-form input-output system [14, Th. 2.1.5]. Let $\boldsymbol{Y}=\left(Y_{1}, \ldots, Y_{k}\right)$ and $\boldsymbol{Z}=\left(Z_{1}, \ldots, Z_{k}\right)$ be two random vectors, $k \geq 1$, related as $\boldsymbol{Z}=\boldsymbol{g}(\boldsymbol{Y})$, where $\boldsymbol{g}: D \subseteq \mathbb{R}^{k} \rightarrow \mathbb{R}^{k}$ is a Borel-measurable deterministic mapping. When $\boldsymbol{g}$ is continuously differentiable on an open set $\bar{D}$ containing the support of $\boldsymbol{Y}$, one-to-one, and with non-vanishing Jacobian $J_{\boldsymbol{g}}(y)=\operatorname{det}\left(\frac{\partial \boldsymbol{g}}{\partial \boldsymbol{y}}(\boldsymbol{y})\right)$, the joint PDF of $\boldsymbol{Z}$ is given in terms of the joint PDF of $\boldsymbol{Y}$ by

$$
f_{\boldsymbol{Z}}(\boldsymbol{z})=f_{\boldsymbol{Y}}(\boldsymbol{h}(\boldsymbol{z}))\left|J_{\boldsymbol{h}}(\boldsymbol{z})\right|, \quad \boldsymbol{z} \in \boldsymbol{g}(D)
$$

where $\boldsymbol{h}=\boldsymbol{g}^{-1}$ is the inverse of $\boldsymbol{g}$ on its domain and $J_{\boldsymbol{h}}(\boldsymbol{z})=\operatorname{det}\left(\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}(\boldsymbol{z})\right)$. Indeed, for any Borel set $B$ contained in the support of $\boldsymbol{Z}$, we have

$$
\mathbb{P}[\boldsymbol{Z} \in B]=\mathbb{P}[\boldsymbol{g}(\boldsymbol{Y}) \in B]=\mathbb{P}[\boldsymbol{Y} \in \boldsymbol{h}(B)]=\int_{\boldsymbol{h}(B)} f_{\boldsymbol{Y}}(\boldsymbol{y}) \mathrm{d} \boldsymbol{y}=\int_{B} f_{\boldsymbol{Y}}(\boldsymbol{h}(\boldsymbol{z}))\left|J_{\boldsymbol{h}}(\boldsymbol{z})\right| \mathrm{d} \boldsymbol{z}
$$

First, it is used the principle that an event has the same probability regardless of whether it is described in terms of $\boldsymbol{Z}$ or $\boldsymbol{Y}$, and second, the change of variables formula for Lebesgue integration is applied.

The one-to-one condition may be overcome by dividing the domain of $\boldsymbol{g}$ into sub-domains where it is one-to-one [14, Th. 2.1.8]. Write $D$ as a pairwise disjoint union $D=\cup_{i=1}^{s} D_{i}$, where $\boldsymbol{g}_{i}=\left.\boldsymbol{g}\right|_{D_{i}}$ is continuously differentiable on $D_{i}$, one-to-one, and with non-vanishing Jacobian $J_{\boldsymbol{g}_{i}}(\boldsymbol{y})$. Then the joint PDF of $\boldsymbol{Z}$ is given by

$$
f_{\boldsymbol{Z}}(\boldsymbol{z})=\sum_{i: \boldsymbol{z} \in \boldsymbol{g}\left(D_{i}\right)} f_{\boldsymbol{Y}}\left(\boldsymbol{h}_{i}(\boldsymbol{z})\right)\left|J_{\boldsymbol{h}_{i}}(\boldsymbol{z})\right|, \quad \boldsymbol{z} \in \boldsymbol{g}(D)
$$

where $\boldsymbol{h}_{i}=\boldsymbol{g}_{i}^{-1}$ is the inverse of $\boldsymbol{g}_{i}$ on $D_{i}$.

### 3.2 Alternative formulation

There is an alternative version of the RVT technique when the transformation mapping $g$ consists of sums and products [12]. Let $A$ be an absolutely continuous random variable with explicit PDF $f_{A}$, independent of the random vector $\left(Z_{1}, Z_{2}\right)$ (which is not necessarily absolutely continuous), where $Z_{1} \neq 0$ almost surely. Then the random variable $Z_{1} A+Z_{2}$ is absolutely continuous, with PDF

$$
\begin{equation*}
f_{Z_{1} A+Z_{2}}(z)=\mathbb{E}\left[f_{A}\left(\frac{z-Z_{2}}{Z_{1}}\right) \frac{1}{\left|Z_{1}\right|}\right], \quad z \in \mathbb{R} \tag{2}
\end{equation*}
$$

The proof is presented in an appendix. To provide the analogy with the customary RVT formula, there is a transformation mapping $\boldsymbol{g}\left(A, Z_{1}, Z_{2}\right)=\left(Z_{1} A+Z_{2}, Z_{1}, Z_{2}\right)$ on $D=\mathbb{R}^{3}$, whose inverse is $\boldsymbol{h}\left(Z, Z_{1}, Z_{2}\right)=\left(\left(Z-Z_{2}\right) / Z_{1}, Z_{1}, Z_{2}\right)$. The Jacobian of $\boldsymbol{h}$ is $1 / Z_{1}$.

Whenever possible, the expectation $\mathbb{E}$ in (2) should be computed by integration (quadratures). Otherwise, if the explicit probability law of ( $Z_{1}, Z_{2}$ ) is too complicated (because it depends on a significant number of random variables), then Monte Carlo simulation may be applied to (2) [12]:

$$
\begin{equation*}
f_{Z_{1} A+Z_{2}}(z) \approx \frac{1}{M} \sum_{k=1}^{M} f_{A}\left(\frac{z-Z_{2}\left(\omega_{k}\right)}{Z_{1}\left(\omega_{k}\right)}\right) \frac{1}{\left|Z_{1}\left(\omega_{k}\right)\right|}, \tag{3}
\end{equation*}
$$

where $Z_{1}\left(\omega_{1}\right), \ldots, Z_{1}\left(\omega_{M}\right)$ and $Z_{2}\left(\omega_{1}\right), \ldots, Z_{2}\left(\omega_{M}\right)$ are randomly drawn samples of length $M$. Notice that the approximation integrates 1 and is still a PDF, since

$$
\begin{aligned}
\int_{\mathbb{R}}\left(\frac{1}{M} \sum_{k=1}^{M} f_{A}\left(\frac{z-Z_{2}\left(\omega_{k}\right)}{Z_{1}\left(\omega_{k}\right)}\right) \frac{1}{\left|Z_{1}\left(\omega_{k}\right)\right|}\right) \mathrm{d} z & =\frac{1}{M} \sum_{k=1}^{M} \int_{\mathbb{R}} f_{A}\left(\frac{z-Z_{2}\left(\omega_{k}\right)}{Z_{1}\left(\omega_{k}\right)}\right) \frac{1}{\left|Z_{1}\left(\omega_{k}\right)\right|} \mathrm{d} z=\frac{1}{M} \sum_{k=1}^{M} \int_{\mathbb{R}} f_{A}(z) \mathrm{d} z \\
& =\frac{1}{M} \sum_{k=1}^{M} 1=1
\end{aligned}
$$

Convergence of the approximation as $M \rightarrow \infty$ is always guaranteed by the law of large numbers. The PDF estimation becomes a parametric problem, since an expectation parameter is estimated. The convergence rate, given $M$ independent realizations of $\left(Z_{1}, Z_{2}\right)$, is $\mathcal{O}\left(M^{-1 / 2}\right)$, due to the central limit theorem (the constant of $\mathcal{O}$ depends on the evaluation point $z \in \mathbb{R}$ ). Variance reduction methods may be applied, such as antithetic or control variates [15]. Since the parametric method acts pointwise, the discontinuities and non-differentiability points of the target PDF are correctly captured, without smoothing them out. Thus, the method is robust.

These features are in contrast to kernel density estimation, which is non-parametric because it reconstructs a distribution. Recall that, given a random variable $Y$ with $\operatorname{PDF} f_{Y}$, the kernel density estimate is defined as

$$
y \mapsto \frac{1}{M h} \sum_{k=1}^{M} \kappa\left(\frac{y-Y\left(\omega_{k}\right)}{h}\right),
$$

where $Y\left(\omega_{1}\right), \ldots, Y\left(\omega_{M}\right)$ are randomly drawn realizations, $\kappa$ is a kernel (a nonnegative function) and $h>0$ is a smoothing parameter called the bandwidth. Under sufficient regularity of the target PDF and optimality of the bandwidth selected, the root-mean-square error of the estimate is $\mathcal{O}\left(M^{-r}\right), r<1 / 2$ [16]. Kernel density estimates are highly influenced by smoothness; without prior knowledge on the features of the target PDF, the optimal kernel may not be known. The kernel density estimate may consider wrong tails or ignore discontinuities and peaks, for instance. Finally, notice that, for a fixed $M$, the kernel density estimation and the parametric estimation have practically the same cost, since both rely on $M$ realizations of $Z_{1}$ and $Z_{2}$ (the kernel density estimation also needs realizations of $A$, evaluates the kernel function and considers a bandwidth, while the parametric estimation evaluates $f_{A}$ ).

Despite all the favorable properties of the parametric estimation method, there are some situations, which were not analyzed in [12], in which it may present slow convergence: since (2) involves random denominators, the variance of the random quantity inside the expectation may be high for some $z$, which produces "noise" that plagues the PDF estimate $[17,18]$. This issue is not observed for kernel density estimation.

Remark 1 When applying the new alternative formulation, there is no need to identify the support of the output random variable analytically. In (2), the variable $z$ belongs to $\mathbb{R}$. When $z$ is not in the support of $Z_{1} A+Z_{2}$, then $f_{A}\left(\left(z-Z_{2}\right) / Z_{1}\right)$ is 0 almost surely, and $f_{Z_{1} A+Z_{2}}(z)=0$, as expected. In numerical computations, one estimates the target PDF without prior specification of its domain; outside the domain, the numerical estimate will be exactly 0 and no problems will arise.

## 4 The PDF

The solution (1) has the special form $N_{m}(t)=N_{1}(0) U_{m}(t)+V_{m}(t)$, where

$$
U_{m}(t)=\left(\prod_{j=1}^{m-1} \lambda_{j}\right) \sum_{j=1}^{m} \frac{\mathrm{e}^{-\lambda_{j} t}}{\prod_{p=1, p \neq j}^{m}\left(\lambda_{p}-\lambda_{j}\right)}
$$

and

$$
V_{m}(t)=\sum_{i=2}^{m}\left[N_{i}(0)\left(\prod_{j=i}^{m-1} \lambda_{j}\right) \sum_{j=i}^{m} \frac{\mathrm{e}^{-\lambda_{j} t}}{\prod_{p=i, p \neq j}^{m}\left(\lambda_{p}-\lambda_{j}\right)}\right]
$$

Thus, if $N_{1}(0)$ is independent of the rest of random variables, formula (2) is applicable with $Z_{1}=U_{m}(t), Z_{2}=V_{m}(t)$ and $N_{1}(0)=A$ :

$$
\begin{aligned}
f_{N_{m}}\left(x_{m} ; t\right) & =\mathbb{E}\left[f_{N_{1}(0)}\left(\frac{x_{m}-V_{m}(t)}{U_{m}(t)}\right) \frac{1}{\left|U_{m}(t)\right|}\right] \\
& =\int_{\mathbb{R}^{m-1}} \int_{\mathbb{R}^{m-1}} f_{N_{1}(0)}\left(\frac{x_{m}-V_{m}(t)}{U_{m}(t)}\right) \frac{1}{\left|U_{m}(t)\right|} \\
& \times f_{\left(N_{2}(0), \ldots, N_{m}(0), \lambda_{1}, \ldots, \lambda_{m-1}\right)}\left(N_{2}(0), \ldots, N_{m}(0), \lambda_{1}, \ldots, \lambda_{m-1}\right) \\
& \times \mathrm{d} \lambda_{1} \cdots \mathrm{~d} \lambda_{m-1} \mathrm{~d} N_{2}(0) \cdots \mathrm{d} N_{m}(0)
\end{aligned}
$$

This is the RVT formula after marginalizing. The case studied in [1] arises for $m=1,2,3, n=3, N_{1}(0)=N_{1,0}$ and $N_{2}(0)=N_{3}(0)=0$ (so that $f_{N_{2}}(x ; 0)=f_{N_{3}}(x ; 0)=\delta_{0}(x)$ is a Dirac delta function). The authors assumed that $\lambda_{1}, \lambda_{2}$ and $N_{1,0}$ are independent random variables, which gives a double integral for $f_{N_{m}}\left(x_{m} ; t\right)$. In general, when the random dimensionality is low, the integrals may be solved numerically. However, for moderate or high random dimensionality, it is preferable to estimate the expectation via Monte Carlo simulation (see (3)). This has advantages compared to kernel density estimation, as discussed in the preceding section.

When $N_{1}(0)$ is not independent of the remaining random variables, the RVT formula gives

$$
\begin{aligned}
f_{N_{m}}\left(x_{m} ; t\right) & =\int_{\mathbb{R}^{m-1}} \int_{\mathbb{R}^{m-1}} f_{\left(N_{1}(0), N_{2}(0), \ldots, N_{m}(0), \lambda_{1}, \ldots, \lambda_{m-1}\right)}\left(\frac{x_{m}-V_{m}(t)}{U_{m}(t)}, N_{2}(0), \ldots, N_{m}(0), \lambda_{1}, \ldots, \lambda_{m-1}\right) \\
& \times \frac{1}{\left|U_{m}(t)\right|} \mathrm{d} \lambda_{1} \cdots \mathrm{~d} \lambda_{m-1} \mathrm{~d} N_{2}(0) \cdots \mathrm{d} N_{m}(0) .
\end{aligned}
$$

That is, the joint PDF $f_{\left(N_{1}(0), N_{2}(0), \ldots, N_{m}(0), \lambda_{1}, \ldots, \lambda_{m-1}\right)}$ does not factorize as a product $f_{N_{1}(0)} \times f_{\left(N_{2}(0), \ldots, N_{m}(0), \lambda_{1}, \ldots, \lambda_{m-1}\right)}$. In this case, $f_{N_{m}}\left(x_{m} ; t\right)$ is not expressible as an expectation, therefore the only possibility is to rely on integration methods.

If $f_{N_{m}}\left(x_{m} ; t\right)$ is computable by numerical integration methods, then the statistics of $N_{m}(t)$ may be determined by integration:

$$
\begin{equation*}
\mathbb{E}\left[G\left(N_{m}(t)\right)\right]=\int_{\mathbb{R}} G\left(x_{m}\right) f_{N_{m}}\left(x_{m} ; t\right) \mathrm{d} x_{m} \tag{4}
\end{equation*}
$$

In particular, the mean and the variance of $N_{m}(t)$ are

$$
\begin{gathered}
\mathbb{E}\left[N_{m}(t)\right]=\int_{\mathbb{R}} x_{m} f_{N_{m}}\left(x_{m} ; t\right) \mathrm{d} x_{m}, \\
\mathbb{V}\left[N_{m}(t)\right]=\int_{\mathbb{R}} x_{m}^{2} f_{N_{m}}\left(x_{m} ; t\right) \mathrm{d} x_{m}-\left(\mathbb{E}\left[N_{m}(t)\right]\right)^{2} .
\end{gathered}
$$

When $f_{N_{m}}\left(x_{m} ; t\right)$ is not computable by numerical integration methods, but by parametric Monte Carlo simulation on $\mathbb{E}$ instead, then it is preferable to directly apply Monte Carlo simulation or spectral techniques [3] for statistics, rather than an integration (4).

## 5 Input uncertainty

In the task of uncertainty quantification, there are two main goals: random-input representation from data (inverse uncertainty quantification), and quantification of the model stochastic output (forward uncertainty quantification) [3]. The computation of the PDF of the model output, which is the focus of this paper, corresponds to forward uncertainty quantification.

For inverse uncertainty quantification, the maximum entropy principle (MEP) [19-21] derives probability distributions for the parameters consistently. Subject to constraints on the support and the statistical moments of the parameters, the entropy (ignorance) on the density functions described by the Shannon measure is maximized using Lagrange multipliers. Given a random input parameter $\theta$ with PDF $f_{\theta}$ and support $[a, b]$, its Shannon entropy is
$\mathcal{S}\left[f_{\theta}\right]=-\int_{a}^{b} f_{\theta}(\theta) \log f_{\theta}(\theta) \mathrm{d} \theta$. Prior information about $\theta$ is $\mathbb{E}\left[\theta^{k}\right]=\int_{a}^{b} \theta^{k} f_{\theta}(\theta) \mathrm{d} \theta=f_{k}, 0 \leq k \leq m$. For example, $f_{1}$ (the mean) may be a pointwise (deterministic) estimate. By calculus of variations, the maximum of $\mathcal{S}$ is attained at

$$
f_{\theta}(\theta)=\mathcal{X}_{[a, b]}(\theta) \exp \left(-\lambda_{0}-\sum_{k=1}^{m} \lambda_{k} \theta^{k}\right)
$$

where $\lambda_{0}, \ldots, \lambda_{m}$ are the Lagrange constants.
There are different maximum entropy distributions depending on the prior information:

1. Only a bounded support $[a, b]$ is known: $\theta \sim \operatorname{Uniform}(a, b)$.
2. Only the support $[0, \infty)$ and the mean $f_{1}$ are known: $\theta \sim \operatorname{Exponential}\left(1 / f_{1}\right)$ with rate parameter $1 / f_{1}$.
3. Only the support $(-\infty, \infty)$, the mean $f_{1}$ and the variance $f_{2}-\left(f_{1}\right)^{2}$ are known: $\theta \sim \operatorname{Normal}\left(f_{1}, f_{2}-\left(f_{1}\right)^{2}\right)$.
4. Only the support $[a, b]$ and the mean $f_{1}$ are known: $\left.\theta \sim \operatorname{Exponential}\left(1 / f_{1}\right)\right|_{[a, b]}$.
5. Otherwise, the Lagrange constants and the maximum entropy distribution are calculated numerically by solving the nonlinear system of equations defined by the restrictions.

## 6 Example

Paper [1] demonstrated that, for small $n$ (in their case $n=3$ ), the RVT technique is successfully applied by means of numerical integration. In this section, we focus on a higher $n, n=10$, for which numerical integration cannot be performed and parametric Monte Carlo simulation is conducted. The methodology from [1] cannot tackle this problem.

For a test problem in forward uncertainty quantification, consider the following distributions for $\lambda_{1}, \ldots, \lambda_{9}$ (recall that $\lambda_{10}=0$ ):

$$
\begin{gathered}
\left.\lambda_{1} \sim \operatorname{Exponential}(0.5)\right|_{[1.97,2.03]},\left.\quad \lambda_{2} \sim \operatorname{Exponential}(0.8)\right|_{[1.22,1.28]}, \\
\left.\lambda_{3} \sim \operatorname{Exponential}(1)\right|_{[0.97,1.03]},\left.\quad \lambda_{4} \sim \operatorname{Exponential}(0.4)\right|_{[2.47,2.53]}, \\
\left.\lambda_{5} \sim \operatorname{Exponential}(0.6)\right|_{[1.637,1.697]},\left.\quad \lambda_{6} \sim \operatorname{Exponential}(0.3)\right|_{[3.303,3.363]}, \\
\left.\lambda_{7} \sim \operatorname{Exponential}(0.9)\right|_{[1.081,1.141]},\left.\quad \lambda_{8} \sim \operatorname{Exponential(1)}\right|_{[0.97,1.03]}, \\
\left.\lambda_{9} \sim \operatorname{Exponential}(1.2)\right|_{[0.803,0.863]}
\end{gathered}
$$

These are test Exponential distributions with rate parameter, truncated in the domain mean $\pm 0.03$. For $N_{1}(0), \ldots, N_{10}(0)$, the following test distributions are considered, respectively:

$$
\operatorname{Exponential}(\eta), \quad \eta \in\{2,3,1,4,2,3,2,2,1,3\}
$$

Based on the MEP, the input probability distributions are selected according to prior information (pointwise/deterministic estimates, variability, support, etc.), in a consistent manner by maximizing the Shannon entropy functional. In modeling, this is the first step, before uncertainty quantification for the model output. Here, the prior information would be a pointwise estimate, which would be regarded as the mean value, and a positive support. The obtainment of prior information is not a trivial task and shall be further studied in the future.

In Fig. 1, the estimated PDFs of $N_{1}(t), N_{5}(t), N_{6}(t)$ and $N_{10}(t)(m=1,5,6,10)$ are plotted in four different panels. Several times $t$ are shown to illustrate the evolution of the PDF. Formula (2)-(3) is employed, with 50,000 realizations. It is observed that, as $t$ grows, the concentrations $N_{1}(t), N_{5}(t)$ and $N_{6}(t)$ decay: the densities tend to the vertical axis (i.e. to zero mean and zero variance). By contrast, the concentration $N_{10}(t)$ increases as $t$ grows. This is an analogous behavior to the deterministic counterpart. In order to better appreciate this behavior, we plot in Fig. 2 the time evolution of the deterministic solution, the expectation and the standard deviation, in three panels. For the deterministic solution, the mean values of the input parameters are fixed as deterministic values (the deterministic value for $\lambda_{8}$ was slightly modified by adding an $\epsilon=0.001$, so that $\lambda_{3} \neq \lambda_{8}$ and (1) is well-defined). It is observed that the deterministic solution and the expectation are very similar.

It can be seen that for some estimates (mainly for lower $t$ and larger $m$ ) there is a noise due to the large variance of the estimator (see the discussion at the end of Sect. 3); in those cases, more realizations are required. In this regard, Fig. 3 examines the convergence of the estimated PDFs and the reduction of noise as the number of realizations gets larger, for $m=10$ and $t=4$ (in the fourth panel of Fig. 1, the PDF was represented with 50,000 realizations).


Fig. 1. Estimated PDFs of $N_{1}(t), N_{5}(t), N_{6}(t)$ and $N_{10}(t)$ at different time instants.

## 7 Conclusions

The main results from [1] on the randomized RDC model have been extended to a general number of nuclear species, by applying the RVT technique appropriately. The target PDF has been obtained semi-explicitly, in terms of an expectation. The expression is independent of the input distributions, which may be consistently selected according to the MEP. When the number of random inputs is low, numerical integrations give the PDF. However, when the number of random inputs is moderate or large, the expectation that defines the PDF is estimated via Monte Carlo simulation. This is a parametric estimation of the PDF, in contrast to the classical kernel estimation. Parametric estimation may show many advantages, in terms of rate of convergence, capture of density features, robustness and acceleration via variance reduction techniques, although care must be exercised due to possible noisy features.

## Appendix

We prove (2). Let $\mathcal{C}$ be a Borel set in $\mathbb{R}$. By definition of conditional law,

$$
\begin{aligned}
\mathbb{P}\left(Z_{1} A+Z_{2} \in \mathcal{C}\right) & =\int_{\mathbb{R}^{2}} \mathbb{P}\left(Z_{1} A+Z_{2} \in \mathcal{C} \mid Z_{1}=z_{1}, Z_{2}=z_{2}\right) \mathbb{P}_{\left(Z_{1}, Z_{2}\right)}\left(\mathrm{d} z_{1}, \mathrm{~d} z_{2}\right) \\
& =\int_{\mathbb{R}^{2}} \mathbb{P}\left(z_{1} A+z_{2} \in \mathcal{C}\right) \mathbb{P}_{\left(Z_{1}, Z_{2}\right)}\left(\mathrm{d} z_{1}, \mathrm{~d} z_{2}\right)
\end{aligned}
$$

Since $A$ has a PDF,

$$
\begin{aligned}
\mathbb{P}\left(Z_{1} A+Z_{2} \in \mathcal{C}\right) & =\int_{\mathbb{R}^{2}} \int_{\left(\mathcal{C}-z_{2}\right) / z_{1}} f_{A}(a) \mathrm{d} a \mathbb{P}_{\left(Z_{1}, Z_{2}\right)}\left(\mathrm{d} z_{1}, \mathrm{~d} z_{2}\right) \\
& =\int_{\mathbb{R}^{2}} \int_{\mathcal{C}} f_{A}\left(\frac{a-z_{2}}{z_{1}}\right) \frac{1}{\left|z_{1}\right|} \mathrm{d} a \mathbb{P}_{\left(Z_{1}, Z_{2}\right)}\left(\mathrm{d} z_{1}, \mathrm{~d} z_{2}\right)
\end{aligned}
$$



Fig. 2. Time evolution of the deterministic solution, the expectation and the standard deviation, for $N_{1}(t), N_{5}(t), N_{6}(t)$ and $N_{10}(t)$.


Fig. 3. Convergence of estimated PDFs as the amount of realizations grows, for $N_{10}(4)$.

By Fubini's Theorem (justified because the integrand is nonnegative) and the expression of the expectation,

$$
\begin{aligned}
\mathbb{P}\left(Z_{1} A+Z_{2} \in \mathcal{C}\right) & =\int_{\mathcal{C}} \int_{\mathbb{R}^{2}} f_{A}\left(\frac{a-z_{2}}{z_{1}}\right) \frac{1}{\left|z_{1}\right|} \mathbb{P}_{\left(Z_{1}, Z_{2}\right)}\left(\mathrm{d} z_{1}, \mathrm{~d} z_{2}\right) \mathrm{d} a \\
& =\int_{\mathcal{C}} \mathbb{E}\left[f_{A}\left(\frac{a-Z_{2}}{Z_{1}}\right) \frac{1}{\left|Z_{1}\right|}\right] \mathrm{d} a .
\end{aligned}
$$

This proves (2).
Though not used in the current paper, (2) may be generalized as follows. Let $\boldsymbol{A}$ be an absolutely continuous random vector of length $m$. Let $\boldsymbol{M}$ be an $m \times m$ random matrix and $\boldsymbol{Z}$ be a random vector of length $m$. Suppose that $\boldsymbol{A}$ is
independent of $(\boldsymbol{M}, \boldsymbol{Z})$ and that $\boldsymbol{M}$ is invertible almost surely. Then $\boldsymbol{M} \boldsymbol{A}+\boldsymbol{Z}$ is absolutely continuous, with PDF

$$
f_{\boldsymbol{M} \boldsymbol{A}+\boldsymbol{Z}}(\boldsymbol{a})=\mathbb{E}\left[f_{\boldsymbol{A}}\left(\boldsymbol{M}^{-1}(\boldsymbol{a}-\boldsymbol{Z})\right) \frac{1}{|\operatorname{det}(\boldsymbol{M})|}\right]
$$

## Funding

Marc Jornet has been supported by a postdoctoral contract from Universitat Jaume I, Spain (Acció 3.2 del Pla de Promoció de la Investigació de la Universitat Jaume I per a l'any 2020).

## Conflict of Interest Statement

The authors declare that there is no conflict of interests regarding the publication of this article.

## Data availability statement

Data sharing not applicable to this article as no datasets were generated or analyzed during the current study.

## References

1. A. Hussein, M.M. Selim, Eur. Phys. J. Plus. 135(5), 418 (2020). https://doi.org/10.1140/epjp/s13360-020-00389-6
2. T. Neckel, F. Rupp, Random Differential Equations in Scientific Computing, (Walter de Gruyter, 2013)
3. R.C. Smith, Uncertainty Quantification: Theory, Implementation, and Applications, (SIAM, 2013)
4. A. Hussein, M.M. Selim, Eur. Phys. J. Plus. 130(12), 249 (2015). https://doi.org/10.1140/epjp/i2015-15249-3
5. F.A. Dorini, M.S. Cecconello, L.B. Dorini, Commun. Nonlinear Sci. Numer. Simulat. 33, 160-173 (2016). https://doi.org/10.1016/j.cnsns.2015.09.009
6. H. Slama, N.A. El-Bedwhey, A. El-Depsy, M.M. Selim, Eur. Phys. J. Plus. 132(12), 505 (2017). https://doi.org/10.1140/epjp/i2017-11763-6
7. J. Calatayud, J.C. Cortés, F.A. Dorini, Fluct. Noise Lett. 20(4, 2150038), 10 pages (2021). https://doi.org/10.1142/S0219477521500383
8. T.T. Soong, Random Differential Equations in Science and Engineering, (Academic Press, New York, 1973)
9. W.J. Padgett, G. Schultz, C.P. Tsokos, SIAM J. Appl. Math. 32(2), 467-483 (1977). https://doi.org/10.1137/0132039
10. M. Ehrendorfer, Mon. Weather Rev. 122(4), 714-728 (1994).
11. A. Halder, R. Bhattacharya, J. Guid. Control Dynam. 34(2), 459-474 (2011). https://doi.org/10.2514/1.51196
12. J.-C. Cortés, M. Jornet, Mathematical and Computational Applications, 25(2), 33-41 https://doi.org/10.3390/mca25020033
13. H. Bateman, Proc. Camb. Philos. Soc. 15, 423-427 (1910)
14. G. Casella, R.L. Berger, Statistical Inference, 2nd edn. (Duxbury Pacific Grove, CA, 2002)
15. Z. Botev, A. Ridder, Wiley StatsRef: Statistics Reference Online, 1-6 (2017). https://doi.org/10.1002/9781118445112.stat07975
16. B.W Silverman, Density Estimation for Statistics and Data Analysis, (Chapman and Hall, 1986)
17. M. Jornet, J. Calatayud, O.P. Le Maître, J.-C. Cortés, J. Comput. Appl. Math. 374, 112770 (2020). https://doi.org/10.1016/j.cam.2020.112770
18. M. Jornet, J. Calatayud, O.P. Le Maître, J.-C. Cortés, Int. J. Uncertain. Quant. 10(5), 467-497 (2020). https://doi.org/10.1615/Int.J.UncertaintyQuantification. 2020032659
19. F. Udwadia, SIAM Rev. 31(1), 103-109 (1989). https://doi.org/10.1137/1031004
20. F.A. Dorini, R. Sampaio, J. Appl. Mech. 79(5), 051008-051014 (2012). https://doi.org/10.1115/1.4006453
21. M. Jornet, Stoch. Anal. Appl. 39, 22-32 (2021). https://doi.org/10.1080/07362994.2020.1777163
