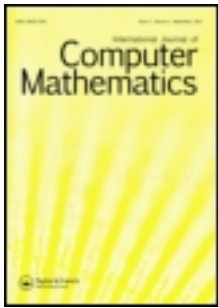


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# Stochastic dynamics simulation with generalized interval probability

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Two types of uncertainties are generally recognized in modelling and simulation, including variability caused by inherent randomness and incertitude due to the lack of perfect knowledge. In this paper, a generalized interval-probability theory is used to model both uncertainty components simultaneously, where epistemic uncertainty is quantified by generalized interval in addition to probability measure. Conditioning, independence, and Markovian probabilities are uniquely defined in generalized interval probability such that its probabilistic calculus resembles that in the classical probability theory. A path-integral approach can be taken to solve the interval Fokker–Planck equation for diffusion processes. A Krylov subspace projection method is proposed to solve the interval master equation for jump processes. Thus, the time evolution of both uncertainty components can be simulated simultaneously, which provides the lower and upper bound information of evolving probability distributions as an alternative to the traditional sensitivity analysis.

**Keywords:** aleatory uncertainty; epistemic uncertainty; imprecise probability; reliable simulation; multi-scale simulation

2010 AMS Subject Classifications: 60A86; 60J60; 60J75; 65G40

## 1. Introduction

Reliable simulation requires uncertainty to be quantified. Uncertainty in simulation and computation is composed of two components. One is the inherent *randomness* because of fluctuation and perturbation, called *aleatory* uncertainty, and the other is due to *lack of perfect knowledge* about the system, called *epistemic* uncertainty. Aleatory uncertainty is also referred to as variability, stochastic uncertainty, irreducible uncertainty, and random error, whereas epistemic uncertainty is also known as incertitude, model form uncertainty, reducible uncertainty, and systematic error.

The two types of uncertainties have distinctively different sources and should be differentiated. In modelling and simulation (M&S), epistemic uncertainty is the result of bias and error associated with the models and input data. For instance, in finite-element analysis, epistemic uncertainty comes from the truncation error involved in linear and nonlinear approximations of strain fields using polynomials, imprecise input parameters in the model, mismatch of structures and geometric configurations between the modelled and the true physical ones, etc. In molecular dynamics simulation, epistemic uncertainty is mainly from the inaccurate interatomic potential functions.

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In kinetic Monte Carlo simulation, it is largely from the imperfect knowledge about transition and reaction rates. In contrast to epistemic uncertainty, sources such as disturbed boundary and loading conditions, different sampling sizes and simulation times, inherent variations of material compositions, and other randomness and fluctuation form the aleatory component of uncertainty.

Given the very different natures of the two types of uncertainties, it is important to distinguish and treat them separately. Neglecting epistemic uncertainty in modelling, simulation, and analysis may lead to decisions that are not robust. The typical way to assess the robustness of stochastic simulation because of epistemic uncertainty is sensitivity analysis (SA), which is to check how much variation the analysis result may have if input distribution parameters or types deviate from the ones used in the analysis. Conflating epistemic and aleatory uncertainties may increase the cost of risk management. If extra knowledge of the collected data is available, they can be further clustered into smaller groups or intrinsic mathematical relations can be identified so that variance can be reduced, which reflects pure randomness more accurately for risk analysis.

### 1.1 Sources of epistemic uncertainty in M&S

The sources of epistemic uncertainty in M&S are summarized as follows.

- *Lack of data or missing data*: the parameters of models, probability distributions, and distribution types are uncertain when the sample size for input analysis and data fitting is small. In some situations, it may not be possible to collect enough data on the random variables of interest. The lack of enough information will introduce errors in models and requires the analyst to find new ways to describe the associated uncertainty more rigorously.
- *Conflicting information*: if there are multiple sources of information, the analyst may face conflicts among them. It is not appropriate to draw a simple conclusion of distributions from several pieces of contradictory evidence. The absence of relevant information has to be properly modelled and incorporated in M&S.
- *Conflicting beliefs*: when data are not available, the analyst usually depends on experts' judgments, opinions, and beliefs. The information obtained from experts is subjective due to the diversity of their past experiences, which can lead to inconsistent observations.
- *Lack of introspection*: in some cases, the analyst cannot afford the necessary time to think deliberately about an uncertain event or an accurate description of physical systems. The lack of introspection increases the risk of inaccurate model of the system under study. The associated uncertainties have to be reflected in the simulation input distributions to receive more reliable outputs.
- *Lack of information about dependency*: lack of knowledge about the correlations among factors and variables as well as unknown time dependency of these factors contribute in the increased uncertainties of M&S. The consideration of unknown dependency among variables will build more reliable simulation models.
- *Numerical errors because of truncation and round-off*: approximation and truncation errors are inherent in numerical methods used for simulations, as well as rounding and cancellation errors.
- *Measurement errors*: all measurements are approximated values (instead of true values) due to the limitations of measuring device, measuring environment, process of measurement, and human errors. The uncertainties associated with the collected quantities should be addressed in parameterization in order to give more reliable outputs.

Since aleatory and epistemic uncertainties come from separate sources and have very different characteristics in nature, we should represent them differently, preferably in different forms, so that they can be easily differentiated. Aleatory uncertainty is traditionally and predominantly modelled

by probability distributions. In contrast, epistemic uncertainty has been modelled in several ways, such as probability, interval, fuzzy set, random set, and basic probability assignment. In this paper, interval is used to quantify epistemic uncertainty.

## 1.2 Interval to quantify epistemic uncertainty

Interval is as simple as a pair of numbers, i.e. the lower and upper bounds. The reason to choose interval is twofold. First, interval is natural to human users and simple to use. It has been widely used to represent a range of possible values, an estimate of lower and upper bounds for numerical errors, and the measurement error because of the available precision as the result of instrument calibration. Second, interval can be regarded as the most suitable way to represent the lack of knowledge. Compared to other forms, interval has the least assumption. It only needs two values for the bounds. In contrast, statistical distributions need assumptions of distribution types, distribution parameters, and the functional mapping from events to real values between 0 and 1. Fuzzy sets need assumptions of not only lower and upper bounds, but also membership functions. Given that the lack of knowledge is the nature of epistemic uncertainty, a representation with the least assumption is the most desirable. Notice that an interval  $[L, U]$  only specifies its lower bound  $L$  and upper bound  $U$ . It does not assume a uniform distribution of values between  $L$  and  $U$ .

The analysis of systems based on intervals has computational advantages over the traditional probabilistic approach when the worst-case scenario is of the main concern in uncertainty quantification and risk assessment. In many applications, such as engineering and decision-making, we would like to know what could be the worst and best possible situations. Interval analysis allows us to estimate the bounds in the worst-case scenario analytically with interval arithmetic. Although uniform distributions can also be used as the input to estimate the lower and upper bounds of outputs as in Monte Carlo sampling, extensive sampling is required in order to cover all possible scenarios and receive the good estimations of lower and upper bounds. Interval analysis does not require sampling, and guarantees that all possible scenarios are enclosed by the analytically estimated bounds. On the other hand, the bounds estimated by interval analysis could be too pessimistic or too wide. The generalized interval used in this paper is a new approach to avoid the over-estimation of bounds, which will be introduced later in Section 2.3.

Probability itself has its limitations in representing epistemic uncertainty. The accuracy of simulation prediction heavily depends on the fundamental understanding of the underlying physical and chemical processes. Lack of perfect knowledge and fundamental insight inevitably makes models imperfect. Any assumption made about distributions in M&S has introduced a bias. The most significant limitation of probability is that it does not differentiate total ignorance from other probability distributions. Total ignorance means that the analyst has zero knowledge about the system under study. Based on the principle of maximum entropy, uniform distributions are usually assumed when traditional probability theory is applied in this case. A problem arises because introducing a uniform or any particular form of distribution has itself introduced extra information that is not justifiable by the zero knowledge. The commonly used uniform distribution where all possible values are equally likely is not guaranteed to be true because we are totally ignorant. This leads to the Bertrand-style paradoxes such as van Fraassen's cube factory [50]. 'Knowing the unknown' does not represent the total ignorance. Although the Bayesian approach has been proposed to reduce the bias introduced in the distribution assumption, and it serves the purpose well in an ideal situation with the premise that we have plenty of data supply with no measurement errors, its limitation remains in the real-world applications where lack of data or imperfect measurement lingers. Arguably if there are plenty of data available, we would gain enough knowledge and the uncertainty has become aleatory in nature instead of epistemic. Other limitations of probability include capturing group inconsistency and personal indeterminacy where precise

values of probabilities are difficult to determine. Therefore, it is desirable to have more general and efficient approaches to incorporate epistemic uncertainty in M&S, with the least assumptions of probability distributions and their parameters and less computationally demanding than the traditional sampling or Bayesian learning approaches.

Interval can overcome the limitation of probability in quantifying the lack of knowledge. Imprecise probability  $[p, \bar{p}]$  combines epistemic uncertainty (as an interval) with aleatory uncertainty (as probability measure), which is regarded as a generalization of traditional probability. Gaining more knowledge can reduce the level of imprecision and indeterminacy, i.e. the interval width. When  $p = \bar{p}$ , the degenerated interval probability becomes a traditional precise one.

To model the simultaneous evolution of aleatory and epistemic uncertainties in dynamic systems, computationally tractable algorithms based on imprecise probabilities are desirable. In this paper, a generalized interval-probability approach is taken to quantify the two components of uncertainty, where epistemic uncertainty is represented by generalized interval, in combination with probability measure. Similar to the traditional probability, generalized interval probability is defined as a probability measure that obeys the axioms of Kolmogorov, which is different from other forms of imprecise probability. In addition, a logic coherence constraint for a mutually disjoint partition of events is required. As a result, we can define conditional probability, the generalized interval Bayes' rule (GIBR), and independence in the forms that resemble those in the precise probability theory. These fundamental properties enable ease of computation and distinguish the proposed generalized interval probability from other imprecise probabilities. It provides the unification between imprecise and precise probabilities.

It is well known that the dynamics of stochastic systems can be generally described by the differential Chapman–Kolmogorov equation (CKE). There are two special cases of the CKE. When the rates of transition in a CKE vanish, the CKE degenerates to a Fokker–Planck equation (FPE) that describes drift–diffusion processes. When the coefficients of drift and diffusion in a CKE are zeros, the CKE becomes a chemical master equation (CME) that describes jump processes. Therefore, FPE's and CME's can be used to simulate stochastic dynamics from two different perspectives at two different length and time scales. In this paper, we present the generalized versions of FPE's and CME's so that a system under both aleatory and epistemic uncertainties can be simulated.

To model diffusion processes under uncertainties, a generalized version of FPE was recently developed [54], where coefficients of drift and diffusion are interval-valued parameters and probability distributions follow the generalized interval probability. In this paper, the stochastic modelling based on generalized interval probability is extended to describe jump processes under aleatory and epistemic uncertainties. It is demonstrated that the simulation based on generalized interval probability are algebraically tractable, as an efficient alternative to SA.

In the remainder of this paper, the background of imprecise probability and generalized interval is introduced in Section 2. Section 3 presents the basics of generalized interval probability. The Markov chain model with generalized interval probability is shown in Section 4. Section 5 describes a path-integral approach to solve the interval FPE to simulate drift–diffusion processes. Section 6 presents a new Krylov subspace projection method to solve the interval master equation to simulate jump processes.

## 2. Background

### 2.1 Existing approaches for robustness in M&S

The ultimate goal of incorporating both components of uncertainty in M&S is to improve the robustness of predictions. Some of the standard approaches that have been used to explore the

impact of input uncertainties are SA and design of experiment (DOE) [19,22,26]. When input probability distributions with associated parameters are selected, the analyst needs to know how sensitive the simulation output performance is, with respect to (w.r.t.) the selected input parameter values. A straightforward way is to vary the input values and study the impact resulted on the output. We can also determine which input factors have the most significant impact on the output by evaluating the amount of output variations as the direct result of modifying the inputs. The sensitivity can be numerically estimated with finite differences. Similarly, the DOE approach is performed by varying the input parameters by levels and examining the output changes. In addition to these direct (forward) methods, adjoint (backward) SA approaches were also developed for deterministic simulation, such as solving ordinary differential equations (ODE's) [2,40,42] and partial differential equations (PDE's) [13,35,58] when a large number of sensitivity parameters but few objective functions are involved, in which case the adjoint methods are more efficient than the direct methods.

A more efficient SA approach that is specific for stochastic simulation is to estimate the derivatives of the expected values of output performance, i.e. the expected values of stochastic derivatives or gradients, from simulation directly. This can be achieved by either varying output performance w.r.t. input parameters such as the infinitesimal perturbation analysis (IPA) alike methods [14,20,48], or by varying the probability measures w.r.t. inputs such as the likelihood ratio method [15,37,39].

Another popular simulation technique that represents the total uncertainty is based on the second-order probability and second-order Monte Carlo (SOMC) [49]. A second-order probabilistic SA is superimposed on the traditional simulation so that uncertainties are quantified by sampling the parameters of the first-order probabilistic distributions. In the double-loop simulation, the inner loop is the variability loop, whereas the outer loop represents the uncertainty of the input parameters of the inner loop. Computationally, SOMC is very expensive. Other approaches to consider input uncertainties in deterministic and stochastic simulation include the Bayesian analysis approach [4,59] and the bootstrap approaches [1,3].

The issue of the traditional SA for stochastic simulation is the computational efficiency. In SOMC, a large number of samples have to be drawn as the possible values of the inputs in order to make robust conclusions. Each sample is one complete run of simulation itself. Similarly, in the IPA methods and Bayesian approaches, the number of runs should be large enough to draw credible conclusions. The result of Bayesian update is sensitively dependent on the prior distribution, unless the amount of data available for the update is substantially large. Therefore, computational efficiency is the bottom-neck of those approaches to assess the robustness of stochastic simulation. The SA methods for ODE's and PDE's are not directly applicable to assess the robustness of stochastic differential equations that describe stochastic dynamics. Although the special formulation of CME and FPE employed in this paper can convert stochastic differential equations to deterministic ODE's, overhead for solving extra equations is still involved if direct or adjoint methods are applied, which will be discussed in detail in Section 6.

## 2.2 Imprecise probability

Many forms of imprecise probabilities have been developed. For example, the Dempster-Shafer theory [6,43] characterizes evidence with discrete probability masses associated with a power set of values. The theory of coherent lower previsions [51] models uncertainties with the lower prevision (supremum acceptable buying price) and the upper prevision (infimum acceptable selling price) following the notations of de Finetti's subjective probability theory. The possibility theory [9] represents uncertainties with Necessity-Possibility pairs. Probability bound analysis [10] captures uncertain information with pairs of lower and upper distribution functions or  $p$ -boxes.

Interval probability [25] characterizes statistical properties as intervals.  $F$ -probability [56] incorporates intervals and represents an interval probability as a set of probabilities which maintain the Kolmogorov properties. A random set [29] is a multi-valued mapping from the probability space to the value space. Fuzzy probability [30] considers probability distributions with fuzzy parameters. A cloud [33] is a combination of fuzzy sets, intervals, and probability distributions.

In the applications of interval probability, the interval bounds  $\underline{p}$  and  $\bar{p}$  can be solicited as the lowest and highest subjective probabilities about a particular event, when the domain expert may hesitate to offer just a precise value of probability. In addition, different experts could have different beliefs. In both cases, the range of probabilities gives the interval bounds. The bounds can also be obtained from the basic probability assignments formulated in the Dempster–Shafer theory [6,43]. When used in data analysis with frequency interpretation, the bounds can be confidence intervals that are calculated from data to enclose a cumulative distribution function.

Imprecise probability quantifies aleatory and epistemic uncertainties simultaneously and can be used as an alternative to SA in assessing robustness of M&S. In this paper, a new form of imprecise probability, generalized interval probability, is described and applied in M&S. This new form is based on a generalized interval, which is an algebraic and semantic extension of the classical set-based interval. As a result, the probabilistic calculus in generalized interval probability is greatly simplified.

### 2.3 Generalized interval

The classical set-based interval [31] is defined as  $\llbracket a, b \rrbracket := \{x \in \mathbb{R} \mid a \leq x \leq b\}$ . Therefore,  $\llbracket a, b \rrbracket$  is invalid when  $a > b$ . In contrast, generalized interval [8,12,27] does not have such restriction. A generalized interval is defined as a pair of numbers  $\mathbf{x} := [\underline{x}, \bar{x}] (\underline{x}, \bar{x} \in \mathbb{R})$ .

The calculation of generalized interval is based on the Kaucher interval arithmetic [21]. Compared to the semi-group formed by the classical set-based intervals without invertibility, generalized intervals form a group. This property significantly simplifies the computational structure. The set of generalized intervals is denoted by  $\mathbb{K}\mathbb{R} = \{[\underline{x}, \bar{x}] \mid \underline{x}, \bar{x} \in \mathbb{R}\}$ . The set of *proper* intervals is  $\mathbb{I}\mathbb{R} = \{[\underline{x}, \bar{x}] \mid \underline{x} \leq \bar{x}\}$ , and the set of *improper* intervals is  $\mathbb{II}\mathbb{R} = \{[\underline{x}, \bar{x}] \mid \underline{x} \geq \bar{x}\}$ . The relationship between proper and improper intervals is established with the operator *dual* as  $\text{dual}([\underline{x}, \bar{x}]) := [\bar{x}, \underline{x}]$ . Thus, the group of generalized intervals is formed with  $\mathbf{x} - \text{dual}\mathbf{x} = 0$  and  $\mathbf{x} \div \text{dual}\mathbf{x} = 1$ .

The *inclusion* relationship  $\subseteq$  between generalized intervals  $\mathbf{x} = [\underline{x}, \bar{x}]$  and  $\mathbf{y} = [\underline{y}, \bar{y}]$  is defined as

$$[\underline{x}, \bar{x}] \subseteq [\underline{y}, \bar{y}] \iff \underline{x} \geq \underline{y} \wedge \bar{x} \leq \bar{y}. \quad (1)$$

The *less-than-or-equal-to* relationship  $\leq$  is defined as

$$[\underline{x}, \bar{x}] \leq [\underline{y}, \bar{y}] \iff \underline{x} \leq \underline{y} \wedge \bar{x} \leq \bar{y}. \quad (2)$$

The relationship between generalized interval and classical interval is established with the operator  $\Delta$  defined as

$$[\underline{x}, \bar{x}]^\Delta := \llbracket \min(\underline{x}, \bar{x}), \max(\underline{x}, \bar{x}) \rrbracket \quad (3)$$

The absolute value of  $\mathbf{x} = [\underline{x}, \bar{x}]$  is defined as

$$|\mathbf{x}| := \begin{cases} [-\bar{x}, -\underline{x}] & (\underline{x} < 0, \bar{x} < 0), \\ [0, \max(-\underline{x}, \bar{x})] & (\underline{x} < 0, \bar{x} \geq 0), \\ [\max(\underline{x}, -\bar{x}), 0] & (\underline{x} \geq 0, \bar{x} < 0), \\ [\underline{x}, \bar{x}] & (\underline{x} \geq 0, \bar{x} \geq 0). \end{cases}$$

Table 1. Illustrations of the semantic extension of generalized interval.

Algebraic relation $[\underline{x}, \bar{x}] + [\underline{y}, \bar{y}] = [\underline{z}, \bar{z}]$	Corresponding logic interpretation	Quantifier of $[\underline{z}, \bar{z}]$	Range estimation of $[\underline{z}, \bar{z}]$
$[2, 3] + [2, 4] = [4, 7]$	$(\forall x \in [2, 3])(\forall y \in [2, 4])(\exists z \in [4, 7])(x + y = z)$	$\exists$	$[4, 7]$ is <i>complete</i>
$[2, 3] + [4, 2] = [6, 5]$	$(\forall x \in [2, 3])(\forall z \in [5, 6])(\exists y \in [2, 4])(x + y = z)$	$\forall$	$[5, 6]$ is <i>sound</i>
$[3, 2] + [2, 4] = [5, 6]$	$(\forall y \in [2, 4])(\exists x \in [2, 3])(\exists z \in [5, 6])(x + y = z)$	$\exists$	$[5, 6]$ is <i>complete</i>
$[3, 2] + [4, 2] = [7, 4]$	$(\forall z \in [4, 7])(\exists x \in [2, 3])(\exists y \in [2, 4])(x + y = z)$	$\forall$	$[4, 7]$ is <i>sound</i>

The absolute value of a vector  $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n]^T$  is  $|\mathbf{X}| := [|\mathbf{x}_1|, \dots, |\mathbf{x}_n|]^T$ , where T denotes matrix transpose. The L2-norm of the vector  $\mathbf{X}$  is  $\|\mathbf{X}\|_2 := \sqrt{|\mathbf{X}^T \mathbf{X}|}$ . An interval function as a pair of real-valued functions is defined as  $\mathbf{f}(x) := [\underline{f}(x), \bar{f}(x)]$ . The integral of  $\mathbf{f}(x)$  is defined as  $\int \mathbf{f}(x) dx := [\int \underline{f}(x) dx, \int \bar{f}(x) dx]$  [27].

Not only generalized interval based on the Kaucher arithmetic simplifies the computational structure, it also provides more semantics than the classical set-based interval. In a functional relation, each generalized interval has an associated logic quantifier, either existential ( $\exists$ ) or universal ( $\forall$ ). The semantics of a generalized interval  $\mathbf{x} \in \mathbb{K}\mathbb{R}$  is denoted by  $(Q_{\mathbf{x}} \mathbf{x} \in \mathbf{x}^\Delta)$  where  $Q : \mathbb{K}\mathbb{R} \mapsto \{\exists, \forall\}$ .  $\mathbf{x}$  is called *existential* if  $Q_{\mathbf{x}} = \exists$ , or *universal* if  $Q_{\mathbf{x}} = \forall$ . If a real relation  $z = f(x_1, \dots, x_n)$  is extended to the interval relation  $\mathbf{z} = \mathbf{f}(\mathbf{x}_1, \dots, \mathbf{x}_n)$ , the interval relation  $\mathbf{z}$  is interpretable if there is a semantic relation

$$(Q_{x_1} x_1 \in \mathbf{x}_1^\Delta) \cdots (Q_{x_n} x_n \in \mathbf{x}_n^\Delta) (Q_z z \in \mathbf{z}^\Delta) (z = f(x_1, \dots, x_n)).$$

Generalized interval provides more semantic power to help verify completeness and soundness of range estimations by logic interpretations. A *complete* range estimation of possible values includes all possible occurrences without underestimation. A *sound* range estimation does not include impossible occurrences without overestimation. The four examples in Table 1 illustrate the interpretations for operator ‘+’.

### 3. Basics of generalized interval probability

The basics of generalized interval probability are defined as follows [52].

DEFINITION 3.1 Given a sample space  $\Omega$  and a  $\sigma$ -algebra  $\mathcal{A}$  of random events over  $\Omega$ , we define the generalized interval probability  $\mathbf{p} \in \mathbb{K}\mathbb{R}$  as  $\mathbf{p} : \mathcal{A} \rightarrow [0, 1] \times [0, 1]$  which obeys the axioms of Kolmogorov: (1)  $\mathbf{p}(\Omega) = [1, 1]$ ; (2)  $[0, 0] \leq \mathbf{p}(E) \leq [1, 1] (\forall E \in \mathcal{A})$ ; and (3) for any countable mutually disjoint events  $E_i \cap E_j = \emptyset (i \neq j)$ ,  $\mathbf{p}(\bigcup_{i=1}^n E_i) = \sum_{i=1}^n \mathbf{p}(E_i)$ .

A generalized interval probability  $\mathbf{p} = [p, \bar{p}]$  is a generalized interval without the restriction of  $p \leq \bar{p}$ . The new definition of interval probability also implies  $\mathbf{p}(\emptyset) = [0, 0]$ .

DEFINITION 3.2 (Union) The probability of union is defined as  $\mathbf{p}(A) := \sum_{S \subseteq A} (-\text{dual})^{|A|-|S|} \mathbf{p}(S)$  for  $A \subseteq \Omega$ .

#### 3.1 Logic coherence constraint

The assignments of interval-valued probabilities to events are not arbitrary. They should meet certain requirements. In generalized interval probability, the interval-probability values should satisfy the *logic coherence constraint* (LCC).



DEFINITION 3.3 [LCC] For a mutually disjoint event partition  $\bigcup_{i=1}^n E_i = \Omega$ ,  $\sum_{i=1}^n \mathbf{p}(E_i) = [1, 1]$ . If the sample space is continuous,  $\int_{x \in \Omega} \mathbf{p}(x) dx = [1, 1]$ .

Notice that the LCC is more restrictive than Walley's coherence and avoid sure loss constraints [51]. The LCC ensures that generalized interval probability is logically coherent with precise probability. Suppose that  $\mathbf{p}(E_i) \in \mathbb{IR}$  (for  $i = 1, \dots, k$ ) and  $\mathbf{p}(E_i) \in \overline{\mathbb{IR}}$  (for  $i = k + 1, \dots, n$ ). It can be interpreted as

$$\forall p_1 \in \mathbf{p}^\Delta(E_1), \dots, \forall p_k \in \mathbf{p}^\Delta(E_k), \exists p_{k+1} \in \mathbf{p}^\Delta(E_{k+1}), \dots, \exists p_n \in \mathbf{p}^\Delta(E_n), \sum_{i=1}^n p_i = 1.$$

For instance, given that  $\mathbf{p}(\text{down}) = [0.2, 0.3]$ ,  $\mathbf{p}(\text{idle}) = [0.3, 0.5]$ , and  $\mathbf{p}(\text{working}) = [0.5, 0.2]$  for a system's working status, we can interpret it as

$$(\forall p_1 \in [0.2, 0.3])(\forall p_2 \in [0.3, 0.5])(\exists p_3 \in [0.2, 0.5])(p_1 + p_2 + p_3 = 1).$$

With different quantifier assignments, we differentiate non-focal events from focal events based on the respective logic interpretation. An event  $E$  is called *focal* if the associated semantics for  $\mathbf{p}(E)$  is universal. Otherwise, it is called *non-focal* if the associated semantics is existential. While the epistemic uncertainty associated with focal events is critical to the analyst, the one associated with non-focal events is not. In the above example, *down* and *idle* are focal events while *working* is non-focal. If the analyst is more interested in *working* and *down*, he/she may assign a different set of interval-probability values, for instance,  $\mathbf{p}(\text{working}) = [0.2, 0.5]$ ,  $\mathbf{p}(\text{down}) = [0.2, 0.3]$ , and  $\mathbf{p}(\text{idle}) = [0.6, 0.2]$ .

### 3.2 Conditional probability, independence, and GIBR

The concepts of conditional probability, independence, and Bayes' rule are critical for the classical probability theory. With independence, we can decompose a complex problem into simpler and manageable components. With Bayes' rule, information can be combined and updated for assessment. Similarly, they are essential for imprecise probabilities.

Different from all other forms of imprecise probabilities, which are based on convex probability sets, the conditional probability in the generalized interval-probability theory is defined directly from marginal probability.

DEFINITION 3.4 The conditional interval probability  $\mathbf{p}(E | C)$  for all  $E, C \in \mathcal{A}$  is defined as

$$\mathbf{p}(E | C) := \frac{\mathbf{p}(E \cap C)}{\text{dual}\mathbf{p}(C)} = \left[ \frac{\underline{p}(E \cap C)}{\underline{p}(C)}, \frac{\bar{p}(E \cap C)}{\bar{p}(C)} \right], \quad (4)$$

when  $\mathbf{p}(C) > 0$ .

Thanks to the unique algebraic properties of generalized intervals, this definition can greatly simplify computation in applications. Only algebraic computation is necessary.

DEFINITION 3.5 For  $A, B, C \in \mathcal{A}$ ,  $A$  is said to be conditionally independent with  $B$  on  $C$  if and only if

$$\mathbf{p}(A \cap B | C) = \mathbf{p}(A | C)\mathbf{p}(B | C). \quad (5)$$

DEFINITION 3.6 For  $A, B \in \mathcal{A}$ ,  $A$  is said to be independent with  $B$  if and only if

$$\mathbf{p}(A \cap B) = \mathbf{p}(A)\mathbf{p}(B). \quad (6)$$

The independence in Definition 3.6 is a special case of conditional independence in Definition 3.5, where  $C$  is the complete sample space  $\Omega$ . The conditional independence also has a second form, as shown in Theorem 3.7.

THEOREM 3.7 For  $A, B, C \in \mathcal{A}$ ,  $\mathbf{p}(A \cap B | C) = \mathbf{p}(A | C)\mathbf{p}(B | C) \iff \mathbf{p}(A | B \cap C) = \mathbf{p}(A | C)$ .

*Proof* From the definition of conditional probability,  $\mathbf{p}(A \cap B | C) = \mathbf{p}(A | C)\mathbf{p}(B | C) \iff \mathbf{p}(A \cap B \cap C)/\text{dual}\mathbf{p}(C) = \mathbf{p}(A | C)\mathbf{p}(B \cap C)/\text{dual}\mathbf{p}(C) \iff \mathbf{p}(A \cap B \cap C)/\text{dual}\mathbf{p}(B \cap C) = \mathbf{p}(A | C) \iff \mathbf{p}(A | B \cap C) = \mathbf{p}(A | C)$ . ■

COROLLARY 3.8 For  $A, B, C, D \in \mathcal{A}$  and  $A \cap D = \emptyset$ , the conditional independence between  $A$  and  $B$  given  $C$  and between  $A$  and  $D$  given  $C$  infers the independence between  $A \cup D$  and  $B$  given  $C$ .

*Proof*  $\mathbf{p}(A \cup D | B \cap C) = \mathbf{p}((A \cup D) \cap B \cap C)/\text{dual}\mathbf{p}(B \cap C) = [\mathbf{p}(A \cap B \cap C) + \mathbf{p}(D \cap B \cap C)]/\text{dual}\mathbf{p}(B \cap C) = \mathbf{p}(A \cap B \cap C)/\text{dual}\mathbf{p}(B \cap C) + \mathbf{p}(D \cap B \cap C)/\text{dual}\mathbf{p}(B \cap C) = \mathbf{p}(A | B \cap C) + \mathbf{p}(D | B \cap C) = \mathbf{p}(A | C) + \mathbf{p}(D | C) = \mathbf{p}(A \cup D | C)$ . ■

The most intuitive meaning of ‘independence’ is that an independence relationship satisfies several graphoid properties. It has been shown that generalized interval probability with the defined independence is graphoid [53]. With  $X, Y, Z$ , and  $W$  as sets of disjoint random variables and ‘ $\perp$ ’ denoting independence, the conditional independence in Definition 3.5 satisfies all of the following graphoid properties.

COROLLARY 3.9 (Symmetry [53])  $X \perp Y | Z \Rightarrow Y \perp X | Z$

*Remark 1* If knowing  $Y$  does not tell us more about  $X$ , then similarly knowing  $X$  does not tell us more about  $Y$ .

COROLLARY 3.10 (Decomposition [53])  $X \perp (W, Y) | Z \Rightarrow X \perp Y | Z$

*Remark 2* If combined two pieces of information is irrelevant to  $X$ , either individual one is also irrelevant to  $X$ .

COROLLARY 3.11 (Composition [53])  $(X \perp Y | Z) \wedge (X \perp W | Z) \Rightarrow X \perp (W, Y) | Z$

*Remark 3* The combined two pieces of information that are individually irrelevant to  $X$  is also irrelevant to  $X$ .

COROLLARY 3.12 (Contraction [53])  $(X \perp Y | Z) \wedge (X \perp W | (Y, Z)) \Rightarrow X \perp (W, Y) | Z$

*Remark 4* If two pieces of information  $X$  and  $Y$  are irrelevant with prior knowledge of  $Z$  and  $X$  is also irrelevant to a third piece of information  $W$  after knowing  $Y$ , then  $X$  is irrelevant to both  $W$  and  $Y$  before knowing  $Y$ .

COROLLARY 3.13 (Reduction [53])  $(X \perp Y | Z) \wedge (X \perp (W, Y) | Z) \Rightarrow X \perp W | (Y, Z)$

*Remark 5* If two pieces of information  $X$  and  $Y$  are irrelevant with prior knowledge of  $Z$  and at the same time  $X$  is also irrelevant to both  $W$  and  $Y$ , then  $X$  is irrelevant to the third piece of information  $W$  even after knowing  $Y$ .

COROLLARY 3.14 (Weak union [53])  $X \perp (W, Y) \mid Z \Rightarrow X \perp W \mid (Y, Z)$

*Remark 6* Gaining more information about irrelevant  $Y$  does not affect the irrelevance between  $X$  and  $W$ .

COROLLARY 3.15 (Redundancy [53])  $X \perp Y \mid X$

*Remark 7* Knowing that  $X$  is irrelevant to  $Y$  also tells us about  $X$ .

COROLLARY 3.16 (Intersection [53])  $(X \perp W \mid (Y, Z)) \wedge (X \perp Y \mid (W, Z)) \Rightarrow X \perp (W, Y) \mid Z$

*Remark 8* If combined information  $W$  and  $Y$  is relevant to  $X$ , then at least either  $W$  or  $Y$  is relevant to  $X$  after learning the other.

The stochastic independence in precise probability is semi-graphoid satisfying symmetry, decomposition, weak union, and contraction. When the probability distributions are strictly positive, intersection is also satisfied. Then, it becomes graphoid.

With Definition 3.4 of the conditional probability, a GIBR can be directly derived.

THEOREM 3.17 (GIBR) For  $A \in \mathcal{A}$  and a mutually disjoint event partition  $\bigcup_{j=1}^n E_j = \Omega$  with  $\sum_{j=1}^n \mathbf{p}(E_j) = [1, 1]$ ,

$$\mathbf{p}(E_i \mid A) = \frac{\mathbf{p}(A \mid E_i)\mathbf{p}(E_i)}{\sum_{j=1}^n \text{dual}\mathbf{p}(A \mid E_j)\text{dual}\mathbf{p}(E_j)} \quad (7)$$

*Proof* From the definition of conditional probability in Definition 3.4,  $\sum_{j=1}^n \text{dual}\mathbf{p}(A \mid E_j)\text{dual}\mathbf{p}(E_j) = \sum_{j=1}^n \text{dual}[\mathbf{p}(A \mid E_j)\mathbf{p}(E_j)] = \text{dual} \sum_{j=1}^n \mathbf{p}(A \cap E_j) = \text{dual}\mathbf{p}(A)$ . Therefore,  $\mathbf{p}(A \mid E_i)\mathbf{p}(E_i)/\text{dual}\mathbf{p}(A) = \mathbf{p}(A \cap E_i)/\text{dual}\mathbf{p}(A) = \mathbf{p}(E_i \mid A)$ . ■

With the conditional probability and independence defined, a Markov chain model with generalized interval probabilities is used to describe the evolution of a system as transitions of states which we do not have perfect knowledge about, as described in the next section.

#### 4. Markov chain model with generalized interval probabilities

Markov chain is commonly used to model and simulate time evolution of stochastic systems. In addition to the stochasticity, epistemic uncertainty associated with model parameters have been studied. The early work on Markov chain model with imprecise transition probabilities appeared in the study of Markovian decision processes [41,57]. Hartfiel [18] used the name *Markov set-chains* and developed a so-called Hi-Lo algorithm based on convexity to calculate lower and upper bounds of state probabilities with interval transition probabilities. In the more general setting of interval probability, Kozine and Utkin [24] developed a linear programming based algorithm to estimation lower and upper bounds of  $F$ -probability with interval transition probabilities. Škulj [45,46] developed formulations of  $F$ -probability and coherent lower prevision to predict transitions. With

a formulation of coherent upper prevision, de Cooman *et al.* [5] developed an algorithm with linear complexity to estimate the credal set evolution in imprecise Markov chains.

Different from the above, here the imprecise Markov chain is defined based on the generalized interval probability, which can be intuitively kept track of with its resemblance to the classical Markov chain. Given  $n$  possible states of a system, a stationary discrete-time imprecise Markov chain is defined by a state transition matrix  $\mathbf{P} \in \mathbb{K}\mathbb{R}^{n \times n}$  with interval-valued transition probabilities  $\mathbf{p}_{ij} = \mathbf{p}(X = i \mid X = j)$  with  $i = 1, \dots, n$  and  $j = 1, \dots, n$ . Given the probabilistic estimates of the states  $\mathbf{Q}^{(k)} \in \mathbb{K}\mathbb{R}^n$  at time  $k$  with elements  $\mathbf{q}_i^{(k)}$  with  $i = 1, \dots, n$ , the probabilistic estimates of states at time  $k + 1$  is  $\mathbf{Q}^{(k+1)} = \mathbf{P}\mathbf{Q}^{(k)}$ .

Notice that  $\mathbf{Q}^{(k+1)} = \mathbf{P}\mathbf{Q}^{(k)}$  holds because the multiplication distributivity of three probability intervals  $\mathbf{p}_1, \mathbf{p}_2$ , and  $\mathbf{p}_3$  ( $0 \leq \mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3 \leq 1$ ) exists [11,28,36]. That is,  $(\mathbf{p}_1 + \mathbf{p}_2)\mathbf{p}_3 = \mathbf{p}_1\mathbf{p}_3 + \mathbf{p}_2\mathbf{p}_3$ .

The logic coherence constraint of state probabilities is automatically satisfied during the transition process, stated as follows.

**THEOREM 4.1 (Markov logic coherence constraint)** *Given an interval matrix  $\mathbf{P}$  and an interval vector  $\mathbf{Q}^{(k)}$  with their respective elements  $\mathbf{p}_{ij}$  ( $i = 1, \dots, n, j = 1, \dots, n$ ) and  $\mathbf{q}_i^{(k)}$  ( $i = 1, \dots, n$ ) as generalized interval probabilities, if  $\sum_{i=1}^n \mathbf{p}_{ij} = [1, 1]$  ( $\forall j = 1, \dots, n$ ) and  $\sum_{i=1}^n \mathbf{q}_i^{(k)} = [1, 1]$ , then the elements of  $\mathbf{Q}^{(k+1)} = \mathbf{P}\mathbf{Q}^{(k)}$  denoted as  $\mathbf{q}_i^{(k+1)}$  ( $i = 1, \dots, n$ ) also satisfy  $\sum_{i=1}^n \mathbf{q}_i^{(k+1)} = [1, 1]$ .*

*Proof* 
$$\begin{aligned} \sum_{i=1}^n \mathbf{q}_i^{(k+1)} &= \sum_{i=1}^n \{ \sum_{j=1}^n \mathbf{p}_{ij} \mathbf{q}_j^{(k)} \} = \sum_{j=1}^n \{ \sum_{i=1}^n \mathbf{p}_{ij} \mathbf{q}_j^{(k)} \} = \sum_{j=1}^n \{ \mathbf{q}_j^{(k)} \sum_{i=1}^n \mathbf{p}_{ij} \} \\ &= \sum_{j=1}^n \{ \mathbf{q}_j^{(k)} \cdot [1, 1] \} = [1, 1] \end{aligned}$$
 ■

If the system is in the steady state, there is an equilibrium distribution  $\Pi$  of the possible states satisfying the stationary transition

$$\Pi = \mathbf{P}\Pi. \tag{8}$$

The elements  $\pi_i$  ( $i = 1, \dots, n$ ) of  $\Pi$  and  $\mathbf{p}_{ij}$  ( $i = 1, \dots, n; j = 1, \dots, n$ ) of  $\mathbf{P}$  are divided into two categories, proper and improper. Let  $\mathcal{P}$  denote the set of indices for those proper interval elements, i.e.  $\pi_i \in \mathbb{IR}$  if  $i \in \mathcal{P}$  and  $\mathbf{p}_{ij} \in \mathbb{IR}$  if  $ij \in \mathcal{P}$ . Let  $\mathcal{I}$  denote the set of indices for those improper interval elements, i.e.  $\pi_i \in \overline{\mathbb{IR}}$  if  $i \in \mathcal{I}$  and  $\mathbf{p}_{ij} \in \overline{\mathbb{IR}}$  if  $ij \in \mathcal{I}$ . Equation (8) can then be re-arranged as

$$\begin{bmatrix} \Pi_{\mathcal{P}} \\ \Pi_{\mathcal{I}} \end{bmatrix} = \begin{bmatrix} \mathbf{P}^{(1)} & \mathbf{P}^{(2)} \\ \mathbf{P}^{(3)} & \mathbf{P}^{(4)} \end{bmatrix} \cdot \begin{bmatrix} \Pi_{\mathcal{P}} \\ \Pi_{\mathcal{I}} \end{bmatrix}. \tag{9}$$

Let  $\mathbf{P}_{\mathcal{P}}^{(i)}$  and  $\mathbf{P}_{\mathcal{I}}^{(i)}$  be the respective proper and improper components of  $\mathbf{P}^{(i)}$  ( $i = 1, 2, 3, 4$ ). The first set of equations  $\Pi_{\mathcal{P}} = \mathbf{P}^{(1)} \cdot \Pi_{\mathcal{P}} + \mathbf{P}^{(2)} \cdot \Pi_{\mathcal{I}}$  in Equation (9) can be interpreted as

$$\begin{aligned} \forall P_{\mathcal{I}}^{(1)} \in \mathbf{P}_{\mathcal{I}}^{(1)\Delta}, \quad \forall P_{\mathcal{I}}^{(2)} \in \mathbf{P}_{\mathcal{I}}^{(2)\Delta}, \quad \forall \pi_{\mathcal{I}} \in \Pi_{\mathcal{I}}^{\Delta}, \\ \exists P_{\mathcal{P}}^{(1)} \in \mathbf{P}_{\mathcal{P}}^{(1)\Delta}, \quad \exists P_{\mathcal{P}}^{(2)} \in \mathbf{P}_{\mathcal{P}}^{(2)\Delta}, \quad \exists \pi_{\mathcal{P}} \in \Pi_{\mathcal{P}}^{\Delta}, \\ P^{(1)} \cdot \pi_{\mathcal{P}} + P^{(2)} \cdot \pi_{\mathcal{I}} = \pi_{\mathcal{P}}. \end{aligned} \tag{10}$$

The second set of equations  $\mathbf{P}^{(3)} \cdot \Pi_{\mathcal{P}} + \mathbf{P}^{(4)} \cdot \Pi_{\mathcal{I}} = \Pi_{\mathcal{I}}$  in Equation (9) can be interpreted as

$$\begin{aligned} \forall P_{\mathcal{P}}^{(3)} \in \mathbf{P}_{\mathcal{P}}^{(3)\Delta}, \quad \forall P_{\mathcal{P}}^{(4)} \in \mathbf{P}_{\mathcal{P}}^{(4)\Delta}, \quad \forall \pi_{\mathcal{P}} \in \Pi_{\mathcal{P}}^{\Delta}, \\ \exists P_{\mathcal{I}}^{(3)} \in \mathbf{P}_{\mathcal{I}}^{(3)\Delta}, \quad \exists P_{\mathcal{I}}^{(4)} \in \mathbf{P}_{\mathcal{I}}^{(4)\Delta}, \quad \exists \pi_{\mathcal{I}} \in \Pi_{\mathcal{I}}^{\Delta}, \\ P^{(3)} \cdot \pi_{\mathcal{P}} + P^{(4)} \cdot \pi_{\mathcal{I}} = \pi_{\mathcal{I}}. \end{aligned} \tag{11}$$

The combination of Equations (10) and (11) leads to the interpretation of Equation (8) or Equation (9) as

$$\begin{aligned} \forall P_{\mathcal{I}}^{(1)} \in \mathbf{P}_{\mathcal{I}}^{(1)\Delta}, \quad \forall P_{\mathcal{I}}^{(2)} \in \mathbf{P}_{\mathcal{I}}^{(2)\Delta}, \quad \forall P_{\mathcal{P}}^{(3)} \in \mathbf{P}_{\mathcal{P}}^{(3)\Delta}, \quad \forall P_{\mathcal{P}}^{(4)} \in \mathbf{P}_{\mathcal{P}}^{(4)\Delta}, \\ \exists P_{\mathcal{P}}^{(1)} \in \mathbf{P}_{\mathcal{P}}^{(1)\Delta}, \quad \exists P_{\mathcal{P}}^{(2)} \in \mathbf{P}_{\mathcal{P}}^{(2)\Delta}, \quad \exists P_{\mathcal{I}}^{(3)} \in \mathbf{P}_{\mathcal{I}}^{(3)\Delta}, \quad \exists P_{\mathcal{I}}^{(4)} \in \mathbf{P}_{\mathcal{I}}^{(4)\Delta}, \quad \exists \pi \in \Pi^{\Delta}, \quad (12) \\ P \cdot \pi = \pi. \end{aligned}$$

The existential quantifiers associated with the elements of  $\Pi$  in Equation (12) indicate the controllable stability of the equilibrium distribution in the steady state. If there are uncontrollable deviations associated with transition probabilities  $P_{\mathcal{I}}^{(1)}$ ,  $P_{\mathcal{I}}^{(2)}$ ,  $P_{\mathcal{P}}^{(3)}$ , and  $P_{\mathcal{P}}^{(4)}$ , we should be able to choose  $P_{\mathcal{P}}^{(1)}$ ,  $P_{\mathcal{P}}^{(2)}$ ,  $P_{\mathcal{I}}^{(3)}$ , and  $P_{\mathcal{I}}^{(4)}$  such that the steady state is maintained. Therefore, Equation (12) provides the logic basis to maintain the stability of the system subject to incomplete knowledge of states and state transitions, which can improve the robustness of the dynamic control in stochastic systems.

## 5. Solving interval FPE

As mentioned in Section 1, FPE's and CME's are intrinsically related. Diffusion processes and jump processes can be regarded as two views of stochastic dynamics at two different time and length scales. The numerical solving procedures for FPE's and CME's can be both based on the state transition scheme, which is different from the traditional trajectory sampling procedure. For the sake of completeness, the interval FPE and a path-integral approach for solving the interval FPE [54] are summarized in this section.

Instead of sampling trajectories, FPE simulates the processes by computing the probability distributions of all states at each time step. Particularly, the path-integral method has been shown as a simple yet numerically efficient and accurate approach. It uses a short-time transition probability density matrix to approximate the evolution of drift-diffusion processes [38,55]. Interpolation [32] can be used to approximate continuous probability density functions in order to improve numerical efficiency and accuracy. It has also been demonstrated that the computation efficiency can be improved under special conditions such as specific probability distributions [7] and constant diffusion coefficients [23].

The traditional FPE does not differentiate the two types of uncertainties. Therefore, extra effort of SA is needed to assess the robustness of results. Here we would like to show a path-integral approach that can be used to solve the *interval FPE* [54]

$$\frac{\partial}{\partial t} \mathbf{p}(x, t | y, t') = -\text{dual} \sum_{i=1}^n \frac{\partial}{\partial x_i} [\mathbf{A}_i(x, t) \mathbf{p}(x, t | y, t')] + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \frac{\partial^2}{\partial x_i \partial x_j} [\mathbf{B}_{ij}(x, t) \mathbf{p}(x, t | y, t')], \quad (13)$$

where  $\mathbf{A} \in \mathbb{K}\mathbb{R}^n$  is an interval vector of drift rates,  $\mathbf{B} \in \mathbb{K}\mathbb{R}^{n \times n}$  is an interval matrix of diffusion coefficients,  $x, y \in \mathbb{R}^n$  represent states in an  $n$ -dimensional configuration space, and  $\mathbf{p}(x, t | y, t')$  is the generalized interval-probability density that the system is in state  $x$  at time  $t$  given that it was in state  $y$  at time  $t'$ . The generalized FPE simultaneously models the time evolution of both aleatory and epistemic uncertainties.

With the short-time transition probability density

$$\mathbf{p}(x', t + \tau | x, t) \propto \exp \left( -\frac{1}{2\tau} [x' - x - \mathbf{A}(x, t)\tau]^T \mathbf{B}^{-1}(x, t) [x' - x - \mathbf{A}(x, t)\tau] \right), \quad (14)$$

where  $\mathbf{B}^{-1}$  is the inverse matrix of  $\mathbf{B}$  such that  $\mathbf{B} \cdot \text{dual}\mathbf{B}^{-1} = I$ . Let the initial probability distribution at time  $t_0$  be  $\mathbf{q}(x, t_0)$  and the discrete time intervals  $t_k = t_0 + k\tau$  for  $k = 1, 2, \dots$ . The distributions at time  $t = t_k$  is calculated by

$$\mathbf{q}(t, t_k) = \int_{\mathbb{R}^n} dy_{k-1} \mathbf{p}(x, t_k | y_{k-1}, t_{k-1}) \cdots \int_{\mathbb{R}^n} dy_0 \mathbf{p}(y_1, t_1 | y_0, t_0).$$

The numerical implementation is based on matrices. Suppose that the number of states  $N$  is finite. The initial probability distribution is an  $N \times 1$  interval vector  $\mathbf{Q}(t_0)$ . The short-time transition probability density is an  $N \times N$  interval matrix  $\mathbf{P}(t)$  calculated in Equation (14). Its element  $\mathbf{P}_{ij}(t)$  represents the probability of transition from state  $x_j$  to state  $x_i$  at time  $t$ . Then, the distribution at time  $t = t_k$  is

$$\mathbf{Q}(t_k) = \mathbf{P}(t_{k-1}) \cdots \mathbf{P}(t_0) \mathbf{Q}(t_0).$$

Each column of  $\mathbf{P}(t)$  should sum up to 1, which is required by the LCC. That is, if the transition rate is calculated by Equation (14) as

$$\mathbf{P}'_{ij}(t) = \exp\left(-\frac{1}{2\tau} [x_i - x_j - \mathbf{A}(x_j, t)\tau]^T \mathbf{B}^{-1}(x_j, t) [x_i - x_j - \mathbf{A}(x_j, t)\tau]\right)$$

then the normalized transition probability density is

$$\mathbf{P}_{ij}(t) = \frac{\mathbf{P}'_{ij}(t)}{\text{dual} \sum_{l=1}^N \mathbf{P}'_{lj}(t)}. \tag{15}$$

### 6. Solving interval master equation

The CME is used to model jump processes such as chemical kinetics. With parameter uncertainty incorporated, an interval master equation is [54]

$$\frac{\partial}{\partial t} \mathbf{p}(x, t | y, t') = \int dz \mathbf{w}(x | z, t) \mathbf{p}(z, t | y, t') - \text{dual} \int dz \mathbf{w}(z | x, t) \mathbf{p}(x, t | y, t'), \tag{16}$$

where  $\mathbf{w}(y | x, t) := \lim_{\delta t \rightarrow 0} \mathbf{p}(y, t + \delta t | x, t) / \delta t$  is the interval-valued rate of transition from state  $x$  to state  $y$  at time  $t$ . With the discrete state space of  $N$  possible states, Equation (16) becomes

$$\frac{\partial}{\partial t} \mathbf{q}_i(t) = \sum_{j \neq i} \mathbf{w}_{ij}(t) \mathbf{q}_j(t) - \text{dual} \sum_{j \neq i} \mathbf{w}_{ji}(t) \mathbf{q}_i(t) \quad (i = 1, \dots, N), \tag{17}$$

where  $\mathbf{w}_{ij}(t)$  is the interval rate of transition from state  $x_j$  to state  $x_i$  at time  $t$ , and  $\mathbf{q}_j(t)$  is the interval probability that the system is in state  $x_j$  at time  $t$ . Equation (17) can be represented in a matrix form as

$$\frac{\partial}{\partial t} \mathbf{Q}(t) = \mathbf{H}(t) \mathbf{Q}(t), \tag{18}$$

where the elements of matrix  $\mathbf{H}(t)$  are  $\mathbf{h}_{ii}(t) = -\text{dual} \sum_j \mathbf{w}_{ji}(t)$  and  $\mathbf{h}_{ij}(t) = \mathbf{w}_{ij}(t)$  ( $j \neq i$ ). Notice that  $\sum_i \mathbf{h}_{ij}(t) = 0$  for any  $j$ . The interval matrix  $\mathbf{H}$  is regarded an infinitesimal generator of a generalized Markovian process.

Given the initial probabilities of states  $\mathbf{Q}(t_0)$ , numerically the time is divided into small steps  $t_0, t_0 + \tau, t_0 + 2\tau, \dots$  and  $\mathbf{H}_k$  remains constant between time  $t_0 + k\tau$  and  $t_0 + (k + 1)\tau$ . The corresponding numerical solution of Equation (18) is

$$\mathbf{Q}(t + k\tau) = \exp(\tau\mathbf{H}_{k-1}) \cdots \exp(\tau\mathbf{H}_0)\mathbf{Q}(t_0).$$

Notice that the CME models stochastic jump processes by a deterministic ODE of probability distributions. Therefore, the sensitivity of CME can also be assessed by other methods such as the direct and adjoint methods. In both the direct and adjoint methods, Jacobi matrices need to be computed. In the direct methods, sensitivity equations need to be solved to check the sensitivity change along time. In the adjoint methods, adjoint equations need to be solved to evaluate adjoint variables in a reverse order, after the state variables are calculated in a forward calculation. Thus, a large amount of memory must be allocated to store the state variables in the forward run. The sensitivity of objectives is estimated by further computing the integral of gradient-adjoint product along time numerically. In contrast, the interval-based approach converts the original ODE to an interval-valued ODE. The solving process is based on interval analysis. The interval extensions of numerical methods for interval ODE's are similar to the ones for ODE's without additional equations and therefore more tractable. However, one caveat of interval analysis is that the interval results can be overly pessimistic and interval estimations can be too wide. The proposed generalized interval approach is to resolve this over-estimation issue by using Kaucher arithmetic.

### 6.1 Computing interval matrix exponential

The computation of interval matrix exponential  $\exp(\tau\mathbf{H}_k)$  is the major task in solving the interval master equation. Several approaches have been proposed to calculate the interval matrix exponential. Oppenheimer and Michel [34] used the centred form of interval and Taylor series approximation in the range estimation. Goldsztejn [16] reduced the interval over-estimation by a scaling and squaring process. Škulj [47] took a partitioning approach to reduce step sizes to avoid interval over-estimation. Different from these approaches, here we use generalized interval. The complete enclosure of the possible variation ranged by the lower and upper bounds is not the only purpose in solving Equation (18), since the LCC is enforced by the generalized interval probability. In addition, the state space of interval master equation has very high dimensions. The infinitesimal generator  $\mathbf{H}$  is a very large but sparse matrix. Therefore, a Krylov subspace projection approach is taken here.

Our approach can be regarded as an extension of the Krylov-based matrix exponential computation [44] from real numbers to generalized intervals, listed as follows.

The core part of the algorithm is an Arnoldi process to search the interval-valued orthonormal basis  $\{\mathbf{V}_1, \dots, \mathbf{V}_{m+1}\}$  forming a matrix  $\mathcal{V} = [\mathbf{V}_1, \dots, \mathbf{V}_{m+1}]$  and the upper Hessenberg matrix  $\mathcal{G} = [g_{ij}]$  such that  $e^{\tau\mathbf{H}}\mathbf{Q}$  can be estimated as  $\mathbf{U}(\tau) = \beta\mathcal{V}e^{\tau\mathcal{G}}\mathbf{e}_1$  where  $\mathbf{e}_1$  is the first unit basis. Here, the lower and upper bound matrices of  $e^{\tau\mathcal{G}}$  are calculated as  $e^{\tau\underline{\mathcal{G}}}$  and  $e^{\tau\bar{\mathcal{G}}}$  respectively, with real-valued matrices  $\underline{\mathcal{G}} = [g_{ij}]$  and  $\bar{\mathcal{G}} = [\bar{g}_{ij}]$ .

For each orthogonal projection in  $\mathbf{R} = \mathbf{R} - \text{dual}g_{ij}\mathbf{V}_i$  in the algorithm, if 0 is included in any element of residual  $\mathbf{R}$ , this element will be assigned to be 0. In a real-valued orthogonal projection, if the residual  $R - g_{ij}V_i$  becomes very small and close to 0, it indicates an orthogonal basis vector is found. However, for interval-valued vectors, the residual may not be zero. Here generalized intervals are applied.  $\mathbf{E} = \mathbf{R} - \text{dual}g_{ij}\mathbf{V}_i$  can always be interpreted as

$$(\forall E \in \mathbf{E}^\Delta)(\forall \mathbf{R} \in \mathbf{R}^\Delta)(\forall g_{ij} \in g_{ij}^\Delta)(\forall V_i \in V_i^\Delta)(R - g_{ij}V_i = E),$$

---

**Algorithm 1** Compute  $\mathbf{U} = e^{\tau\mathbf{H}}\mathbf{Q}$ , where  $\mathbf{H} \in \mathbb{K}\mathbb{R}^{n \times n}$  and  $\mathbf{Q} \in \mathbb{K}\mathbb{R}^n$

---

```

t = 0;
choose an m ≪ n;
β ← ‖Q‖2;
U ← Q;
WHILE t < τ DO
    V1 ← U/dual(β);
    FOR j = 1 to m
        R ← H · Vj where R = [r1, ..., rn]T;
        FOR i = 1 to j
            gij ← ViT · R;
            R ← R - dualgijVi;
            FOR k = 1 to n
                IF 0 ∈ rkΔ;
                    rk ← 0;
                END IF
            END FOR
        END FOR
        gj+1,j ← ‖R‖2;
        IF ‖gj+1,j‖2 < ε;
            BREAK;
        END IF
        Vj+1 ← R/dualgj+1,j;
    END FOR
    gm+2,m+1 = 1;
    G ← [g1:m+2,1:m+1];
    V ← [V1, ..., Vm+1];
    Δt = τ - t;
    DO
        F ← eΔtG;
        U ← βV(1 : n, 1 : m + 1)F(1 : m + 1, 1);
        err = min(|βF(m + 1, 1)|, |βF(m + 2, 1)| · ‖HVm+1‖2);
        Δt ← αΔt where 0 < α < 1;
    WHILE (err > ε)
        t ← t + Δt;
    END WHILE

```

---

where  $\mathbf{Q}_R$ ,  $\mathbf{Q}_{g_{ij}}$ , and  $\mathbf{Q}_{V_i}$  can be either  $\forall$  or  $\exists$ . If  $0 \in \mathbf{E}^\Delta$ , then the interpretation is

$$(\mathbf{Q}_R R \in \mathbf{R}^\Delta)(\mathbf{Q}_{g_{ij}} g_{ij} \in \mathbf{g}_{ij}^\Delta)(\mathbf{Q}_{V_i} V_i \in \mathbf{V}_i^\Delta)(R - g_{ij} V_i = 0).$$

That is, with the zero residual, an orthogonal basis can be found with the given intervals  $\mathbf{R}$ ,  $\mathbf{g}_{ij}$ , and  $\mathbf{V}_i$ . In other words, two generalized interval vectors  $\mathbf{E}_1$  are  $\mathbf{E}_2$  called orthogonal to each other if  $0 \in (\mathbf{E}_1^T \cdot \mathbf{E}_2)^\Delta$ .

If the error of Krylov subspace approximation is large, the algorithm iterative reduces the step size  $\Delta t$  such that for each small step the approximation is within a preset threshold  $\epsilon$ . That is, a jump for a time period of  $\tau$  is subdivided into several jumps with smaller step sizes.



$\mathbf{U}$  computed from the algorithm is a vector of probabilities. A normalization procedure

$$\mathbf{U}'_i(t) = \frac{\mathbf{U}_i(t)}{\text{dual} \sum_{l=1}^N \mathbf{U}_l(t)} \tag{19}$$

is required to satisfy the LCC. The normalization at each step of the iterative process for time evolution avoids the problem of overly pessimistic estimation of interval ranges, yet at the cost of enclosure completeness.

### 6.2 Numerical illustration

Here we use two numerical examples to illustrate the developed algorithm for solving the interval master equation. The first example is the well-known Lotka–Volterra predatory–prey model, and the second one is the Michaelis–Menten enzyme kinetics.

The first example is the Lotka–Volterra predatory–prey model with two species, predator and prey. The dynamics of the system is described by three kinetic equations, as given in Table 2. The first equation is the growth of prey, the second one is the growth of predatory, and the third one is the death of predator.  $N_{\text{predator}}$  and  $N_{\text{prey}}$  are the numbers of species. With the initial distributions  $p(N_{\text{predator}} = 5) = 1.0$  and  $p(N_{\text{prey}} = 5) = 1.0$  and the time step  $\tau = 0.1$ , the simulation results are shown in Figure 1 where the distributions for the numbers of predator and prey evolve along time. The lower and upper bounds of probability density is compared with the result of a real-valued traditional simulation, where the rate constants take the values of  $c_1 = 0.1$ ,  $c_2 = 0.01$ , and  $c_3 = 0.1$ .

The combination of different numbers of species form the state space. For a system of  $M$  species with the maximal numbers as  $N$ , the numbers of possible states is in the order of  $N^M$ . Yet the probabilities that most of the states are occupied are zeros. Therefore, both the infinitesimal generator  $\mathbf{H}$  and probability vector  $e^{\tau\mathbf{H}}\mathbf{Q}$  are very sparse.

Table 2. An example of Lotka–Volterra predatory–prey model.

Reaction	Propensity	Rate constant
Prey $\xrightarrow{c_1}$ 2Prey	$\alpha_1 = c_1 N_{\text{Prey}}$	$c_1 = [0.09, 0.11]$
Predator + Prey $\xrightarrow{c_2}$ Predator	$\alpha_2 = c_2 N_{\text{Predator}} N_{\text{Prey}}$	$c_2 = [0.009, 0.011]$
Predator $\xrightarrow{c_3}$ $\emptyset$	$\alpha_3 = c_3 N_{\text{Predator}}$	$c_3 = [0.09, 0.11]$

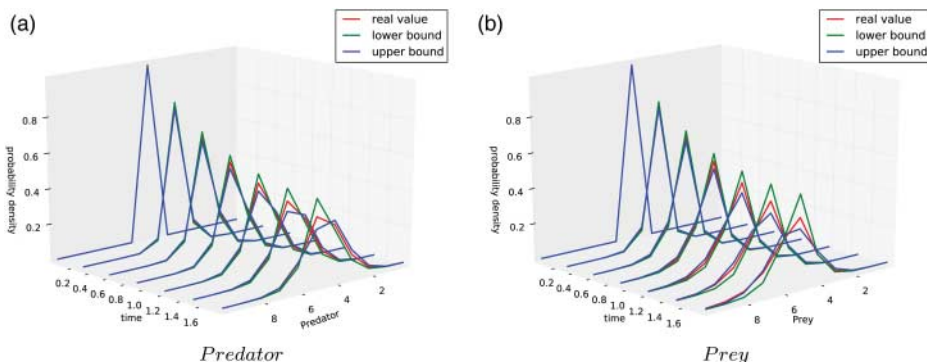


Figure 1. Evolution of probability densities in the predator–prey model: (a) predator and (b) prey.

Table 3. An example of Michaelis–Menten enzyme kinetics [17].

Reaction	Propensity	Rate constant
$S + E \xrightarrow{c_1} ES$	$\alpha_1 = c_1 N_S N_E$	$c_1 = [0.9, 1.1]$
$ES \xrightarrow{c_2} E + S$	$\alpha_2 = c_2 N_{ES}$	$c_2 = [0.9, 1.1]$
$ES \xrightarrow{c_3} P + E$	$\alpha_3 = c_3 N_{ES}$	$c_3 = [0.09, 0.11]$

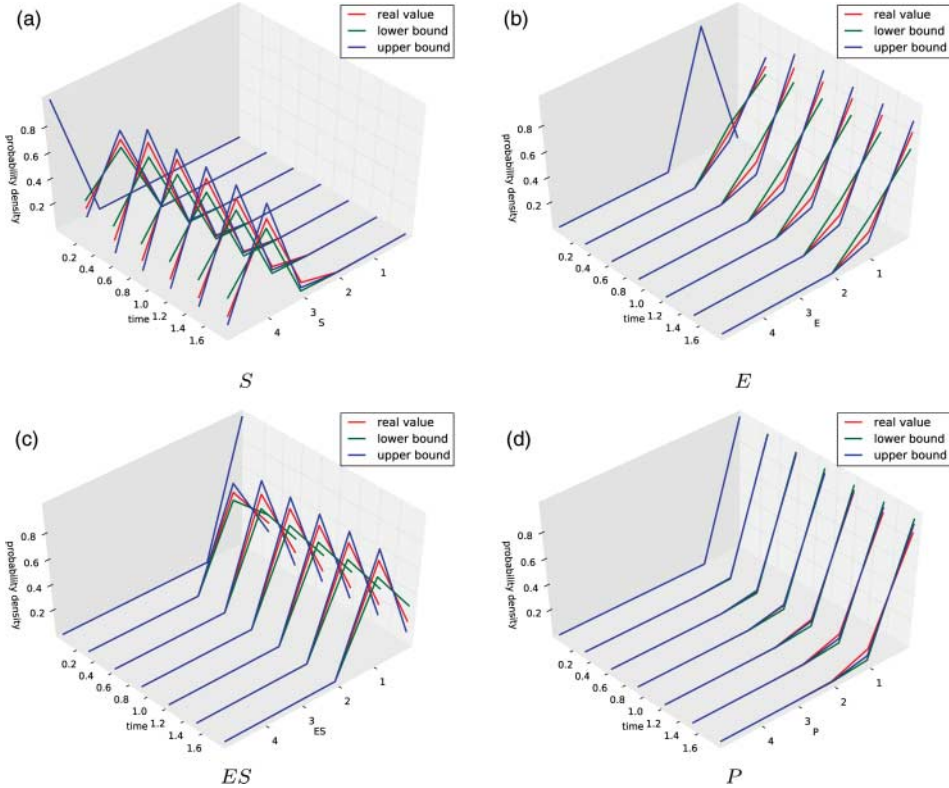


Figure 2. Time evolution of probability densities in the Michaelis–Menten enzyme kinetics example: (a) S, (b) E, (c) ES, and (d) P.

The second example is the Michaelis–Menten enzyme kinetics [17]. The involved reactions and species are listed in Table 3, where enzymes E catalyse the reaction of substrates S into products P by forming intermediate enzyme/substrate complexes ES. There are three reactions with the respective interval-valued rate constants specified. The propensities are functions of the number of reactant species  $N_S$ ,  $N_E$ , and  $N_{ES}$ .

The combination of different numbers of species forms the state space. For a system of  $M$  species with the maximal numbers as  $N$ , the numbers of possible states is in the order of  $N^M$ . Yet the probabilities that most of the states are occupied are zeros. Therefore, both the infinitesimal generator  $\mathbf{H}$  and probability vector  $e^{\tau\mathbf{H}}\mathbf{Q}$  are very sparse.

In this example, the initial numbers of species are  $N_S = 5$ ,  $N_E = 1$ ,  $N_{ES} = 0$ , and  $N_P = 0$ . The time step size is  $\tau = 0.1$ . Figure 2 shows the evolution of the probability densities for the four species.

## 7. Concluding remarks

In this paper, a new approach to perform stochastic simulation under both aleatory and epistemic uncertainties is presented. The underlying theoretical basis is generalized interval probability, which integrates generalized interval and probability. The new approach simulates the dynamics of stochastic systems with imprecise model parameters without the need of the traditional SA to assess the robustness of simulation results.

Different from other imprecise probability theories, generalized interval probability has an algebraic framework that resembles the traditional precise probability so that probabilistic calculus and reasoning can be greatly simplified. Its definitions of conditioning, independence, and Markovian properties provide a convenient calculation structure. Its unique semantics with logic interpretations also allows us to assess the interval range estimation for completeness and soundness.

The FPE and master equations are extended with generalized interval probability to model the time evolution of both uncertainty components simultaneously. The drift–diffusion and jump processes with uncertain models and parameters thus can be simulated. A path-integral algorithm is used to solve the interval FPE, whereas a Krylov subspace projection method is proposed for the interval master equation. Numerical examples demonstrated that the developed approach provides an insight on the effect of uncertain model and parameters. Confidence of the simulation reliability and robustness can be obtained directly from the resulted lower and upper probabilities without introducing the overhead of SA.

The logic coherence constraint of generalized interval probability ensures that the interval-valued probabilities satisfy the three axioms of Kolmogorov. It greatly simplifies the calculus structure. Yet, the completeness of interval range estimation is not guaranteed any more during the computation, just as in the classical interval arithmetic. More work of completeness and soundness analysis is needed so that confidence of robustness can be further improved.

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