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SOLVING INTERVAL MASTER EQUATION IN SIMULATION OF JUMP PROCESSES UNDER UNCERTAINTIES

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ABSTRACT

Two types of uncertainty are generally recognized in modeling and simulation, including variability caused by inherent randomness and incertitude due to the lack of perfect knowledge. Generalized interval probability is able to model both uncertainty components simultaneously, where epistemic uncertainty is quantified by the generalized interval in addition to the probabilistic measure. With the conditioning, independence, and Markovian property uniquely defined, the calculus structures in generalized interval probability resembles those in the classical probability theory. An imprecise Markov chain model is proposed with the ease of computation. A Krylov subspace projection method is developed to solve the interval master equation to simulate jump processes with finite state transitions under uncertainties. The state transitions with interval-valued probabilities can be simulated, which provides the lower and upper bound information of evolving distributions as an alternative to the traditional sensitivity analysis.

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.

In modeling and simulation, epistemic uncertainty is the result of the errors 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 modeled and the true physical ones, etc. In molecular dynamics simulation, epistemic uncertainty is mainly from the inaccurate potential functions. In kinetic Monte Carlo simulation, it is largely from the imperfect knowledge about transition and reaction rates. In contrast to epistemic uncertainty, various sources such as disturbed boundary and loading conditions, different sampling sizes and running times, inherent variations of material compositions, and other randomness and fluctuation form the aleatory component of uncertainty.

1.1 Sources of epistemic uncertainty in modeling and simulation

The sources of epistemic uncertainty [1–6] in modeling and simulation (M&S) are summarized as follows .

1. 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.
2. Conflicting information: if there are multiple sources of information, the analyst may face conflicts among them. It is

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not appropriate to draw a simple conclusion of distributions from several pieces of contradictory evidence. The absence of relevant information has to be properly modeled and incorporated in M&S.

3. 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.
4. Lack of introspection: in some cases the analyst can not 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.
5. 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.
6. 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.
7. 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 modeled by probability distributions. In contrast, epistemic uncertainty has been modeled in several ways, such as probability, interval, fuzzy set, random set, basic probability assignment, etc. 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 two-fold. 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.

Probability 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 the van Fraassen's cube factory [7]. "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 where 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. 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 Bayesian learning and update approach.

In this paper, a generalized interval probability is used to quantify the two components of uncertainty, where epistemic uncertainty is represented by generalized intervals, in combination with probability measures that capture aleatory uncertainty. 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. The conditional probabil-

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ity, independence, and generalized interval Bayes' rule are in a very similar form of those in the traditional probability theory. As a result, the proposed imprecise Markov chain model based on these fundamental properties enables the ease of computation. An interval master equation is used to describe jump processes under both uncertainty components. The master equation models state transitions in jump processes and has been widely applied in simulations of chemical reactions, quantum systems, and others. Here a Krylov subspace projection method is developed to compute interval matrix exponentials with the large and sparse generator matrices. It is demonstrated that the simulation based on generalized interval probability is algebraically tractable, as an efficient alternative to sensitivity analysis.

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. Section 4 describes the new imprecise Markov chain model with generalized interval probability and the Krylov subspace projection method to solve the interval master equation to simulate jump processes under both uncertainty components. Two numerical examples are used to illustrated the proposed method in Section 5.

2 BACKGROUND

2.1 Existing approaches for robustness in modeling and simulation

The ultimate goal of incorporating both components of uncertainty in modeling and simulation is to improve the robustness of predictions. Some of the standard approaches that have been used to explore the impact of input uncertainties are sensitivity analysis (SA) and design of experiment(DOE) [8–10]. 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.

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 [11–13], or by varying the probability measures w.r.t. inputs such as the likelihood ratio method [14–16].

Another popular simulation technique that represents the total uncertainty is based on the second order probability and second order Monte Carlo (SOMC) (e.g. [17]). A second-order probabilistic sensitivity analysis 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 [18, 19] and the bootstrap approaches [20, 21].

The biggest issue of the above sensitivity analysis 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 for robust simulation.

2.2 Imprecise probability

Imprecise probability $[\underline{p}, \overline{p}]$ 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 $\underline{p} = \overline{p}$, the degenerated interval probability becomes a traditional precise one.

Many forms of imprecise probabilities have been developed. For example, the Dempster-Shafer theory [22, 23] characterizes evidence with discrete probability masses associated with a power set of values. The theory of coherent lower previsions [24] models uncertainties with the lower and upper previsions with behavioral interpretations. The possibility theory [25] represents uncertainties with Necessity-Possibility pairs. Probability bound analysis [26] captures uncertain information with pairs of lower and upper distribution functions or p-boxes. Interval probability [27] characterizes statistical properties as intervals. F-probability [28] 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 [31] is a combination of fuzzy sets, intervals, and probability distributions.

In the applications of interval probability, the interval bounds $\underline{p}$ and $\overline{p}$ can be solicited as the lowest and highest subjective probabilities about a particular event from a domain expert,

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where probability represents the degree of belief. One expert may hesitate to offer just a precise value of probability. Different experts could have different beliefs. In both cases, the range of probabilities gives the interval bounds. When used in data analysis with frequency interpretation, the interval bounds can be confidence intervals that are calculated from data (e.g. the Kolmogorov-Smirnov confidence band) to enclose a cumulative distribution function. If extra data are collected, the interval distribution converges toward a precise distribution function. For parametric distributions such as exponential and Gaussian, the epistemic uncertainty is represented by interval values of the parameters.

2.3 Imprecise Markov chain models

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 [32, 33]. Hartfiel [34] 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 [35] developed a linear programming based algorithm to estimation lower and upper bounds of F-probability with interval transition probabilities. Škulj [36, 37] developed formulations of F-probability and coherent lower prevision to predict transitions. With a formulation of coherent upper prevision, de Cooman et al. [38] developed an algorithm with linear complexity to estimate the credal set evolution in imprecise Markov chains.

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

2.4 Generalized interval

The classical set-based interval [39] is defined as $[\![a,b]\!] := \{x \in \mathbb{R} | a \le x \le b\}$. Therefore $[\![a,b]\!]$ is invalid when $a > b$. In contrast, generalized interval [40–42] does not have such restriction. A generalized interval is defined as a pair of numbers $\mathbf{x} := [\underline{x}, \overline{x}] (\underline{x}, \overline{x} \in \mathbb{R})$.

The calculation of generalized interval is based on the Kaucher interval arithmetic [43]. 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 $\mathbb{KR} = \{[\underline{x}, \overline{x}] | \underline{x}, \overline{x} \in \mathbb{R}\}$. The set of *proper* intervals is $\mathbb{IR} = \{[\underline{x}, \overline{x}] | \underline{x} \le \overline{x}\}$, and the set of *improper* intervals is $\overline{\mathbb{IR}} = \{[\underline{x}, \overline{x}] | \underline{x} \ge \overline{x}\}$. The relationship between proper and improper intervals is established with the operator *dual* as $\mathrm{dual}([\underline{x}, \overline{x}]) := [\overline{x}, \underline{x}]$ Thus, the group of generalized intervals is formed with $\mathbf{x} - \mathrm{dual}\mathbf{x} = 0$ and $\mathbf{x} \div \mathrm{dual}\mathbf{x} = 1$.

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

$$[\underline{x}, \overline{x}] \subseteq [\underline{y}, \overline{y}] \iff \underline{x} \ge \underline{y} \wedge \overline{x} \le \overline{y} \tag{1}$$

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

$$[\underline{x}, \overline{x}] \le [\underline{y}, \overline{y}] \iff \underline{x} \le \underline{y} \wedge \overline{x} \le \overline{y} \tag{2}$$

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

$$[\underline{x}, \overline{x}]^{\triangle} := [\![\min(\underline{x}, \overline{x}), \max(\underline{x}, \overline{x})]\!] \tag{3}$$

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

$$|\mathbf{x}| := \begin{cases} [-\overline{x}, -\underline{x}] & (\underline{x} < 0, \overline{x} < 0) \\ [0, \max(-\underline{x}, \overline{x})] & (\underline{x} < 0, \overline{x} \ge 0) \\ [\max(\underline{x}, -\overline{x}), 0] & (\underline{x} \ge 0, \overline{x} < 0) \\ [\underline{x}, \overline{x}] & (\underline{x} \ge 0, \overline{x} \ge 0) \end{cases} \tag{4}$$

The absolute value of a vector $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n]^T$ is $|\mathbf{X}| := [|\mathbf{x}_1|, \ldots, |\mathbf{x}_n|]^T$, where T denotes matrix transpose. The L_2-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 $\mathbf{f}(x) := [\underline{f}(x), \overline{f}(x)]$. The integral of $\mathbf{f}(x)$ is defined as $\int \mathbf{f}(x)dx := [\int \underline{f}(x)dx, \int \overline{f}(x)dx]$ [41].

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 $\mathbf{x} \in \mathbb{KR}$ is denoted by $(\mathrm{Q}_{\mathbf{x}} x \in \mathbf{x}^{\triangle})$ where $\mathrm{Q} : \mathbb{KR} \mapsto \{\exists, \forall\}$. $\mathbf{x}$ is called *existential* if $\mathrm{Q}_{\mathbf{x}} = \exists$, or *universal* if $\mathrm{Q}_{\mathbf{x}} = \forall$. If a real relation $z = f(x_1, \ldots, x_n)$ is extended to the interval relation $\mathbf{z} = \mathbf{f}(\mathbf{x}_1, \ldots, \mathbf{x}_n)$, the interval relation $\mathbf{z}$ is interpretable if there is a semantic relation

$$(\mathrm{Q}_{\mathbf{x}_1} x_1 \in \mathbf{x}_1^{\triangle}) \cdots (\mathrm{Q}_{\mathbf{x}_n} x_n \in \mathbf{x}_n^{\triangle})(\mathrm{Q}_{\mathbf{z}} z \in \mathbf{z}^{\triangle})(z = f(x_1, \ldots, x_n))$$

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 "+".

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Table 1. Illustrations of the semantic extension of generalized interval

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

3 Basics of generalized interval probability

The basics of generalized interval probability are defined as follows [44].

Given a sample space Ω and a σ-algebra $\mathcal{A}$ of random events over Ω, we define the generalized interval probability $\mathbf{p}\in\mathbb{KR}$ as $\mathbf{p}:\mathcal{A}\to[0,1]\times[0,1]$ which obeys the axioms of Kolmogorov: (1) $\mathbf{p}(\Omega)=[1,1]$; (2) $[0,0]\le\mathbf{p}(E)\le[1,1]\,(\forall E\in\mathcal{A})$; 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 $\mathbf{p}=[\underline{p},\overline{p}]$ is a generalized interval without the restriction of $\underline{p}\le\overline{p}$. The new definition of interval probability also implies $\mathbf{p}(\emptyset)=[0,0]$. 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 (LCC)

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

Notice that the LCC is more restrictive than Walley's coherence and avoid sure loss constraints [24]. The LCC ensures that generalized interval probability is logically coherent with precise probability. Suppose that $\mathbf{p}(E_i)\in\mathbb{IR}$ (for $i=1,\ldots,k$) and $\mathbf{p}(E_i)\in\overline{\mathbb{IR}}$ (for $i=k+1,\ldots,n$). It can be interpreted as

$$\begin{aligned}&\forall p_1\in\mathbf{p}^{\triangle}(E_1),\ldots,\forall p_k\in\mathbf{p}^{\triangle}(E_k),\\&\exists p_{k+1}\in\mathbf{p}^{\triangle}(E_{k+1}),\ldots,\exists p_n\in\mathbf{p}^{\triangle}(E_n),\\&\sum_{i=1}^n p_i=1\end{aligned}$$

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

$$\begin{aligned}&(\forall p_1\in[\![0.2,0.3]\!])(\forall p_2\in[\![0.3,0.5]\!])(\exists p_3\in[\![0.2,0.5]\!])\\&(p_1+p_2+p_3=1)\end{aligned}$$

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, $\mathbf{p}(working)=[0.2,0.5]$, $\mathbf{p}(down)=[0.2,0.3]$, and $\mathbf{p}(idle)=[0.6,0.2]$.

3.2 Conditional probability and independence

The concepts of conditional probability and independence are critical for the classical probability theory. With independence, we can decompose a complex problem into simpler and manageable components. 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.

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

$$\mathbf{p}(E|C):=\frac{\mathbf{p}(E\cap C)}{\text{dual}\mathbf{p}(C)}=\left[\frac{\underline{p}(E\cap C)}{\underline{p}(C)},\frac{\overline{p}(E\cap C)}{\overline{p}(C)}\right]\tag{5}$$

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.

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

$$\mathbf{p}(A\cap B|C)=\mathbf{p}(A|C)\mathbf{p}(B|C)\tag{6}$$

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

$$\mathbf{p}(A\cap B)=\mathbf{p}(A)\mathbf{p}(B)\tag{7}$$

4 MODELING JUMP PROCESSES UNDER UNCERTAINTIES

The jump process in a stochastic system is typically modeled as a continuous-time Markov chain. The system dynamics

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is modeled as a special case of the Chapman-Kolmogorov equation where the state space is discontinuous, also known as the master equation. When epistemic uncertainty is incorporated in the model, generalized interval probability can be used to construct a compact form of the *interval master equation*, as [45]

$$\begin{aligned}\frac{\partial}{\partial t}\mathbf{p}(x,t|y,t') = \int dz\mathbf{w}(x|z,t)\mathbf{p}(z,t|y,t') \\ - \text{dual}\int dz\mathbf{w}(z|x,t)\mathbf{p}(x,t|y,t')\end{aligned} \tag{8}$$

where $\mathbf{w}(y|x,t) := \lim_{\delta t\to 0}\mathbf{p}(y,t+\delta t|x,t)/\delta t$ is the interval-valued rate of transition from state x to state y at time t.

Solving Eq.(8) depends the formalism of imprecise Markov chain. With the conditional probability and independence defined, a Markov chain model with generalized interval probability is proposed to describe the system as transitions of states which we do not have perfect knowledge about, as described next.

4.1 Imprecise Markov chain with generalized interval probability

Different from the ones in Section 2.3, the imprecise Markov chain defined here is based on 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 $\mathbf{P}\in\mathbb{KR}^{n\times n}$ with interval-valued transition probabilities $\mathbf{p}_{ij}=\mathbf{p}(X=i|X=j)$ with $i=1,\ldots,n$ and $j=1,\ldots,n$. Given the probabilistic estimates of the states $\mathbf{Q}^{(k)}\in\mathbb{KR}^n$ at time k with elements $\mathbf{q}_i^{(k)}$ with $i=1,\ldots,n$, 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 $\mathbf{p}_3$ ($0\le \mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3\le 1$) exists [46–48]. 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 1 (*Markov logic coherence constraint*): Given an interval matrix $\mathbf{P}$ and an interval vector $\mathbf{Q}^{(k)}$ with their respective elements $\mathbf{p}_{ij}$ ($i=1,\ldots,n, j=1,\ldots,n$) and $\mathbf{q}_i^{(k)}$ ($i=1,\ldots,n$) as generalized interval probabilities, if $\sum_{i=1}^n\mathbf{p}_{ij}$ ($\forall j=1,\ldots,n$) and $\sum_{i=1}^n\mathbf{q}_i^{(k)}$, then the elements of $\mathbf{Q}^{(k+1)}=\mathbf{P}\mathbf{Q}^{(k)}$ denoted as $\mathbf{q}_i^{(k+1)}$ ($i=1,\ldots,n$) also satisfy $\sum_{i=1}^n\mathbf{q}_i^{(k+1)}=1$.

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

$$\Pi=\mathbf{P}\Pi \tag{9}$$

The elements Π_i ($i=1,\ldots,n$) of Π and $\mathbf{p}_{ij}$ ($i=1,\ldots,n; j=1,\ldots,n$) 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 I denote the set of indices for those improper interval elements, i.e. $\Pi_i\in\overline{\mathbb{IR}}$ if $i\in I$ and $\mathbf{p}_{ij}\in\overline{\mathbb{IR}}$ if $ij\in I$. Eq.(9) can then be re-arranged as

$$\begin{bmatrix}\Pi_{\mathcal{P}}\\ \Pi_I\end{bmatrix}=\begin{bmatrix}\mathbf{P}^{(1)} & \mathbf{P}^{(2)}\\ \mathbf{P}^{(3)} & \mathbf{P}^{(4)}\end{bmatrix}\cdot\begin{bmatrix}\Pi_{\mathcal{P}}\\ \Pi_I\end{bmatrix} \tag{10}$$

Let $\mathbf{P}_{\mathcal{P}}^{(i)}$ and $\mathbf{P}_I^{(i)}$ be the respective proper and improper components of $\mathbf{P}^{(i)}$ ($i=1,2,3,4$). The first set of equations $\Pi_{\mathcal{P}}=\mathbf{P}^{(1)}\cdot\Pi_{\mathcal{P}}+\mathbf{P}^{(2)}\cdot\Pi_I$ in Eq.(10) can be interpreted as

$$\begin{aligned}\forall P_I^{(1)}\in\mathbf{P}_I^{(1)\triangle},\forall P_I^{(2)}\in\mathbf{P}_I^{(2)\triangle},\forall\pi_I\in\Pi_I^{\triangle},\\ \exists P_{\mathcal{P}}^{(1)}\in\mathbf{P}_{\mathcal{P}}^{(1)\triangle},\exists P_{\mathcal{P}}^{(2)}\in\mathbf{P}_{\mathcal{P}}^{(2)\triangle},\exists\pi_{\mathcal{P}}\in\Pi_{\mathcal{P}}^{\triangle},\\ P^{(1)}\cdot\pi_{\mathcal{P}}+P^{(2)}\cdot\pi_I=\pi_{\mathcal{P}}\end{aligned} \tag{11}$$

The second set of equations $\mathbf{P}^{(3)}\cdot\Pi_{\mathcal{P}}+\mathbf{P}^{(4)}\cdot\Pi_I=\Pi_I$ in Eq.(10) can be interpreted as

$$\begin{aligned}\forall P_{\mathcal{P}}^{(3)}\in\mathbf{P}_{\mathcal{P}}^{(3)\triangle},\forall P_{\mathcal{P}}^{(4)}\in\mathbf{P}_{\mathcal{P}}^{(4)\triangle},\forall\pi_{\mathcal{P}}\in\Pi_{\mathcal{P}}^{\triangle},\\ \exists P_I^{(3)}\in\mathbf{P}_I^{(3)\triangle},\exists P_I^{(4)}\in\mathbf{P}_I^{(4)\triangle},\exists\pi_I\in\Pi_I^{\triangle},\\ P^{(3)}\cdot\pi_{\mathcal{P}}+P^{(4)}\cdot\pi_I=\pi_I\end{aligned} \tag{12}$$

The combination of Eq.(11) and Eq.(12) leads to the interpretation of Eq.(9) or Eq.(10) as

$$\begin{aligned}\forall P_I^{(1)}\in\mathbf{P}_I^{(1)\triangle},\forall P_I^{(2)}\in\mathbf{P}_I^{(2)\triangle},\forall P_{\mathcal{P}}^{(3)}\in\mathbf{P}_{\mathcal{P}}^{(3)\triangle},\forall P_{\mathcal{P}}^{(4)}\in\mathbf{P}_{\mathcal{P}}^{(4)\triangle},\\ \exists P_{\mathcal{P}}^{(1)}\in\mathbf{P}_{\mathcal{P}}^{(1)\triangle},\exists P_{\mathcal{P}}^{(2)}\in\mathbf{P}_{\mathcal{P}}^{(2)\triangle},\exists P_I^{(3)}\in\mathbf{P}_I^{(3)\triangle},\\ \exists P_I^{(4)}\in\mathbf{P}_I^{(4)\triangle},\exists\pi\in\Pi^{\triangle},\\ P\cdot\pi=\pi\end{aligned} \tag{13}$$

The existential quantifiers associated with the elements of Π in Eq.(13) indicate the controllable stability of the equilibrium distribution in the steady state. If there are uncontrollable deviations associated with transition probabilities $P_I^{(1)}$, $P_I^{(2)}$, $P_{\mathcal{P}}^{(3)}$, and $P_{\mathcal{P}}^{(4)}$, we should be able to choose $P_{\mathcal{P}}^{(1)}$, $P_{\mathcal{P}}^{(2)}$, $P_I^{(3)}$, and $P_I^{(4)}$ such that the steady state is maintained. Therefore, Eq.(13) 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.

4.2 Solving interval master equation

With the discrete state space of N possible states, Eq.(8) becomes

$$\frac{\partial}{\partial t}\mathbf{q}_i(t)=\sum_{j\neq i}\mathbf{w}_{ij}(t)\mathbf{q}_j(t)-\text{dual}\sum_{j\neq i}\mathbf{w}_{ji}(t)\mathbf{q}_i(t)\ (i=1,\ldots,N) \tag{14}$$

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. Eq.(14) can be represented in a matrix form as

$$\frac{\partial}{\partial t}\mathbf{Q}(t)=\mathbf{H}(t)\mathbf{Q}(t) \tag{15}$$

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where the elements of matrix $\mathbf{H}(t)$ are

$$\mathbf{h}_{ii}(t) = -\text{dual}\sum_j \mathbf{w}_{ji}(t) \tag{16}$$

and

$$\mathbf{h}_{ij}(t) = \mathbf{w}_{ij}(t) \;\; (j \neq i) \tag{17}$$

Note 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 $t_0, t_0+\tau, t_0+2\tau, \ldots$ and $\mathbf{H}_k$ remains constant between time $t_0+k\tau$ and $t_0+(k+1)\tau$. The corresponding numerical solution of Eq.(15) is

$$\mathbf{Q}(t+k\tau) = \exp(\tau\mathbf{H}_{k-1})\cdots\exp(\tau\mathbf{H}_0))\mathbf{Q}(t_0) \tag{18}$$

which is an imprecise Markov chain with k steps of transitions.

4.3 Computing interval matrix exponential

The computation of interval matrix exponential $\exp(\tau\mathbf{H}_k)$ in Eq.(18) is the major task in solving the interval master equation. Several approaches have been proposed to calculate the interval matrix exponential. Oppenheimer and Michel [49] used the centered form of interval and Taylor series approximation in the range estimation. Goldsztejn [50] reduced the interval overestimation by a scaling and squaring process. Škulj [51] took a partitioning approach to reduce step sizes to avoid interval overestimation. Different from these approaches, here we use generalized interval. The complete enclosure of the possible variation ranges by the lower and upper bounds is not the only purpose in solving Eq.(15), 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 developed here.

Our approach can be regarded as an extension of the Krylov-based matrix exponential computation [52] from real numbers to generalized intervals. The new algorithm to compute interval matrix exponential is listed in Table 2. The core part of the algorithm is an Arnoldi process to search the interval-valued orthonormal basis $\{\mathbf{V}_1, \ldots, \mathbf{V}_{m+1}\}$ forming a matrix $\mathcal{V} = [\mathbf{V}_1, \ldots, \mathbf{V}_{m+1}]$ and the upper Hessenberg matrix $\mathcal{G} = [\mathbf{g}_{ij}]$ such that $e^{\tau\mathbf{H}}\mathbf{Q}$ can be estimated as

$$\mathbf{U}(\tau) = \beta\mathcal{V}e^{\tau\mathcal{G}}\mathbf{e}_1 \tag{19}$$

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 $e^{\tau\overline{\mathcal{G}}}$ respectively, with real-valued matrices $\underline{\mathcal{G}} = [\underline{g}_{ij}]$ and $\overline{\mathcal{G}} = [\overline{g}_{ij}]$.

For each orthogonal projection in $\mathbf{R} = \mathbf{R} - \text{dual}\mathbf{g}_{ij}\mathbf{V}_i$ in the algorithm, if zero 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. $\mathbf{E} = \mathbf{R} - \text{dual}\mathbf{g}_{ij}\mathbf{V}_i$ can always be interpreted as

$$(\forall E \in \mathbf{E}^{\triangle})(\mathrm{Q}_{\mathbf{R}} R \in \mathbf{R}^{\triangle})(\mathrm{Q}_{\mathbf{g}_{ij}} g_{ij} \in \mathbf{g}_{ij}^{\triangle})(\mathrm{Q}_{\mathbf{V}_i} V_i \in \mathbf{V}_i^{\triangle})(R - g_{ij}V_i = E)$$

where $\mathrm{Q}_{\mathbf{R}}$, $\mathrm{Q}_{\mathbf{g}_{ij}}$, and $\mathrm{Q}_{\mathbf{V}_i}$ can be either $\forall$ or $\exists$. If $0 \in \mathbf{E}^{\triangle}$, then the

Table 2. A Krylov subspace projection algorithm to compute interval matrix exponentials

Compute $\mathbf{U} = e^{\tau\mathbf{H}}\mathbf{Q}$
Input: $\mathbf{H} \in \mathbb{KR}^{n\times n}$ and $\mathbf{Q} \in \mathbb{KR}^n$
Output: $\mathbf{U}$

```
t = 0;
choose an m ≪ n;
β ← ‖Q‖_2;
U ← Q;
WHILE t < τ DO
    V_1 ← U/dual(β);
    FOR j = 1 to m
        R ← H · V_j where R = [r_1, ..., r_n]^T;
        FOR i = 1 to j
            g_ij ← V_i^T · R;
            R ← R − dual g_ij V_i;
            FOR k = 1 to n
                IF 0 ∈ r_k^△;
                    r_k ← 0;
                END IF
            END FOR
        END FOR
        g_{j+1,j} ← ‖R‖_2;
        IF ‖g_{j+1,j}‖_2 < ε;
            BREAK;
        END IF
        V_{j+1} ← R/dual g_{j+1,j};
    END FOR
    g_{m+2,m+1} = 1;
    G ← [g_{1:m+2,1:m+1}];
    V ← [V_1, ..., V_{m+1}];
    Δt = τ − t;
    DO
        F ← e^{ΔtG};
        U ← βV(1 : n, 1 : m+1)F(1 : m+1, 1);
        err = min(|βF(m+1,1)|, |βF(m+2,1)| · ‖HV_{m+1}‖_2);
        Δt ← αΔt where 0 < α < 1;
    WHILE (err > ε)
    t ← t + Δt;
END WHILE
```


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interpretation is

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

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 $0 \in (\mathbf{E}_1^T \cdot \mathbf{E}_2)^{\triangle}$.

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

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

$$\mathbf{U}_i'(t) = \mathbf{U}_i(t) / \mathrm{dual} \sum_{l=1}^{N} \mathbf{U}_l(t) \tag{20}$$

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.

5 NUMERICAL EXAMPLES

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.

5.1 Predatory-prey model

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 shown in Table 3. 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. $N_{predator}$ and N_{prey} are the numbers of species.

Table 3. An example of Lotka-Volterra predatory-prey model

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

With the propensities given in Table 3, the elements of the infinitesimal generator $\mathbf{H}$ are calculated as follows. If the total numbers of species for predator and prey under consideration are n_a and n_b respectively, the total number of states in simulation is $n = n_a \times n_b$. Let the state of the system at a particular time be represented by a vector $x \in \mathbb{Z}^{n \times 2}$ where $x(i,1)$ and $x(i,2)$ the respective number of predator and prey at state i. The three reactions that correspond to the transitions from state $x(j,\cdot)$ to $x(i,\cdot)$ are $[x(j,1) \to x(i,1), x(j,2) \to x(i,2)+1]$, $[x(j,1) \to x(i,1)+1, x(j,2) \to x(i,2)-1]$, and $[x(j,1) \to x(i,1)-1, x(j,2) \to x(i,2)]$ respectively. The two-dimensional vector x needs to be mapped to a one-dimensional state space so that Eq.18 can be applied for simulation. The value of the non-diagonal element $\mathbf{h}_{ij}$ $(i \neq j)$ in $\mathbf{H}$ corresponding to the transition from state j to state i is assigned to be $\mathbf{h}_{ij} = \mathbf{c}_1 x(j,2)$ for the first reaction, $\mathbf{h}_{ij} = \mathbf{c}_2 x(j,1) x(j,2)$ for the second reaction, $\mathbf{h}_{ij} = \mathbf{c}_3 x(j,1)$ for the third reaction, as in Eq.17, by going through each column of $\mathbf{H}$. Any other elements that are not involved in reactions are assigned to be zero. Once the non-diagonal elements $\mathbf{h}_{ij}$'s are assigned, the diagonal elements are calculated by Eq.16.

With the initial distributions $p(N_{predator} = 5) = 1.0$ and $p(N_{prey} = 5) = 1.0$ 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 $c_3 = 0.1$.

To demonstrate the effectiveness of the proposed interval-based approach in incorporating uncertainty, the results are compared with the ones from the traditional Monte Carlo sampling method for sensitivity analysis, as shown in Figure 2. As samples of parameters c_1, c_2, and c_3 within the given intervals are taken randomly from uniform distributions, 40 runs of simulations provide a collection of probability densities at time $t = 2.0$, shown as the 'band' in the figure. For a large portion, they are enclosed by the interval lower and upper bounds generated by the proposed method. Because LCC is enforced, the over-estimation at the portion with higher probability leads to the under-estimation at the portion with lower probability.

The combinations 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.

5.2 Enzyme kinetics

The second example is the Michaelis-Menten enzyme kinetics [53]. The involved reactions and species are listed in Table 4, where enzymes E catalyze 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}.

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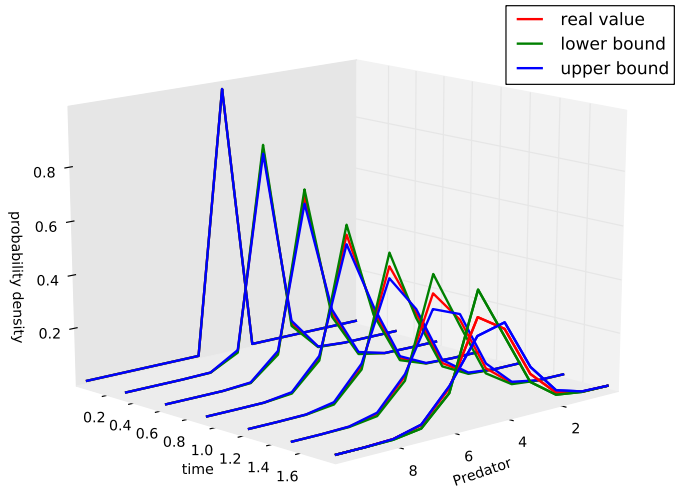
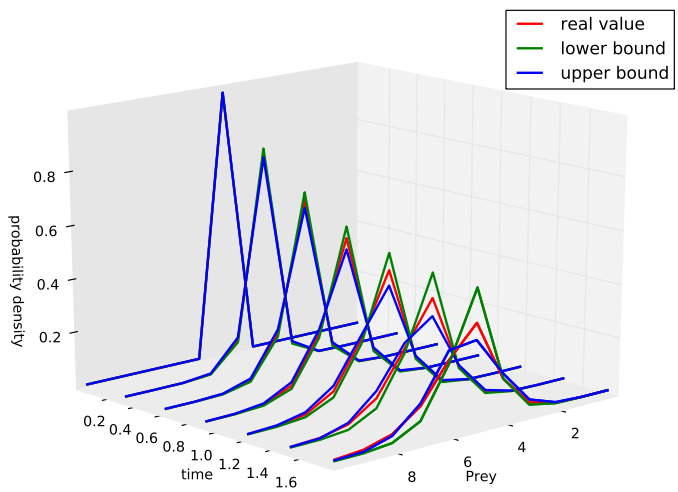
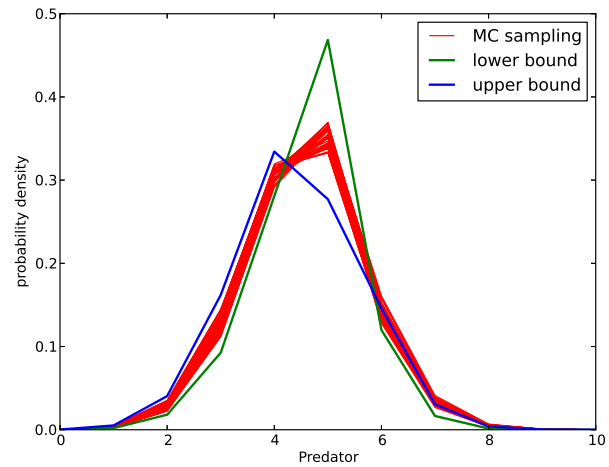


(a) *Predator*

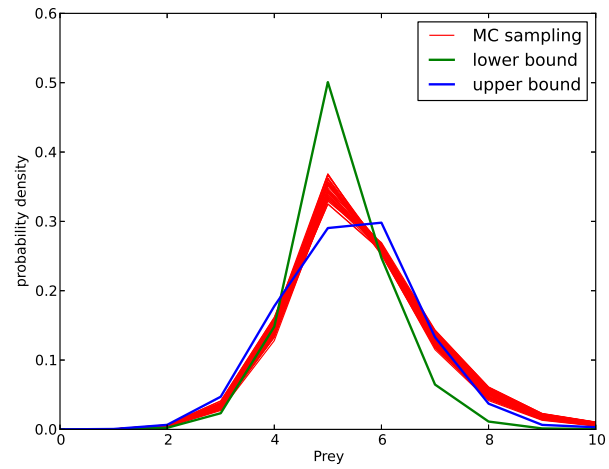


(b) *Prey*

Figure 1. Evolution of probability densities in the Predator-Prey model



(a) *Predator*



(b) *Prey*

Figure 2. Comparison of the results between the proposed interval-based method and Monte Carlo sampling

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 3 shows the evolution of the lower and upper probability densities for the four species, with the comparison with the traditional real-valued ones.

6 CONCLUDING REMARKS

In this paper, a new approach to perform stochastic simulation of finite state transitions under both aleatory and epistemic uncertainties are presented. The underlying theoretical basis is generalized interval probability, which integrates generalized interval and probability. The dynamics of stochastic systems with imprecise model parameters can be simulated without the need of the traditional sensitivity analysis 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 estima-

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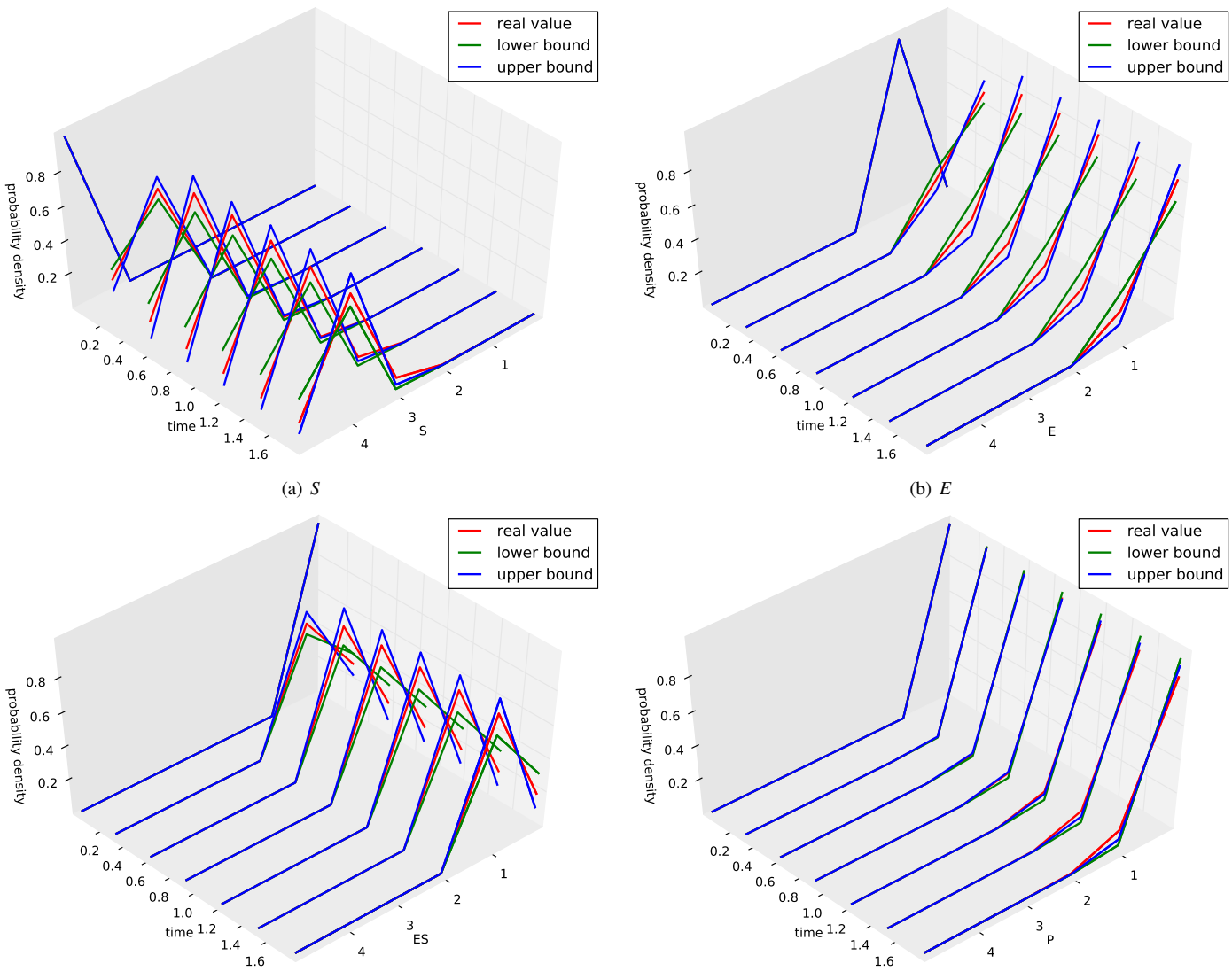

(a) S (b) E

(c) ES (d) P

Figure 3. Time evolution of probability densities in the Michaelis-Menten enzyme kinetics example

Table 4. An example of Michaelis-Menten enzyme kinetics [53]

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

tion for completeness and soundness.

The master equation extended with generalized interval probability models the time evolution of both uncertainty components simultaneously in jump processes. A Krylov subspace projection method is proposed for solving the interval master equation. Numerical examples demonstrated that the developed approach provides insight on the effect of uncertainty associated with models and parameters. Simulation reliability and robustness can be assessed directly from the resulted lower and upper probabilities without introducing the overhead of sensitivity analysis.

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