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14. ABSTRACT
Many engineering systems can be modeled as a large collection of stochastically evolving particles, whose dynamics are weakly coupled by an interaction that depends only on the empirical distribution of the particles. Good design of these systems requires accurate estimation of key performance measures of interest, such as the expected exit time from the neighborhood of a desirable operating point. This requires an understanding of stability, mestastability and other related aspects of the long-time behavior of the system. The focus of this proposal is to develop general analytical and computational methods for quantitative characterizations of these properties. The

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Final Report: 3.4.1 Rare Events, Control and Metastability of Weakly Interacting Particle Systems

ABSTRACT

Many engineering systems can be modeled as a large collection of stochastically evolving particles, whose dynamics are weakly coupled by an interaction that depends only on the empirical distribution of the particles. Good design of these systems requires accurate estimation of key performance measures of interest, such as the expected exit time from the neighborhood of a desirable operating point. This requires an understanding of stability, mestastability and other related aspects of the long-time behavior of the system. The focus of this proposal is to develop general analytical and computational methods for quantitative characterizations of these properties. The techniques developed will include partial differential equation characterizations and control representations for the construction of Lyapunov functions, formulation and solution of optimization problems that identify the most likely large way in which certain rare events of interest occur and the development of efficient importance sampling algorithms for accurate estimation the probabilities of rare events of interest. Additionally, these methods developed will be applied to shed insight into the performance and design of real-world systems.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
08/27/2015	16.00	Amarjit Budhiraja, Paul Dupuis, Markus Fischer, Kavita Ramanan. Limits of relative entropies associated with weakly interacting particle systems, Electronic Journal of Probability, (08 2015): 1. doi: 10.1214/EJP.v20-4003
08/27/2015	17.00	Amarjit Budhiraja, Paul Dupuis, Markus Fischer, Kavita Ramanan. Local stability of Kolmogorov forward equations for finite state nonlinear Markov processes, Electronic Journal of Probability, (08 2015): 1. doi: 10.1214/EJP.v20-4004
08/31/2013	1.00	Amarjit Budhiraja, Jiang Chen, Paul Dupuis. Large deviations for stochastic partial differential equations driven by a Poisson random measure, Stochastic Processes and their Applications, (02 2013): 523. doi:
08/31/2013	2.00	Jim Doll, Nuria Plattner, David Freeman, Yufei Liu, Paul Dupuis. Rare-event sampling: occupation-based performance measures for parallel tempering and infinite swapping Monte Carlo methods, Journal of Chemical Physics, (11 2012): 986. doi:
08/31/2013	3.00	Paul Dupuis, Konstantinos Spiliopoulos, Hui Wang. Importance sampling for multiscale diffusions, Multiscale Modeling & Simulation, (01 2012): 1. doi:
08/31/2013	4.00	Yi Cai, Paul Dupuis. Analysis of an interacting particle method for rare event estimation, Queueing Systems, (02 2013): 345. doi: 10.1007/s11134-013-9344-z
09/15/2014	13.00	Weining Kang, Kavita Ramanan. Characterization of Stationary Distributions of Reflected Diffusions, Annals of Applied Probability, (08 2014): 1329. doi:

TOTAL: **7**

Number of Papers published in peer-reviewed journals:

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Received	Paper
08/28/2015 18.00	Paul Dupuis, Yufei Liu. On the Large Deviation Rate Function for the Empirical Measures of Reversible Jump Markov Processes, The Annals of Applied Probability, (08 2015): 1121. doi:
08/28/2015 19.00	Paul Dupuis, Dane Johnson. Moderate Deviations for Recursive Stochastic Algorithms, Stochastic Systems, (08 2015): 1. doi:
TOTAL:	**2**

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received	Paper
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Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

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TOTAL:	

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(d) Manuscripts

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08/22/2016	5.00	Paul Dupuis, Yufei Liu. On the large deviation rate function for the empirical measures of reversible jump Markov processes, The Annals of Probability (02 2013)
08/22/2016	6.00	Weining Kang, Kavita Ramanan. Characterization of stationary distributions of reflected diffusions, Annals of Applied Probability (10 2012)
08/30/2015	20.00	Nina Gantert, Steven Kim, Kavita Ramanan. Cramer's Theorem is Atypical, http://arxiv.org/abs/1508.04402 (08 2015)
TOTAL:		**3**

Number of Manuscripts:

Books

Received	Book
TOTAL:	

Received	Book Chapter
TOTAL:	

Patents Submitted

Patents Awarded

Awards

Kavita Ramanan

i) IMS (Institute of Mathematical Statistics) Fellow, 2013
ii) IMS (Institute of Mathematical Statistics) Medallion, 2015
iii) Invited Tutorial Speaker at INFORMS International Meeting, Honolulu, June 2016
iv) Invited Tutorial Speaker at the Midwest Probability Colloquium, Evanston, October 2015
v) Keynote Speaker, INFORMS Annual meeting, Philadelphia, November 2015
vi) Plenary speaker, Applied Probability Meeting, Istanbul, July 2015
vii) Plenary speaker, Stochastic Processes and their Applications meeting, Colorado, Boulder, July 2013
viii) Keynote lecture at the Sigma-Xi Northeast Regional Meeting, WCSU, Connecticut, April, 2015

Paul Dupuis

i) Fellow, American Mathematical Society, 2015
ii) Plenary lecture for the workshop Computational Statistics and Molecular Simulation, École de Ponts, Paris, 2^{nd} of February, 2016.
iii) Invited Lecture Series of 12 lectures at Università degli Studi di Padova from 20 May to 31 May, 2013.

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Wei Wu	0.50	
FTE Equivalent:	**0.50**	
Total Number:	**1**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Kavita Ramanan	0.08	
Paul Dupuis	0.08	
FTE Equivalent:	**0.16**	
Total Number:	**2**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED	Discipline
Katrina Kardassakis	0.00	Applied Mathematics
FTE Equivalent:	**0.00**	
Total Number:	**1**	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

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Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Wei Wu

Total Number: 1

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
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Sub Contractors (DD882)

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Paul Dupuis and Kavita Ramanan

A. Foreword and Problem Statement.

Many systems arising in science and engineering can be modeled as a large collection of stochastically evolving agents or particles that are weakly coupled by an interaction that depends only on the current distribution (or empirical measure) of the particles. Such interactions are often referred to as mean-field interactions in the literature. Systems of Markovian particle systems under mean field interactions arise in many different contexts. They first appear as the approximation of statistical physics models in higher dimensional lattices (for various type of spin dynamics, see [23], [7], and references therein) and kinetic theory [17]. Recently, this type of model also appears in studying game theory [16] and communication networks [14, 15]. As an example, consider the situation where a collection of users must use a communication link, and the bandwidth available to an individual user depends on how the collection of users loads the system. A natural question in such a context is: "How should each user adjust its behavior in response to feedback about the congestion in the system, so as to maximize network throughput?" One would like to design control policies that lead to good overall system performance, but the decisions of individual users are allowed to depend only on this limited information regarding the global system state.

For large systems, the dynamics of the entire particle system is Markovian only on a very high-dimensional state space. This makes the study of these particle systems using standard methods from Markov processes challenging due to the curse of dimensionality. Instead, due to the mean-field nature of the system, one can often obtain much information about the system from either studying a typical particle or the empirical measure of the system. Indeed, achieving good performance in these systems typically requires the design of control policies that keep the empirical measure in a neighborhood of some operating point. The objective of this work is to develop analytical and computational tools for the analysis of stability and equilibrium properties of such weakly interacting systems and their empirical measures. It is of particular interest to characterize the typical behavior of the system as well as large deviations from the typical behavior. We would also like to use insight from the latter to develop accelerated Monte Carlo schemes to estimate performance measures of interest for weakly interacting particle systems that arise in applications.

B. Description of a Class of Models.

The dynamics of the particle systems that we consider have the following common features: a) Particles are exchangeable, i.e., their joint distribution is invariant under permutation of their indices. b) At each time, some group of finitely many particles can switch their state simultaneously. c) The interaction between particles are global and weak. In these models, the jump rate (of each group of particles) is a function of the intial and final configuration, and the empirical measure of all particles. We first focus on the case when the dynamics of the interacting particle system is described by a Markov chain, with each particle taking values in a finite state space $\mathcal{X} = \{1, \ldots, d\}$. This setting captures many models arising in applications, and at the same time exhibits the essential mathematical difficulties characteristic of these models. In this setting, the behavior of a typical particle in the system can be approximated by the solution to a finite-dimensional nonlinear ordinary differential equation (ODE), when the number of particles is large.

Specifically, we consider a collection of N weakly interacting particles, in which each particle evolves as a continuous time pure jump càdlàg stochastic process taking values in a finite state space $\mathcal{X} = \{1, \ldots, d\}$. The evolution of this collection of particles is described by an N-dimensional time-homogeneous Markov process $\mathbf{X}^N = \{X^{i,N}, i = 1, \ldots, N\}$, where for $t \geq 0$, $X^{i,N}(t)$ represents the state of the ith particle in the N-particle system at time t. The jump intensity of any given particle depends on the configuration of other particles only through the empirical measure

$$\mu^N(t) \doteq \frac{1}{N} \sum_{i=1}^{N} \delta_{X^{i,N}(t)}, \quad t \in [0, \infty), \tag{1}$$

where δ_a is the Dirac measure at a, and consequently any given particle's effect on the dynamics of any other particle is $O(1/N)$. For this reason the interaction is referred to as a "weak interaction." Note that the random element $\mu^N(t)$ takes values in the space $\mathcal{P}_N(\mathcal{X}) \doteq \mathcal{P}(\mathcal{X}) \cap [\mathbb{Z}^d/N]$, where $\mathcal{P}(\mathcal{X})$ is the space of probability measures on $\mathcal{X}$, equipped with the usual topology of weak convergence.

Under fairly general conditions on the jump rates, the functional law of large numbers of the empirical measure associated with the interacting jump processes was established in [24], and the limit process μ also describes the evolution of the law of a typical particle in the system, in the limit as $N \to \infty$. Since the forward equation describing the law of the particle is non-linear, the associated process is sometimes referred to as a nonlinear Markov process. In the specific case when at most one particle jumps at a given time, μ is defined as a solution to a certain non-linear ODE:

$$\frac{d\mu}{dt} = \mu(t)\Gamma(\mu(t)), \quad t \geq 0, \tag{2}$$

$\mu(0) = \mu_0$, where for each $p \in \mathcal{P}(\mathcal{X})$, $\Gamma(p)$ is a rate matrix. Here, for $i, j \in \mathcal{X}$, roughly speaking $\Gamma_{ij}(p)$ denotes the infinitesimal rate at which a particle jumps from state i to state j when the empirical measure of the particle system is equal to p.

C. Summary of the most important results during the project.
C1. A Large Deviation Principle. In [11] we consider a finite-state weakly interacting system of N particles, and study the sample path large deviations of the associated empirical measure μ^N process from the law of large number limit μ, as the number of particles tends to infinity. Such a sample path large deviation principle over a finite time interval has a number of applications, including the study of metastability properties (via Freidlin-Wentzell theory [13]), an understanding of which is crucial for the study of performance measures in many applications. For a large class of interacting particle systems, in addition to establishing a sample path large deviation principle, we also establish a certain locally uniform refinement for the associated sequence of empirical measure processes and obtain an explicit form for the so-called rate function. The locally uniform refinement characterizes the decay rate of the probability of hitting a point, and is relevant only for finite-state Markov chains (and not diffusions). The proof of this result entails additional subtleties. In particular, we provide an example where the sample path LDP holds, but the locally uniform LDP does not. This locally uniform refinement is used in [5] to construct candidate Lyapunov functions for these interacting particle systems.

The empirical measure of the finite-state weakly interacting system can be represented as a jump Markov process that takes values on the unit simplex, and whose rates diminish to zero as one approaches the boundary. The large deviation upper bound can be obtained as a special case of a more general result in [8]. However, the lower bound is not covered by standard results which typically assumes that all jump rates are uniformly bounded away from zero (cf. [25]). This makes the proof of the large deviation lower bound rather delicate.

Our strategy for the proof is based on a variational representation for empirical measure process and a perturbation argument near the boundary. The starting point of our variational representations is the representation formula for the functionals of Poisson random measures [4], and the fact that the empirical measure process has an SDE representation in terms of a sequence of Poisson random measures. However, the state dependent nature of the jump rates makes the variational problems more complicated, and we utilize the special structure of the SDE to simplify the representation formula. The second component of our proof is a perturbation argument to deal with jump rates that diminish to zero as one approaches the boundary of the unit simplex (the compact state space on which the empirical measure lies). These two tools enable us to study the large deviation lower bound by an explicit construction of the controlled process, and understand its asymptotic properties.

As a by-product of the proof, we also establish a sample path LDP (and its locally uniform refinement) for a generic class of jump Markov processes on the simplex that statisfy certain communication conditions. We believe our arguments are robust in the sense that they can be applied to generic jump Markov processes on fairly general connected, piecewise smooth domains with vanishing rates near the boundary. Also, the variational representation we establish holds for generic jump processes with bounded jump rates, and we expect it to be useful to show other asymptotics.

C2. Lyapunov Functions and Stability of the Nonlinear ODE.

A goal of our work is to study the stability and metastability properties for the nonlinear ODE (2) that describes the law of large numbers limit of the weakly interacting particle system. An understanding of stability properties of the ODE is crucial to understanding the performance of the system.

Lyapunov functions are the main tool used in the stability analysis of nonlinear systems. Thus, a specific objective of our work is to develop systematic methods to construct Lyapunov functions for the nonlinear ODE (2). Although in practice the construction of a Lyapunov function will use particular properties of the system, there are nonetheless a few general principles that guide their construction. Below, we recall two of these principles, which at first glance would appear to be unrelated. However, our results show that for the class of weakly interacting finite-state Markov chains described above, the two very different large deviations analyses in these approaches in fact lead to precisely the same Lyapunov function.

One approach to the construction of Lyapunov functions for deterministic systems is though the notion of energy storage, which is usually formulated in terms of variational problems, and in particular calculus of variations problems. Within this framework is the particular case when the given deterministic system is a law of large numbers limit for a stochastic system that is “nearly” deterministic. For such problems (and assuming all quantities described below are well defined), the large deviation rate function, and in particular the Freidlin-Wentzell quasipotential that can be defined in terms of this rate function, provides a natural candidate (local) Lyapunov function. The relevant large deviation theory in this setting is considered to be of the "small noise" variety, since the stochastic system is viewed as a small random perturbation of the deterministic nonlinear system of interest. The relevant limit is as N tends to infinity, or equivalently, as $1/N$ (which characterizes the order of magnitude of random perturbations of the empirical measures from the deterministic strong law of large numbers limit) tends to zero.

A second approach to the construction of Lyapunov functions, but this time for stochastic systems and in particular for ergodic Markov processes, is to consider the relative entropy function with respect to the invariant distribution. Relative entropy generically serves as a Lyapunov function, though of course the notion of stability here is different. In comparison with the deterministic setting, the Lyapunov function here is used to prove that the *distribution* or *law* of the process converges to the unique invariant distribution. Moreover the evolution of the distribution satisfies a *linear* (though typically high dimensional) deterministic equation.

In the context of the *weakly interacting particle systems* described above, there is the very high dimensional model characterized by $\mathbf{X}^N$, the process that describes the entire collection of interacting particles, as well as a related model which has a low dimensional aspect. This second model is described by a representative particle (any will do since they are assumed exchangable), together with an empirical measure that captures the relevant properties of all other particles. There is a law of large numbers limit as the number of particles tends to infinity, resulting in a nonlinear deterministic system (the evolution equation for the distribution of the so-called nonlinear Markov process).

Starting with the detailed high-dimensional description, one could consider a study of stability properties of the low dimensional problem that is based on calculating relative entropies at the high dimensional (linear) level, and then projecting down to get a statement regarding the low dimensional (nonlinear) dynamics. We do not provide the details of how this is done in this report. However, we note here that the relative entropies at the high dimensional level will scale proportionally with the number of particles, and that although the calculation involves a large deviation limit, it is large deviations for an empirical measure as N, the number of particles tends to ∞.

In [5, 6], we have identified several candidate Lyapunov functions for the nonlinear ODE, and show that these candidates are indeed Lyapunov functions. In [5, 6], we first consider N-particle systems of "Gibbs" type, for which the explicit form of the stationary distribution π^N is known. For these systems, given a probability distribution p on the state space $\mathcal{X}$, we explicitly calculate the limit of the normalized relative entropy of the product distribution $\otimes^N p$ with respect to the stationary distribution π^N, yielding a function of p. Then, for more general interacting systems that do not have an explicit stationary distribution, we use the locally uniform LDP established in [11], to obtain existence of the limits of normalized relative entropies of the product distribution $\otimes^N p$ with respect to the law of the N-particle system at time T. The idea is that as $T \to \infty$, this function would also be expected to serve as a Lyapunov function. Indeed, in ongoing work (see C3 below), both these limits are shown to lead to Lyapunov functions for the nonlinear system.

C3. Numerical Approximations to the Quasipotential

As mentioned in C2, the quasipotential associated with the sequence of N-particle interacting systems captures a lot of information about the stability (and metastability) properties of the system. While for Gibbs systems the quasipotential can be computed explicitly, more generally it can only be expressed as a variational problem that involves the rate function for the sample path LDP obtained in [11]. In [12], we develop numerical approximations to the quasipotential. A numerical algorithm for the quasipotential associated with diffusion processes (as well as many related deterministic optimal control problems) was developed in [2], and modifications of this algorithm have since been used in a variety of other contexts, and are now referred to as "fast-sweeping" algorithms in the numerical analysis community. However, none of the existing algorithms are suitable for solving variational problems (in particular, the one associated with the quasipotential) arising from Markov chains with values on the unit simplex. In particular, the particular geometry of the state space (a unit simplex) leads to new, interesting and non-trivial questions about the appropriate grid structure of the numerical approximation, how to obtain the fast-sweeping property on this grid, and the associated convergence issues. In [12] we develop a "fast-sweeping" type method for the numerical approximation of the quasipotential associated with the weakly interacting particle system model, establish convergence of the method and also demonstrate the efficacy of the algorithm on a variety of examples.

C4. Related Work. One of the areas of research of the PI is focused on the development of large deviation methods for the design of accelerated Monte Carlo schemes. The research uses large deviation theory for purposes of design and analysis, and when existing theory is not adequate, it is developed in the form suited to such applications. Two important classes of problems are considered. In the first class one is interested in a single critical rare event, such as a buffer overflow in a queueing network, or loss of tracking in a problem of dynamical estimation, or transitions between metastable states in a chemical or biological system. The second class of problems uses a very different large deviation theory (that of the empirical measures of a Markov process), and is concerned with efficient methods for approximating the stationary distribution of a Markov process. This numerical problem arises in many settings, and has generated an enormous literature.

The papers [3] and [10] focus on proving what are called moderate deviation principles for fairly complicated process models. A moderate deviation principle gives information that is not as far out in the tails of the distribution as in the case of large deviation, and hence can be used to study events that are rare but not extremely small. Papers that are nearly complete will use these results to design efficient Monte Carlo schemes based on importance sampling to obtain accurate estimates of rare events. The emphasis on efficiency for these problems is due to the fact that the expense associated with generating even a single sample can be high. As an example of how paper [3] could be used consider the problem of assessing the probability of exceeding an allowed pollution level in the context of groundwater contamination. Pollutants are modeled as entering a waterway according to a spatially distributed Poisson input, after which they diffuse throughout the waterway. The problem of interest might be a rare event, such as exceeding a regulatory threshold for chlorinated hydrocarbons, or a less rare event, such as higher-than-normal levels of plant nutrients, leading to algae bloom and fish kill. The form of the rate function in the moderate deviation setting is generically that of a linear-quadratic-regulator, and we have been exploiting this to develop a more systematic approach to importance sampling design than is possible in the large deviation setting.

Paper [9] develops an explicit expression for the large deviation rate for the empirical measure of a jump Markov process. This rate can be used to define a "rate of convergence" for the numerical approximation defined by the empirical measure. The rate is being further developed as a tool for the analysis and design of the "infinite swapping" schemes recently introduced by the PI.

A different approach to mean-field systems with continuous state space, using measure-valued processes, was introduced in a series of papers by the co-PI, K. Ramanan. In particular, certain models of interacting particle systems arising from smany-server networks were studied in [21, 22, 18, 19] and it was shown that by using an appropriate representation of the state of the network, and applying certain martingale methods, one can obtain a characterization of the mean-field equations as well as fluctuations around a fixed point of the mean-field dynamics. In [1], we identify the limiting deterministic dynamics of a class of networks arising from mean-field load balancing, which is given in terms of a coupled system of measure-valued differential equations. In ongong work, we will study the limiting behavior of these equations to understand the stability and equilibrium properties of these systems.

Once a stochastic system is known to be stable, a natural follow-up question is to identify its stationary distribution. In [20], the co-PI obtained a characterization of the stationary distribution of a large class of reflected diffusions is obtained. In particular, we identify a class of state-dependent diffusions whose stationary distribution takes an explicit form. An unconstrained analog of this stationary distribution can be shown to arise as the stationary distributions associated with a class of interacting particle systems.

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