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Safety, Complexity and Responsibility based design and validation of highly automated Air Traffic Management

Specific Targeted Research Projects (STREP)

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Rare event estimation for a large scale stochastic hybrid system with air traffic application
-IPS extension to large hybrid systems-

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Abstract

This report continues the Hybridge development of the Interacting Particle System (IPS) approach towards rare event estimation. Embedding of rare event estimation theory within a stochastic analysis framework has recently led to significant novel results in rare event estimation for a diffusion process using sequential MC simulation. This report presents this rare event estimation theory for diffusions to a Stochastic Hybrid System (SHS) and extends it in order to handle a large scale SHS where a very huge number of rare discrete modes may contribute significantly to the rare event estimation. Essentially, the approach taken is to introduce a suitable aggregation of the discrete modes, and to develop importance sampling and Rao-Blackwellization relative to these aggregated modes. The practical use of this approach is demonstrated for the estimation of mid-air collision for an advanced air traffic control example.

1 Introduction

The aim of WP7 is to perform a safety risk analysis of the Advanced Automous Aircraft Concept of Operations (A^3 ConOps) that has been developed through the first iFly design cycle conducted within WP1 on the basis of human factors guidelines from WP2. This A^3 ConOps has been documented in [20]. This risk analysis serves two main objectives: 1) it should assess up to which en route traffic demand can be safely accommodated by the A^3 ConOps; and 2) it should provide safety assessment feedback to the refinement of the A^3 ConOps within the second design cycle (to be conducted within WP8 and WP9).

The safety risk analysis within WP7 shall be done through conducting hazard identification and Monte Carlo simulation, and should produce estimated accident risk and flight efficiency as a function of traffic demand, including an analysis what this means in terms of the traffic demand that can safely be accommodated by the A^3 ConOps. The estimated accident risk levels should be in the form of an expected value, a 95 % uncertainty area, and a decomposition of the risk level over the main risk contributing sources. In order to accomplish this assessment through Monte Carlo simulation, a complementary aim of WP7 is to further develop the innovative HYBRIDGE speed up approaches in rare event Monte Carlo simulation [10].

In [10] an overview has been provided of the state-of-the-art in Monte Carlo simulation based accident risk assessment for air traffic, including dedicated speed up techniques developed within HYBRIDGE. These methods have succesfully been applied to the assessment of accident risk [4],[9] of the Autonomous Mediterranean Free Flight (AMFF) concept of operations [40]. The AMFF accident risk assessment studies have shown that the accident risk assessment of the A^3 ConOps poses a much higher challenge to the Monte Carlo speed-up methods. And in addition, a bias and uncertainty assessment should also be conducted. In order to prepare for this, potential candidate approaches were identified that are expected to provide significant room for the development of complementary speed-up and bias and uncertainty assessment techniques, such as

a. Perform a study to identify whether randomization theory provides a new perspective to the problem of Monte Carlo simulation speed up.

b. Develop an effective combination of Interacting Particle System based rare event simulation with Markov Chain Monte Carlo speed up technique

c. Develop a method to assess the sensitivity of multiple aircraft encounter geometries to collision risk, and develop importance sampling approaches which take advantage of these sensitivities.

d. Develop novel ways how Interacting Particle System speed up techniques that

apply to a pair of aircraft can effectively be extended to situations of multiple aircraft.

e. Develop an efficient extension of Interacting Particle System based rare event simulation for application to hybrid systems

f. Combine Monte Carlo simulation based bias and uncertainty assessment with operation design parameter optimization.

The most promising candidates are explored and subsequently the results are integrated with the innovative speed up approaches used in [4],[9].

The aim of this report is to study option e and this is organized as follows. In Section 2, the problem is formulated in the setting of reach probability analysis. Section 3 develops a factorization of the reach probability. Section 4 explains the approach of [17, 18, 22, 23]. Section 5 presents an extension of this approach to hybrid systems. Section 6 develops the aggregation mode process and characterizes key relations with the controlled SHS. Section 7 develops a novel sequential MC simulation approach for estimating reach probabilities. Section 8 shortly describes the free flight air traffic example considered. Section 9 applies the novel approach towards estimating reach probabilities for this air traffic example. Section 10 presents concluding remarks. An early version of this report is [5].

2 SHS Reach probability

This study is motivated by the problem of safety verification of a future air traffic concept of operation through the analysis of reach probabilities. From a control theoretic perspective, such an advanced concept of operations is a blueprint of a controlled Stochastic Hybrid System (SHS) which satisfies the strong Markov property [14]. Recently, Sastry and co-workers [1, 2] studied the optimization of the control policy of a discrete-time SHS, such that the probability of staying within some prescribed safe set remains above some prescribed minimum level. Specifically, Amin et al. [2] developed a theoretical framework which expressed the reach probability as a multiplicative function, and this was used to develop a dynamic programming-based approach to compute probabilistic maximal safe sets, i.e. initial states of a system for which control policies exists that assure the reach probability to stay below some given value. Subsequently, Abate et al. [1] showed this problem to be complementary to the problem of how to optimize the control policy of an SHS such that the reach probability of some prescribed unsafe set remains below some given maximum level, and that the same dynamic programming-based computation of maximal safe sets can be used. The dynamic programming approach becomes computationally

intractable when the SHS considered is of large scale type. Prandini and Hu [42] developed a Markov chain approximation based method for the computation of reach probabilities for a continuous time SHS. This way the dynamic programming challenge is avoided, however the computational load of their method prohibits its application to a large scale SHS. Prajna et al. [41] developed an approach to obtain an upper bound of the reach probability, but this cannot handle large scale SHS either.

In theory, reach probability estimation can be done by simulating many trajectories of the process considered, and counting the fraction of cases where the simulated trajectory reaches the unsafe set within some given period T. When the reach probability value is very small then the number of straightforward MC simulations needed is impractically large. Rare event estimation literature forms a potentially rich source of information for speeding up MC simulation, e.g. through combining methods from large deviation and importance sampling theories [12, 31, 33]. An early successful development in this area is sequential MC simulation for the estimation of the intensity of radiation that penetrates a shield of absorbing material in nuclear physics, e.g. [11]. More recently this approach has also found application in non-nominal delay time and loss estimation in telecommunication networks, e.g. [3]. L'Ecuyer et al. [38] provide a very good recent overview of these sequential MC simulation developments.

In order to exploit rare event estimation theory within probabilistic reachability analysis of controlled SHS, we are in need of establishing a theoretically unambiguous connection between the two concepts. Implicitly, this connection has recently been elaborated by Del Moral and co-workers [17, 18, 19, 22, 23]. They embedded theoretical physics equations, which supported the development of advanced MC simulations, within the stochastic analysis setting that is typically used for probabilistic reachability analysis. They subsequently showed that this embedding provides a powerful background for the development and analysis of sequential MC simulation for rare event simulation. In [39] this novel development is well explained in the broader context of splitting techniques in rare event simulation.

The aim of this report is to present a part of the framework developed by Del Moral et al. [17, 18, 19, 22, 23] in a probabilistic reachability setting, to further develop this for a large scale SHS, and to demonstrate its practical use for safety verification of an advanced air traffic operation. In [8, 9], the practical use of the approach of Del Moral [17, 18, 19, 22, 23] for safety verification of an advanced air traffic operation has already been demonstrated for some specific scenarios. In these scenarios, the main contributions to the reach probability value came from diffusion behavior. It also became clear that the same sequential MC simulation approach failed to work for scenarios of the same air traffic operation where the reach probability is determined by rare switching between modes. This chapter is aimed to handle such more demanding rare event estimation problems for large scale controlled SHS. Essentially

the approach is to introduce an aggregation of the discrete mode process, and to develop importance switching and Rao-Blackwellization relative to these aggregated modes.

3 Factorization of reach probability

Throughout this and the following sections, all stochastic processes are defined on a complete stochastic basis $(\Omega, \mathscr{F}, \mathbb{F}, P, \mathrm{T})$ with $(\Omega, \mathscr{F}, P)$ a complete probability space, and $\mathbb{F}$ an increasing sequence of sub-σ-algebra's on the positive time line $\mathrm{T} = \mathbb{R}_+$, i.e. $\mathbb{F} \triangleq \{\mathscr{J}, (\mathscr{F}_t, t \in \mathrm{T}), \mathscr{F}\}$, $\mathscr{J}$ containing all P-null sets of $\mathscr{F}$ and $\mathscr{J} \subset \mathscr{F}_s \subset \mathscr{F}_t \subset \mathscr{F}$ for every $s < t$.

Let us denote $E' = \mathbb{R}^n \times \mathbb{M}$, with $\mathbb{M}$ a discrete set. Let $\mathscr{E}'$ be the Borel σ-algebra of E'. We consider a time-homogeneous strong Markov process which also is a generalised stochastic hybrid process $\{x_t, \theta_t\}$ [13, 15, 34, 37], with $\{x_t\}$ assuming values in $\mathbb{R}^n$ and $\{\theta_t\}$ assuming values in $\mathbb{M}$. The first component of $\{x_t\}$ equals t and the other components of $\{x_t\}$ form an $\mathbb{R}^{n-1}$ valued cadlag process $\{s_t\}$. The $\mathbb{M}$-valued process $\{\theta_t\}$ is a cadlag switching process. Incorporating t as a state component allows to represent any time-inhomogeneous strong Markov process $\{s_t, \theta_t\}$ as a time-homogeneous strong Markov process $\{t, s_t, \theta_t\}$ [21]. The problem considered is to estimate the probability that $\{s_t\}$ hits a given "small" closed subset $D \subset \mathbb{R}^{n-1}$ within a given time period $[0, T)$, i.e. $P(\exists t \in [0, T);\ s_t \in D)$.

Following Del Moral and co-workers [17, 18, 22, 23], this probability can be characterized in the form of a multiplicative function the terms of which are defined through an arbitrarily assumed nested sequence of closed (time-invariant) subsets $D = D_m \subset D_{m-1} \subset \ldots \subset D_1$, with the constraint that $P(s_0 \in D_1) = 0$ and each component of $\{x_t\}$, that may hit any D_k, is a pathwise continuous process. In order to derive a multiplicative functional characterization of the hitting probability, we set $\tau_0 = 0$ and define $\tau_k, k = 1, .., m$, as the first moment that $\{s_t\}$ hits subset k, i.e.

$$\tau_k = \inf\{t > 0;\ s_t \in D_k\}, \tag{1}$$

which implies $P(\exists t \in [0, T);\ s_t \in D_m) = P(\tau_m < T)$.

We also define $\{0, 1\}$-valued random variables $\{\chi_k, k = 0, .., m\}$ as follows

$$\chi_k = \begin{cases} 1 & \text{if } \tau_k < T \text{ or } k = 0, \\ 0 & \text{otherwise.} \end{cases}$$

By using these τ_k and χ_k definitions and the assumption that each component of $\{s_t\}$ that may hit any D_k, $k = 1, .., m$, has continuous paths (i.e. $\{s_t\}$ can not enter D_k by jumping over the boundary of D_k) we can write the probability of $\{s_t\}$ hitting

D before T as a product of conditional probabilities of reaching D_k given D_{k-1} has been reached at some earlier moment in time, i.e.

$$P(\tau_m < T) = \mathbb{E}[\chi_m] = \mathbb{E}[\prod_{k=1}^{m} \chi_k] = \prod_{k=1}^{m} \mathbb{E}[\chi_k \,|\, \chi_{k-1} = 1]$$
$$= \prod_{k=1}^{m} P(\tau_k < T \,|\, \tau_{k-1} < T) = \prod_{k=1}^{m} \gamma_k \tag{2}$$

with $\gamma_k \triangleq P(\tau_k < T \,|\, \tau_{k-1} < T)$.

With this, the problem can be seen as one to estimate the conditional probabilities γ_k in such a way that the product of the estimators $\tilde{\gamma}_k$ is unbiased. Because of the multiplication of the various individual $\tilde{\gamma}_k$ estimators, which depend on each other, in general such a product may be heavily biased. Garvels et al. [29, 30] showed for a discrete-time Markov process that estimating the γ_k's in (2) by an appropriate sequential MC simulation approach, which is known as "splitting method", guarantees unbiased estimation of $P(\tau_m < T)$. The key novelty of [17, 18, 19, 22, 23] was to develop such convergence type of proof for a sequential MC simulation approach towards the estimation of the γ_k's in (2) under the much weaker condition that $\{s_t\}$ is embedded in (or is) a strong Markov process.

4 Sequential MC simulation

For the process $\{x_t, \theta_t\}$ we follow the approach of [17, 18, 22, 23] to characterize how the evolution proceeds from $\tau_{k-1} \wedge T$ to $\tau_k \wedge T$ with $\tau_k \wedge T = min\{\tau_k, T\}$. For any $B \in \mathscr{E}'$, let $p_{\xi_k|\chi_k}(B \,|\, 1)$ denote the conditional probability of $\xi_k = (x_{\tau_k \wedge T}, \theta_{\tau_k \wedge T}) \in B$ given $\chi_k = 1$. Under the assumption that $P(s_0 \in D_1) = 0$, we characterize the following recursive sequence of transformations:

$$p_{\xi_{k-1}|\chi_{k-1}}(\cdot \,|\, 1) \xrightarrow{\text{prediction}} p_{\xi_k|\chi_{k-1}}(\cdot \,|\, 1) \xrightarrow{\text{conditioning}} p_{\xi_k|\chi_k}(\cdot \,|\, 1).$$
$$\downarrow$$
$$\gamma_k$$

Because $\{x_t, \theta_t\}$ is a strong Markov process, $\{\xi_k\}$ is a Markov sequence. Hence the prediction step satisfies a Chapman-Kolmogorov equation:

$$p_{\xi_k|\chi_{k-1}}(B|1) = \int_{E'} p_{\xi_k|\xi_{k-1}}(B|\xi)\, p_{\xi_{k-1}|\chi_{k-1}}(d\xi|1). \tag{3}$$

Next we characterize the conditional probability of reaching the next subset:

$$\gamma_k = P(\tau_k < T | \tau_{k-1} < T) = P(\chi_k = 1 | \chi_{k-1} = 1)$$
$$= \mathbb{E}[\chi_k \,|\, \chi_{k-1} = 1] = \int_{E'} 1_{Q_k}(\xi)\, p_{\xi_k|\chi_{k-1}}(d\xi|1), \tag{4}$$

where $Q_k \triangleq (0,T) \times D_k \times \mathbb{M}$. Similarly, the condition step satisfies, for any $B \in \mathscr{E}'$:

$$p_{\xi_k|\chi_k}(B|1) = \frac{\int_B 1_{Q_k}(\xi)\, p_{\xi_k|\chi_{k-1}}(d\xi|1)}{\int_{E'} 1_{Q_k}(\xi')\, p_{\xi_k|\chi_{k-1}}(d\xi'|1)}. \tag{5}$$

With this, the γ_k's in (2) are characterized as a solution of the set of recursive equations (3)-(5). Following [17, 18, 22, 23], this recursive characterization can numerically be approximated through a sequential MC simulation to estimate $P(\tau_m < T)$. This is referred to as the IPS (Interacting Particle System) algorithm, and works as follows.

Simulate N_p random trajectories of $\{x_t, \theta_t\}$ over $[0,T)$, each of which starts from a random initial condition $((0,s_0),\theta_0)$, with $s_0 \notin D_1$. Each simulated trajectory stops at $\tau_1 \wedge T$, i.e. upon hitting Q_1 or when the first x-component reaches T. The full hybrid states of these trajectory end points form an empirical density $\tilde{\pi}_1$ as an approximation of $p_{\xi_1|\chi_1}(.|1)$. This empirical density is used to generate (i.e. to resample) N_p initial conditions of trajectories which are subsequently simulated until hitting Q_2 or when the first x-component reaches T; the end points in Q_2 form an empirical density $\tilde{\pi}_2$ as an approximation of $p_{\xi_2|\chi_2}(\cdot|1)$. This cycle repeats from Q_2 to Q_3 ,... , and finally from Q_{m-1} to $Q_m = Q$. During the k-th cycle, a fraction $\tilde{\gamma}_k$ of the N_p simulated trajectories arrives at Q_k. The product of these m fractions forms an estimator for $P(\tau_m < T)$.

Using the recursive characterization of the conditional density, [17, 22] have also shown that the product of these fractions $\tilde{\gamma}_k$ forms an unbiased estimate of the probability of $\{s_t\}$ to hit the set D within the time period $[0,T)$, i.e.

$$\mathbb{E}[\prod_{k=1}^{m} \tilde{\gamma}_k] = \prod_{k=1}^{m} \gamma_k = P(\tau < T).$$

In addition there is a bound on the L^1 estimation error [17, 22], i.e.:

$$\mathbb{E}(\prod_{k=1}^{m} \tilde{\gamma}_k - \prod_{k=1}^{m} \gamma_k) \leq \frac{c_p}{\sqrt{N_p}},$$

with c_p a finite constant which depends on the simulated scenario and the sequence of nested subsets adopted. These convergence results have been obtained under the assumption that the resampling of the empirical density $\tilde{\pi}_k$ is done uniformly,

hence there is a chance of resampling some particles more than once, and other particles not at all. Furthermore, Cérou et al. [19] developed some complementary error bounds, and showed convergence under an alternate resampling approach.

Application of this IPS algorithm to air traffic operation may work well for specific scenarios where rare discrete modes are not significantly contributing to the reach probability [8, 9]. However, there also are relevant scenarios which do not satisfy the latter condition. To tackle this problem, [34, 35, 36] proposed Hybrid versions of the baseline IPS algorithm (HIPS). These approaches work well only if the size of space $\mathbb{M}$ is not too big. However, in many realistic scenarios the state space $\mathbb{M}$ of the discrete valued component $\{\theta_t\}$ is usually very large. Therefore another extension was proposed, namely, Hierarchical Hybrid IPS algorithm (HHIPS), which will be presented and applied in this chapter. For the convenience of the reader, before addressing HHIPS, we first introduce the HIPS algorithm of [35].

5 Importance switching based Hybrid IPS algorithm

Although in theory the IPS approach is applicable virtually to any strong Markov process, in practice the straightforward application of this approach to stochastic hybrid processes may fail to produce reasonable estimates within a reasonable amount of simulation time. First, there may be few or no particles in modes with small probabilities (i.e. "light" modes). This happens because each resampling step tends to sample more "heavy" particles from modes with higher probabilities, thus, "light" particles in the "light" modes tend to be discarded. Second, if the switching rate is small then it is highly unlikely to observe even one switch during a simulation run. In such cases, the possible switching between modes is not properly taken into account. Together with the first problem this badly affects IPS estimation performance. By increasing the number of particles the IPS estimates should improve but only at the cost of substantially increased simulation time which makes the performance of IPS approach similar to one of the standard Monte Carlo.

The HIPS algorithm of [35] incorporates sampling per mode (stratified sampling with modes defining the strata) to cope with large differences in mode weights, and importance switching (an importance sampling form for the discrete valued component $\{\theta_t\}$) to cope with rare mode switching. In what follows, we outline the HIPS algorithm.

If the initial probabilities of some particular modes are very small then it is highly unlikely to draw particles in these modes. To avoid this, at the initial sampling step we start with a fixed number of particles in each mode whatever small the initial probability is and adjust the weights appropriately. Let N_p denote the initial number of particles in each mode $\theta \in \mathbb{M}$. In total the system of particles will consist of $N = N_p \cdot |\mathbb{M}|$ particles. Let J^θ denote the ordered set of indices of particles which are in

mode θ ($J^\theta \cap J^\eta = \varnothing$ for $\theta \neq \eta$). The whole set of indices is defined by

$$J \triangleq \bigcup_{\theta\in\mathbb{M}} J^\theta = \{1,2,\ldots,N\},\ |J| = N.$$

At the initial sampling step we will have $|J^\theta| = N_p$ particles in each mode $\theta \in \mathbb{M}$. As particles evolve and switch from one mode to another one, the numbers of particles in different modes will change, so will the index sets J^θ's. But at each resampling step we will again sample N_p particles for each mode $\theta \in \mathbb{M}$ from a conditional empirical distribution.

Let $\tilde{\gamma}_k$ and $\tilde{\pi}_k$ denote numerical approximations of γ_k and $p_{\xi_k|\chi_k}(\cdot\,|\,1)$ respectively. We choose these numerical approximations in the form of the weighted empirical distributions associated with the particle system $\{\xi_k^i, \omega_k^i\}_{i=1}^N$, where $\xi_k \triangleq (x_{\tau_k\wedge T}, \theta_{\tau_k\wedge T})$ and $\omega \in [0,1]$. When simulating from $\tau_{k-1}\wedge T$ to $\tau_k \wedge T$, only a fraction γ_k of the Monte Carlo simulated trajectories will reach Q_k. The HIPS algorithm estimates these fractions and their product in a recursive way using the following steps:

Step 0 generates, per $\theta \in \mathbb{M}$ value, N_p initial particles at $k = 0$ and then starts the cycling through steps 1 through 3 for $k := 1,2,\ldots,m$.

Step 1 extrapolates each particle from $\tau_{k-1}\wedge T$ to $\tau_k \wedge T$ in time steps of length h, using importance switching for the new value of $\{\theta_t\}$ component.

Step 2 evaluates the particles that have arrived at Q_k. For this, use is made of equations (4)-(5).

Step 3 resamples with replacement, per $\theta \in \mathbb{M}$, N_p particles that have arrived at Q_k; the weights must be adjusted accordingly.

Each of these steps is specified in detail below.

Hybrid Interacting Particle System (HIPS)

HIPS Step 0: Initial sampling for $k = 0$.

- For each $\theta \in \mathbb{M}$, sampling N_p independent initial $\mathbb{R}^n$ values outside D_1: $x_0^j \sim p_{x_0|\theta_0}(\cdot|\theta)$. Set $\theta_0^j = \theta$, then $\xi_0^j = (x_0^j, \theta_0^j)$, $j \in J^\theta$.
- Assigning initial weights:

$$\omega_0^j = P_{\theta_0}(\theta)/N_p, \quad j \in J^\theta, \quad \theta \in \mathbb{M}.$$

- Then $\tilde{\gamma}_0 = 1$ and

$$p_{x_0,\theta_0}(dx,\theta) \approx \sum_{\theta\in\mathbb{M}} \sum_{j\in J^\theta} \omega_0^j \delta_{(x_0^j,\theta_0^j)}(dx,\theta) = \sum_{i=1}^N \omega_0^i \delta_{(x_0^i,\theta_0^i)}(dx,\theta).$$

HIPS iteration cycle: For $k = 1, \dots, m$ cycle over step 1 (prediction), step 2 (assessment) and step 3 (resampling):

HIPS Step 1. Prediction:

- For $i = 1, \dots, N$, using importance switching for $\{\theta_t\}$ component[1], generate path starting at $\xi_{k-1}^i = (x^i_{\tau_{k-1}\wedge T}, \theta^i_{\tau_{k-1}\wedge T})$ until the k-th set Q_k is reached.
- The weight of each particle must be adjusted recursively in time (i.e. at each time discretization step):

$$\omega^i_{t+h} = \omega^i_t \cdot L_{t+h|t}(\theta^i_{t+h} \,|\, \theta^i_t, x^i_t),$$

where

$$L_{t+h|t}(\theta^i_{t+h} \,|\, \theta^i_t, x^i_t) = \frac{p_{\theta_{t+h}|\theta_t, x_t}(\theta^i_{t+h}|\theta^i_t, x^i_t)}{\tilde{p}_{\theta_{t+h}|\theta_t, x_t}(\theta^i_{t+h}|\theta^i_t, x^i_t)}$$

is the likelihood ratio corresponding to the change of switching rates of the $\{\theta_t\}$ component.

- This yields a new set of particles $\{\xi^i_k, \omega^i_k\}_{i=1}^N$.

HIPS Step 2. Evaluation of the Q_k arrived particles:

- Particles which do not reach the set Q_k are killed, i.e. we set $\hat{\omega}^i_k = 0$, else set $\hat{\omega}^i_k = \omega^i_k$ and $\hat{\xi}^i_k = \xi^i_k$.
- The new set of particles is $\{\hat{\xi}^i_k, \hat{\omega}^i_k\}_{i=1}^N$.
- Approximation of γ_k:

$$\gamma_k \approx \tilde{\gamma}_k = \sum_{i=1}^N \hat{\omega}^i_k.$$

If all particles are killed, i.e. $\tilde{\gamma}_k = 0$, then the algorithm stops and $P_{hit}(0, T) \approx 0$.

- If $k = m$, then stop HIPS with the estimate

$$P_{hit} \approx \prod_{k=1}^m \tilde{\gamma}_k.$$

- For each $i = 1, \dots, N$ set $\tilde{\xi}^i_k = \hat{\xi}^i_k$ and normalize the weights: $\bar{\omega}^i_k = \hat{\omega}^i_k / \tilde{\gamma}_k$.

[1] in order to increase frequency of switchings at each time discretization step we replace the original transition probabilities $p_{\theta_{t+h}|\theta_t, x_t}(\cdot|\theta, x)$ by some known transition probabilities $\tilde{p}_{\theta_{t+h}|\theta_t, x_t}(\cdot|\theta, x)$, which guarantees higher switching rates (see [34, 35] for details).

- This yields a new set of particles $\{\tilde{\xi}^i_k, \tilde{\omega}^i_k\}_{i=1}^N$.
- The estimated $p_{\xi_k|\chi_k}(\cdot\,|\,1)$ satisfies:

$$p_{\xi_k|\chi_k}(dx,\theta\,|\,1) \approx \tilde{\pi}_k(dx,\theta) = \sum_{i=1}^{N} \tilde{\omega}^i_k \delta_{(\tilde{x}^i_k,\tilde{\theta}^i_k)}(dx,\theta).$$

HIPS Step 3. Resampling step.

- For each mode $\theta \in \mathbb{M}$ resample with replacement N_p values of $\tilde{\xi}_k$ from the unnormalized conditional empirical measure

$$p_{\xi_k|\chi_k,\theta_k}(\cdot\,|\,1,\theta) \approx \tilde{\pi}_k(dx,\theta\,|\,\theta_k=\theta) = \sum_{j\in J^\theta} \tilde{\omega}^j_k \delta_{(\tilde{x}^j_k,\tilde{\theta}^j_k)}(dx,\theta)$$

  and adjust the weights as follows

$$\omega^j_k = \frac{\sum_{s\in J^\theta} \tilde{\omega}^s_k}{N_p}, \quad j \in J^\theta, \quad \theta \in \mathbb{M}.$$

- This yields a new set of particles $\{\xi^i_k, \omega^i_k\}_{i=1}^N$.
- If $k < m$, then repeat steps 1 - 3 for $k := k+1$.

6 Aggregation of modes

In [34, 35, 36], hybrid versions of the baseline IPS algorithm [17, 18, 22, 23] have been developed, which take into account that rare discrete modes may contribute significantly to the reach probability to be estimated. As has been explained in section 5, the hybrid IPS version of [35] simulates a more frequent switching $\mathbb{M}$-valued process $\{\tilde{\theta}_t\}$ and compensates importance weights for the difference between $\{\tilde{\theta}_t\}$ and $\{\theta_t\}$. In [36] another hybrid IPS version has been developed, which makes use of Rao-Blackwellization by using exact probabilistic equations for certain components and simulated particles for all other components [16]. For filtering of a stochastic hybrid process $\{x_t,\theta_t\}$ two Rao-Blackwellization versions have been developed [6, 24]. The version of [24] uses exact probabilistic equations for $\{x_t\}$ and particle simulation for $\{\theta_t\}$. The version of [6] uses exact probabilistic equations for $\{\theta_t\}$ and particle simulation for $\{x_t\}$. [36] combines the latter approach with IPS. The resulting hybrid IPS version uses exact probabilistic equations for the evolution of $\{\theta_t\}$ and simulates particles for the Euclidean valued $\{x_t\}$. This Rao-Blackwellization based hybrid IPS version also resamples at the end of each IPS cycle N_p x-values from $\tilde{\pi}_k(\cdot,\theta)$ for each

mode $\theta \in \mathbb{M}$, leading to a total of $N_p \times |\mathbb{M}|$ particles, where $|\mathbb{M}|$ is the number of elements in $\mathbb{M}$. Since the computational load increases linearly with $|\mathbb{M}|$, these hybrid IPS approaches are computationally intractable when $|\mathbb{M}|$ is very large. Such condition e.g. applies to the air traffic example (where $|\mathbb{M}| \approx 10^{25}$) considered further on in this chapter.

The idea is to improve the situation for very large $|\mathbb{M}|$ through developing an hybrid IPS approach not for $\{\theta_t, x_t\}$, but for $\{\kappa_t, (\theta_t, x_t)\}$, where $\{\kappa_t\}$ is some complementary $\mathbb{K}$-valued process with $|\mathbb{K}| \ll |\mathbb{M}|$. In order to accomplish this, we group modes that have large differences in mode switching frequencies. This defines a partition $\{\mathbb{M}_\kappa,\ \kappa \in \mathbb{K}\}$, i.e. $\bigcup_{\kappa\in\mathbb{K}} \mathbb{M}_\kappa = \mathbb{M}$ and $\mathbb{M}_\kappa \bigcap \mathbb{M}_{\kappa'} = \emptyset$ for $\kappa \neq \kappa'$, and a $\mathbb{K}$-valued aggregation mode process $\{\kappa_t\}$ as follows:

$$\kappa_t(\omega) = \kappa, \text{ if } \theta_t(\omega) \in \mathbb{M}_\kappa. \tag{6}$$

Because the evolution of the aggregation mode process $\{\kappa_t\}$ depends of the evolution of $\{\theta_t\}$, $\{\kappa_t\}$ may inherit rare mode switching from $\{\theta_t\}$. In order to avoid these rare effects in the evolution of particles, we also define a $\mathbb{K}$-valued Markov chain $\{\check{\kappa}_t\}$ with known non-rare transition rates, and use the transition rates of $\{\check{\kappa}_t\}$ to determine for each particle a new $\check{\kappa}$-value at some time step h later. The particle weight is compensated with the corresponding importance switching ratio

$$p_{\kappa_{\tau+h}|\kappa_\tau,x_\tau,\theta_\tau}(\check{\kappa}|\kappa,x,\theta) \,/\, p_{\check{\kappa}_{\tau+h}|\check{\kappa}_\tau}(\check{\kappa}|\kappa),$$

where κ, x, θ denote the given $(\kappa_\tau, x_\tau, \theta_\tau)$ particle value, and $\check{\kappa}$ denotes the value newly sampled for $\check{\kappa}_{\tau+h}$.

Next, the prediction of the new $\theta_{\tau+h}$ particle from the (x_τ, θ_τ) particle values is done conditional on the newly sampled $\check{\kappa}$ value. Theorem 6.1 provides a probabilistic characterization of such $\check{\kappa}$-conditional θ-prediction.

Theorem 6.1. *($\check{\kappa}$-conditional θ-prediction) Let τ be an arbitrary stopping time, then*

$$p_{\theta_{\tau+h}|x_\tau,\theta_\tau,\kappa_{\tau+h}}(\eta|x,\theta,\check{\kappa}) = \frac{1_{\mathbb{M}_{\check{\kappa}}}(\eta)\, p_{\theta_{\tau+h}|x_\tau,\theta_\tau}(\eta|x,\theta)}{\sum_{\eta'\in\mathbb{M}} 1_{\mathbb{M}_{\check{\kappa}}}(\eta')\, p_{\theta_{\tau+h}|x_\tau,\theta_\tau}(\eta'|x,\theta)}. \tag{7}$$

Proof. Using Bayes yields:

$$p_{\theta_{\tau+h}|x_\tau,\theta_\tau,\kappa_{\tau+h}}(\eta|x,\theta,\check{\kappa}) = \frac{p_{\kappa_{\tau+h}|\theta_{\tau+h}}(\check{\kappa}|\eta)\, p_{\theta_{\tau+h}|x_\tau,\theta_\tau}(\eta|x,\theta)}{\sum_{\eta'\in\mathbb{M}} p_{\kappa_{\tau+h}|\theta_{\tau+h}}(\check{\kappa}|\eta')\, p_{\theta_{\tau+h}|x_\tau,\theta_\tau}(\eta'|x,\theta)}.$$

Substituting $p_{\kappa_{\tau+h}|\theta_{\tau+h}}(\check{\kappa}|\eta) = 1_{\mathbb{M}_{\check{\kappa}}}(\eta)$ yields (7). □

The prediction of the x-part of the particle over time step h is done by drawing a sample from $p_{x_{\tau+h}|x_\tau,\theta_\tau,\theta_{\tau+h}}(\cdot|x,\theta,\eta)$. In order to identify all particles that arrive at Q_k

before time T, the prediction over time step h has to be done up to T/h times. After these prediction steps, there is no guarantee that for each $\breve{\kappa} \in \mathbb{K}$ some minimum number of particles have arrived at Q_k. Hence we resample the Q_k-arrived particles such that we regain N_p particles for each $\kappa \in \mathbb{K}$. In order to make this possible, in Theorem 6.2 we provide a characterization of the (conditional) probabilities $p_{\kappa_{\tau+h}}$ and $p_{x_\tau,\theta_\tau|\kappa_{\tau+h}}$ as a function of p_{x_τ,θ_τ}, for arbitrary stopping time τ and time step h. This characterization allows to sample a fixed number of particles per aggregation mode $\kappa \in \mathbb{K}$, and to sample for each particle a novel θ value conditional on the aggregation mode value.

Theorem 6.2. *(Hierarchical interaction) If $p_{\kappa_{\tau+h}}(\kappa) > 0$ for an arbitrary stopping time τ, then*

$$p_{x_\tau,\theta_\tau|\kappa_{\tau+h}}(dx,\theta|\kappa) = \sum_{\eta\in\mathbb{M}_\kappa} p_{\theta_{\tau+h}|x_\tau,\theta_\tau}(\eta|x,\theta)\, p_{x_\tau,\theta_\tau}(dx,\theta)/p_{\kappa_{\tau+h}}(\kappa) \tag{8}$$

$$p_{\kappa_{\tau+h}}(\kappa) = \sum_{\theta\in\mathbb{M}} \int_{\mathbb{R}^n} \sum_{\eta\in\mathbb{M}_\kappa} p_{\theta_{\tau+h}|x_\tau,\theta_\tau}(\eta|x,\theta)\, p_{x_\tau,\theta_\tau}(dx,\theta). \tag{9}$$

Proof. By definition of the partitioning $\{\mathbb{M}_\kappa,\ \kappa \in \mathbb{K}\}$ we have

$$\begin{aligned} p_{\kappa_{\tau+h},x_\tau,\theta_\tau}(\kappa,dx,\theta) &= \sum_{\eta\in\mathbb{M}_\kappa} p_{\theta_{\tau+h},x_\tau,\theta_\tau}(\eta,dx,\theta) \\ &= \sum_{\eta\in\mathbb{M}_\kappa} p_{\theta_{\tau+h}|x_\tau,\theta_\tau}(\eta|x,\theta)\, p_{x_\tau,\theta_\tau}(dx,\theta). \end{aligned}$$

Dividing left and right hand sides by $p_{\kappa_{\tau+h}}(\kappa)$ yields (8). From the law of total probability we have:

$$p_{\kappa_{\tau+h}}(\kappa) = \sum_{\theta\in\mathbb{M}} \int_{\mathbb{R}^n} p_{\kappa_{\tau+h},x_\tau,\theta_\tau}(\eta,dx,\theta).$$

Substitution of the latter in the former yields (9). □

In order to see what Theorem 6.2 means for the empirical kind of densities that will be used, we assume $p_{x_\tau,\theta_\tau}(\cdot)$ equals an empirical density:

$$p_{x_\tau,\theta_\tau}(dx,\theta) = \sum_{\kappa\in\mathbb{K}} \sum_{i=1}^{N^\kappa} \omega^{\kappa,i}\, \delta_{(x^{\kappa,i},\theta^{\kappa,i})}(dx,\theta) \tag{10}$$

with $\{x^{\kappa,i},\theta^{\kappa,i},\omega^{\kappa,i}\}_{i=1}^{N^\kappa}$, $\kappa \in \mathbb{K}$, a given set of particles. Substituting (10) into (8) and

evaluation yields:

$$p_{x_\tau,\theta_\tau|\kappa_{\tau+h}}(dx,\theta|\kappa) = \sum_{\eta\in\mathbb{M}_\kappa} p_{\theta_{\tau+h}|x_\tau,\theta_\tau}(\eta|x,\theta) \sum_{\kappa'\in\mathbb{K}} \sum_{i=1}^{N^{\kappa'}} \omega^{\kappa',i}\delta_{(x^{\kappa',i},\theta^{\kappa',i})}(dx,\theta)/p_{\kappa_{\tau+h}}(\kappa)$$
$$= \sum_{\kappa'\in\mathbb{K}} \sum_{i=1}^{N^{\kappa'}} \sum_{\eta\in\mathbb{M}_\kappa} p_{\theta_{\tau+h}|x_\tau,\theta_\tau}(\eta|x^{\kappa',i},\theta^{\kappa',i})\omega^{\kappa',i}\delta_{(x^{\kappa',i},\theta^{\kappa',i})}(dx,\theta)/p_{\kappa_{\tau+h}}(\kappa). \tag{11}$$

Similarly, substituting (10) into (9) yields

$$p_{\kappa_{\tau+h}}(\kappa) = \sum_{\kappa'\in\mathbb{K}} \sum_{i=1}^{N^{\kappa'}} \sum_{\eta\in\mathbb{M}_\kappa} p_{\theta_{\tau+h}|x_\tau,\theta_\tau}(\eta|x^{\kappa',i},\theta^{\kappa',i})\omega^{\kappa',i}. \tag{12}$$

The idea is to use equation (11) for resampling N_p particles from $p_{x_{\tau_k},\theta_{\tau_k}|\kappa_{\tau_k+h}}(\cdot|\kappa)$ for each κ-value once at the beginning of a prediction cycle from τ_k to τ_{k+1}. Equation (12) is used to compensate each particle weight for this resampling.

7 Hierarchical Hybrid IPS algorithm

Similar as in the IPS algorithm for an SHS [8, 9], a particle is defined as a triplet (x,θ,ω), $\omega\in[0,1]$, $x\in\mathbb{R}^n$ and $\theta\in\mathbb{M}$. Numerical approximations $\widetilde{\gamma}_k$ and $\widetilde{\pi}_k$ are used for γ_k and $p_{\xi_k|\chi_k}(\cdot|1)$ respectively. When simulating from $\tau_{k-1}\wedge T$ to $\tau_k\wedge T$, a fraction $\widetilde{\gamma}_k$ of the Monte Carlo simulated trajectories only will reach Q_k. The Hierarchical Hybrid Interacting Particle System (HHIPS) algorithm estimates these fractions and their product in a recursive way, using the following steps:

Step 0 generates per κ-value N_p initial particles at $k=0$, and then starts the cycling over steps 1 through 3 for $k:=1,2,...m$.

Step 1 extrapolates each particle from $\tau_{k-1}\wedge T$ to $\tau_k\wedge T$ in time steps of length h, using importance switching for the new κ-value and κ-conditional sampling of a new θ value. For the latter use is made of the κ-conditional θ-prediction characterization in Theorem 6.1.

Step 2 evaluates the particles that have arrived at Q_k. For this, use is made of equations (4)-(5).

Step 3 resamples from the particles that have arrived at Q_k. In order to draw N_p samples per κ-value, use is made of the hierarchical interaction characterization in Theorem 6.2.

Each of these steps is specified in detail below.

Hierarchical Hybrid Interacting Particle System

HHIPS Step 0: Initial sampling for $k = 0$.

- At time $t = 0$ we start with a set of $N^\kappa := N_p$ particles for each aggregation mode $\kappa \in \mathbb{K}$: $\{x^{\kappa,i}, \theta^{\kappa,i}, \omega^{\kappa,i}\}_{i=1}^{N_p}$, $\kappa \in \mathbb{K}$, where the particles are obtained as follows. First, the $\theta^{\kappa,i}$ are independently drawn from $p_{\theta_0|\kappa_0}(\cdot|\kappa)$. Then, the $x^{\kappa,i} \in \{0\} \times \mathbb{R}^{n-1}/D_1$ are independently drawn from $p_{x_0|\theta_0}(\cdot|\theta^{\kappa,i})$ with the first component of $x^{\kappa,i}$ equal to zero. The initial weights satisfy

$$\omega^{\kappa,i} = \frac{p_{\kappa_0}(\kappa)}{N_p},\ i = 1,\dots,N_p, \kappa \in \mathbb{K}.$$

- With this we have $\tilde{\gamma}_0 = 1$ and

$$\tilde{p}_{x_0,\theta_0}(dx,\theta) = \sum_{\kappa\in\mathbb{K}} \sum_{i=1}^{N^\kappa} \omega^{\kappa,i} \delta_{(x^{\kappa,i},\theta^{\kappa,i})}(dx,\theta).$$

- Identify a sufficiently large number J of equal discretization steps of time length $h = T/J$, which allows to use a numerical integration time step h.

- Identify an appropriate positive value for $\alpha < 1/J$.

HHIPS iteration cycle: For $k = 1,\dots,m$ cycle over step 1 (prediction), step 2 (assessment) and step 3 (resampling):

HHIPS Step 1. Prediction:

- Start with empty sets S_k^κ, $\kappa \in \mathbb{K}$, to store all particles that arrive at $Q_k = (0,T) \times D_k \times \mathbb{M}$.

- For $j = 1,\dots,J$, iterate over substeps 1.a, 1.b and 1.c.

Substep 1.a Sample $\kappa_{\tau+h}$ using importance switching.
If $k > 1$ and $j = 1$, then go to substep 1b, else for each $\kappa \in \mathbb{K}$ and $i = 1,\dots,N^\kappa$:

- If $\omega^{\kappa,i} = 0$ then $\breve{\omega}^{\kappa,i} := 0$ and $\breve{\kappa}^{\kappa,i} := \kappa$; else, sample a $\breve{\kappa}^{\kappa,i} \in \mathbb{K}$ with probability α for each of the values in $\mathbb{K}\setminus\{\kappa\}$, and with probability $1-\alpha(|\mathbb{K}|-1)$ for the value κ, and correct the corresponding weight according to this importance switching, i.e.

$$\breve{\omega}^{\kappa,i} = \begin{cases} \omega^{\kappa,i} \frac{p_{\kappa_{\tau+h}|x_\tau,\theta_\tau}(\breve{\kappa}^{\kappa,i}\,|\,x^{\kappa,i},\theta^{\kappa,i})}{1-\alpha(|\mathbb{K}|-1)} & \text{if } \breve{\kappa}^{\kappa,i} = \kappa, \\ \omega^{\kappa,i} \frac{p_{\kappa_{\tau+h}|x_\tau,\theta_\tau}(\breve{\kappa}^{\kappa,i}\,|\,x^{\kappa,i},\theta^{\kappa,i})}{\alpha} & \text{if } \breve{\kappa}^{\kappa,i} \neq \kappa. \end{cases}$$

- The resulting sets of particles are $\{\bar{x}^{\kappa',l}, \bar{\theta}^{\kappa',l}, \breve{\omega}^{\kappa',l}, \breve{\kappa}^{\kappa',l}\}_{l=1}^{N^{\kappa'}}$, $\kappa' \in \mathbb{K}$. For each $\kappa \in \mathbb{K}$, collect from these particles those N^κ particles for which $\breve{\kappa}^{\kappa',l} = \kappa$, i.e.

$$N^\kappa := \sum_{\substack{\kappa' \in \mathbb{K} \\ N^{\kappa'} \neq 0}} \sum_{l=1}^{N^{\kappa'}} 1_{\{\kappa\}}(\breve{\kappa}^{\kappa',l}).$$

- For each $\kappa \in \mathbb{K}$, renumber the indices of these N^κ particles such that the first index equals κ and the second index runs over $\{1, ..., N^\kappa\}$. This yields for each $\kappa \in \mathbb{K}$ the following new set of particles $\{x^{\kappa,i}, \theta^{\kappa,i}, \omega^{\kappa,i}\}_{i=1}^{N^\kappa}$ if $N^\kappa \neq 0$, and an empty set $\varnothing$ if $N^\kappa = 0$.

Substep 1.b $\kappa_{\tau+h}$-conditional prediction of $(x_{\tau+h}, \theta_{\tau+h})$.
For each $\kappa \in \mathbb{K}$, determine the new set of particles $\{\bar{x}^{\kappa,i}, \bar{\theta}^{\kappa,i}, \bar{\omega}^{\kappa,i}\}_{i=1}^{N^\kappa}$ as follows:

- For each κ, i for which $\omega^{\kappa,i} = 0$, set $\bar{x}^{\kappa,i} := x^{\kappa,i}$ and $\bar{\theta}^{\kappa,i} := \theta^{\kappa,i}$. Else, use Theorem 6.1 to sample a new value $\bar{\theta}^{\kappa,i}$ from:

$$p_{\theta_{\tau+h}|x_\tau,\theta_\tau,\kappa_{\tau+h}}(\eta \,|\, x^{\kappa,i}, \theta^{\kappa,i}, \kappa) = \frac{1_{\mathbb{M}_\kappa}(\eta)\, p_{\theta_{\tau+h}|x_\tau,\theta_\tau}(\eta \,|\, x^{\kappa,i}, \theta^{\kappa,i})}{\sum_{\eta' \in \mathbb{M}_\kappa} 1_{\mathbb{M}_\kappa}(\eta')\, p_{\theta_{\tau+h}|x_\tau,\theta_\tau}(\eta' \,|\, x^{\kappa,i}, \theta^{\kappa,i})}$$

  and a new value $\bar{x}^{\kappa,i}$ from

$$p_{x_{\tau+h}|\theta_{\tau+h},x_\tau,\theta_\tau}(dx \,|\, \bar{\theta}^{\kappa,i}, x^{\kappa,i}, \theta^{\kappa,i}).$$

- The weights are not changed, i.e. $\bar{\omega}^{\kappa,i} := \omega^{\kappa,i}$.

Substep 1.c. Memorizing particles that arrived at Q_k:

- If $(\bar{x}^{\kappa,i}, \bar{\theta}^{\kappa,i}) \in Q_k$ and $\omega^{\kappa,i} \neq 0$, then a copy of the particle $\{\bar{x}^{\kappa,i}, \bar{\theta}^{\kappa,i}, \bar{\omega}^{\kappa,i}\}$ is stored in the set S_k^κ.

- Subsequently, we set $\bar{\omega}^{\kappa,i} := 0$ in the original particle.

- If $j = J$, then step 1 is complete, hence go to step 2, else, repeat substeps 1a,b,c for $j := j + 1$.

HHIPS Step 2. Evaluate the Q_k arrived particles:

- The particles which are memorized in S_k^κ, $\kappa \in \mathbb{K}$, provide an estimate of $p_{\xi_k|\chi_k}(\cdot|1)$ and γ_k.

- Renumbering the particles in S_k^κ yields a set of particles $\{\tilde{x}^{\kappa,i}, \tilde{\theta}^{\kappa,i}, \tilde{\omega}^{\kappa,i}\}_{i=1}^{N^\kappa}$ with N^κ the number of particles in S_k^κ.
- Weighted fraction $\tilde{\gamma}_k$ of the Q_k arrived particles:

$$\gamma_k \approx \tilde{\gamma}_k = \sum_{\substack{\kappa \in \mathbb{K} \\ N^\kappa \neq 0}} \sum_{i=1}^{N^\kappa} \tilde{\omega}^{\kappa,i}.$$

- If $N^\kappa = 0$ for all $\kappa \in \mathbb{K}$, then the algorithm stops with estimate $P_{hit}(0,T) \approx 0$.
- If $k = m$, then stop HHIPS with the estimate $P_{hit}(0,T) \approx \prod_{k=1}^m \tilde{\gamma}_k$.
- For each $\kappa \in \mathbb{K}$ and $i = 1, \ldots, N^\kappa$:

$$\tilde{\omega}^{\kappa,i} := \tilde{\omega}^{\kappa,i} / \tilde{\gamma}_k.$$

- The estimated $p_{\xi_k|\chi_k}(\cdot|1)$ satisfies:

$$p_{\xi_k|\chi_k}(dx, d\theta|1) \approx \tilde{\pi}_k(dx, d\theta) = \sum_{\substack{\kappa \in \mathbb{K} \\ N^\kappa \neq 0}} \sum_{i=1}^{N^\kappa} \tilde{\omega}^{\kappa,i} \delta_{(\tilde{x}^{\kappa,i}, \tilde{\theta}^{\kappa,i})}(dx, d\theta).$$

HHIPS Step 3. Copy the Q_k arrived particles through κ_{τ_k+h}-conditional resampling.

- Evaluate aggregated mode probabilities at $\tau := \tau_k$ using (12):

$$p_{\kappa_{\tau+h}|\chi_k}(\kappa|1) \approx \varphi(\kappa) = \sum_{\substack{\kappa' \in \mathbb{K} \\ N^{\kappa'} \neq 0}} \sum_{i=1}^{N^{\kappa'}} \sum_{\eta \in \mathbb{M}_{\kappa'}} p_{\theta_{\tau+h}|x_\tau,\theta_\tau}(\eta|\tilde{x}^{\kappa',i}, \tilde{\theta}^{\kappa',i}) \tilde{\omega}^{\kappa',i}.$$

- For each $\kappa \in \mathbb{K}$ independently draw N_p random pairs $(x^{\kappa,i}, \theta^{\kappa,i})$, $i = 1, \ldots, N_p$ from the particle spanned empirical measure, using (11):

$$p_{x_\tau,\theta_\tau|\kappa_{\tau+h},\chi_k}(dx, d\theta\,|\,\kappa, 1) \approx \sum_{\substack{\kappa' \in \mathbb{K} \\ N^{\kappa'} \neq 0}} \sum_{i=1}^{N^{\kappa'}} \sum_{\eta \in \mathbb{M}_{\kappa'}} p_{\theta_{\tau+h}|x_\tau,\theta_\tau}(\eta|\tilde{x}^{\kappa',i}, \tilde{\theta}^{\kappa',i}) \times$$
$$\times\, \tilde{\omega}^{\kappa',i} \delta_{\{\tilde{x}^{\kappa',i}, \tilde{\theta}^{\kappa',i}\}}(dx, d\theta) / \varphi(\kappa).$$

- This yields, for each $\kappa \in \mathbb{K}$, a set of particles $\{x^{\kappa,i}, \theta^{\kappa,i}, \omega^{\kappa,i}\}_{i=1}^{N_p}$ with $\omega^{\kappa,i} := \varphi(\kappa)/N_p$.
- If $k < m$, then repeat steps 1-3 for $k := k+1$ and $N^{\kappa} := N_p$.

Remark 7.1. The key extensions of HHIPS over IPS for an SHS [8, 9] are:

1. Embedding of an aggregation mode process;
2. Particles are maintained per aggregation mode;
3. Importance switching of aggregation mode is used for the conditional prediction of SHS particles;
4. Hierarchical interaction is used for the resampling of particles that reached Q_k, $k = 1, .., m-1$.

8 Free flight air traffic example

We consider the Autonomous Mediterranean Free Flight (AMFF) operational concept that has been developed within the Mediterranean Free Flight (MFF) project [40]. In this free flight air traffic example, the airspace is an en-route airspace without fixed routes and without support by air traffic control. All aircraft flying in this airspace are assumed to be properly equipped and enabled for free flight: the pilots can try to optimise their trajectory, due to the enlarged freedom to choose path and flight level. The pilots are only limited by their responsibility to maintain airborne separation, in which they are assisted by a system called ASAS (Airborne Separation Assistance System). This system processes the information flows from the data-communication links between aircraft, the navigation systems and the aircraft guidance and control systems. ASAS detects conflicts, determines conflict resolution maneuvers and presents the relevant information to the aircrew. The number of agents involved in the free flight operation is huge and ranges from the Control Flow Management Unit to flight attendants. In the setting chosen for an initial risk assessment, the following agents are taken into account:

- One pilot-flying in each aircraft,
- One pilot-non-flying in each aircraft,
- Various systems and entities per aircraft, like the aircraft position evolution and the conflict management support systems,
- Some global systems and entities, like the communication frequencies and a satellite system.

The approach taken in developing the AMFF concept of operation [40] is to avoid much information exchange between aircraft and to avoid dedicated decision-making by artificial intelligent machines. Although the conflict detection and resolution approach developed for AMFF has its roots in the modified potential field approach [32], it has some significant deviations from this. The main deviation is that conflict resolution in AMFF is intentionally designed not to take the potential field of all aircraft into account. The resulting AMFF design can be summarized as follows:

- All aircraft are supposed to be equipped with Automatic Dependent Surveillance-Broadcast (ADS-B), which is a system that periodically broadcasts own aircraft state information, and continuously receives the state information messages broadcasted by aircraft that fly within broadcasting range (~ 100 Nm).
- To comply with pilot preferences, conflict resolution algorithms are designed to solve multiple conflicts one by one rather than according to a full concurrent way, e.g., see [32].
- Conflict detection and resolution are state-based, i.e., intent information, such as information at which point surrounding aircraft will change course or height, is supposed to be unknown.
- The vertical separation minimum is 1000 ft and the horizontal separation minimum is 5 Nm. A conflict is detected if these separation minima will be violated within 6 minutes.
- The conflict resolution process consists of two phases. During the first phase, one of the aircraft crews should make a resolution maneuver. If this does not work, then during the second phase, both crews should make a resolution maneuver.
- Prior to the first phase, the crew is warned when an ASAS alert is expected to occur if no preventive action would be timely implemented; this prediction is done by a system referred to as P-ASAS (Predictive ASAS).
- Conflict co-ordination does not take place explicitly, i.e., there is no communication on when and how a resolution maneuver will be executed.
- All aircraft are supposed to use the same resolution algorithm, and all crew are assumed to use ASAS and to collaborate in line with the procedures.
- Two conflict resolution maneuver options are presented: one in vertical and one in horizontal direction. The pilot decides which option to execute.

- ASAS related information is presented to the crew through a Cockpit Display of Traffic Information (CDTI).

In order to use the HHIPS algorithm for the estimation of collision risk of this free flight operation, we need to develop a MC simulator of this operation, such that the simulated trajectories constitute realizations of a hybrid state strong Markov process. Everdij and Blom [25, 26, 27, 28] have developed a Stochastically and Dynamically Coloured Petri Net (SDCPN) formalism that ensures the specification of a free flight MC simulation model which is of the appropriate class. In [9] it is explained how the SDCPN formalism has been used to develop a MC simulation model of a particular free flight design. The dimensionality of the resulting MC simulation model is very large, e.g. in simulating two aircraft there are about 10^{25} discrete mode combinations, and the Euclidean state may go up to $\mathbb{R}^{336}$ [9]. For this very large stochastic hybrid system we want to estimate the probability of collision between aircraft. This is practically infeasible using naive MC simulation.

9 Application of HHIPS to air traffic example

In [4, 8, 9] we developed a way to cast the air traffic SHS model within the setting of the IPS formulation, and used the IPS to evaluate demanding high risk bearing multi-aircraft scenarios. This IPS approach, however, does not work properly anymore for low risk bearing scenarios. The aim of this section is to demonstrate that the novel HHIPS works well for such a low risk bearing scenario, using the same SHS model.

In the low risk bearing scenario considered, two aircraft start at the same flight level, some 250 km away from each other, and fly on opposite direction flight plans head-on with a ground speed of 240 m/s. This means that collision may be reached after about 500s simulation, hence we set $T = 600$s. The collision reach probability is estimated through running ten times the HHIPS algorithm[2]. The aggregation modes chosen are all combinations of the following high level mode values: global communication support is 'up' or 'down', and decision-making (DM) loop of aircraft 1 is 'up' or 'down'. This leads to a total of four aggregation mode values.

The D_k's have been identified through an iterative process of learning from conducting MC simulations. This quite easily led to the identification of a series of D_k's that appeared to work well. Although it is likely that further optimization of D_k's may lead to a reduction in the variance and confidence interval of the estimates [39], we did not try to do so yet.

Each D_k is defined by three parameters, the values of which are given in Table 1 for a sequence of eight nested subsets. Here d_k and h_k define a cylinder of diameter

[2] In [7] a similar two-aircraft encounter scenario has been simulated using an initial precursor of the current HHIPS.

d_k and height h_k respectively. The Δ_k value is the time period over which position and velocity differences between the two aircraft are compared. If within Δ_k the predicted position difference falls within the corresponding cylinder, then D_k is said to be reached. The three parameters of D_1, D_2, D_4, D_6 and D_8 are such that reaching them represent a type of conflict that is well known in air traffic, i.e. medium term conflict, short term conflict, minimum separation infringement, conflict, near collision and collision respectively. The extra D_3, D_5 and D_7 appeared useful in avoiding too small fractions remaining from hitting D_4 after D_2, D_6 after D_4 and D_8 after D_6.

Table 1: IPS conflict level parameter values

k	1	2	3	4	5	6	7	8
d_k (Nm)	4.5	4.5	4.5	4.5	2.5	1.25	0.50	0.054
h_k (ft)	900	900	900	900	900	500	250	131
Δ_k (min)	8	2.5	1.5	0	0	0	0	0

The number of particles used is 5,000 per aggregation mode value; hence 20,000 particles are used per HHIPS run. The time step $h = 1$s, and $\alpha = 0.001$. Results of these HHIPS runs are presented in Table 2.

Table 2: $\tilde{\gamma}_k$ values estimated by first five HHIPS runs. IPS based estimation typically yields values 0.0 for $k \geq 4$

k	**Run 1**	**Run 2**	**Run 3**	**Run 4**	**Run 5**
1	1.000	1.000	1.000	0.991	1.000
2	5.77E-04	5.64E-06	6.24E-06	5.04E-06	6.13E-06
3	6.40E-03	7.25E-01	7.20E-01	6.84E-01	7.66E-01
4	0.566	0.569	0.596	0.540	0.608
5	0.344	0.256	0.223	0.401	0.198
6	0.420	0.452	0.402	0.459	0.429
7	0.801	0.845	0.929	0.710	0.949
8	0.814	0.827	0.841	0.828	0.802
Π	1.97E-07	1.89E-07	1.89E-07	2.00E-07	1.85E-07

Table 2 presents the values for $\tilde{\gamma}_k$ which have been estimated during the first five HHIPS runs. The estimated mean probability of collision between the two aircraft equals 1.91×10^{-7}. The estimated standard deviation is 1.6×10^{-8}, which shows that the estimated value is quite accurate. It should be noticed that the variation in the fractions per level is significantly larger than the variation in the product of the frac-

tions. Apparently, the dependency between the fractions $\tilde{\gamma}_k$ reduces the variation in the multiplication of these fractions.

Finally we improved the availability/reliability of the ASAS related systems by a factor 100, and then conducted the ten HHIPS runs again. This resulted in a 100-fold decrease of the collision reach probability. These results demonstrate that HHIPS works well for this large scale SHS.

10 Concluding remarks

This report started to present the rare event estimation theory developed in [17, 18, 19, 22, 23] in the framework of probabilistic reachability analysis of SHS. Subsequently, the theory has been extended with mode aggregation, importance switching and Rao-Blackwellization. This allows probabilistic reachability analysis theory to be applied to large scale SHS, and in particular when the reachability probability considered receives significant contributions from combinatorially many rare modes. The power of the resulting novel sequential MC simulation approach has been demonstrated through a successful application to collision risk estimation in a demanding future air traffic scenario. And, of course, there are several interesting directions for follow up research, such as:

- Extending convergence proof of [17, 19] to the novel speed-up approaches in this report.
- Incorporating parameter sensitivity assessment in the novel speed-up approaches.

The intention is to study these issues within the iFly project.

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