

RESEARCH CENTRE

**Inria Centre at Rennes
University**

IN PARTNERSHIP WITH:
Université de Rennes

2024

ACTIVITY REPORT

Project-Team
SIMSMART

SIMulating Stochastic Models with pARTicles

IN COLLABORATION WITH: Institut de recherche mathématique de
Rennes (IRMAR)

DOMAIN

**Applied Mathematics, Computation and
Simulation**

THEME

Stochastic approaches

The Inria logo is a stylized, red, cursive script of the word "Inria".

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Project-Team SIMSMART

Creation of the Project-Team: 2019 January 01

Keywords

Computer sciences and digital sciences

- A6. – Modeling, simulation and control
 - A6.1. – Methods in mathematical modeling
 - A6.1.1. – Continuous Modeling (PDE, ODE)
 - A6.1.2. – Stochastic Modeling
 - A6.1.4. – Multiscale modeling
 - A6.2. – Scientific computing, Numerical Analysis & Optimization
 - A6.2.1. – Numerical analysis of PDE and ODE
 - A6.2.2. – Numerical probability
 - A6.2.3. – Probabilistic methods
 - A6.2.4. – Statistical methods
 - A6.2.5. – Numerical Linear Algebra
 - A6.2.6. – Optimization
 - A6.3. – Computation-data interaction
 - A6.3.1. – Inverse problems
 - A6.3.2. – Data assimilation
 - A6.3.4. – Model reduction
 - A6.3.5. – Uncertainty Quantification
 - A6.5. – Mathematical modeling for physical sciences
 - A6.5.2. – Fluid mechanics
 - A6.5.3. – Transport
 - A6.5.5. – Chemistry

Other research topics and application domains

- B1. – Life sciences
- B2. – Health
- B3. – Environment and planet
 - B3.2. – Climate and meteorology
- B4. – Energy
 - B4.2. – Nuclear Energy Production
 - B4.2.1. – Fission
- B5.3. – Nanotechnology
- B5.5. – Materials

1 Team members, visitors, external collaborators

Research Scientists

- Mathias Rousset [Team leader, INRIA, Researcher]
- Frederic Cerou [INRIA, Researcher]
- Patrick Heas [INRIA, Researcher]
- Mouad Ramil [INRIA, Researcher, from Nov 2024]

Faculty Member

- Valérie Monbet [Univ. Rennes, Professor]

PhD Student

- Theo Guyard [INSA RENNES, until Sep 2024]

Administrative Assistant

- Gunther Tessier [INRIA]

2 Overall objectives

As the constant surge of computational power is nurturing scientists into simulating the most detailed features of reality, from complex molecular systems to climate or weather forecast, the computer simulation of physical systems is becoming reliant on highly complex stochastic dynamical models and very abundant observational data. The complexity of such models and of the associated observational data stems from intrinsic physical features, which do include high dimensionality as well as intricate temporal and spatial multi-scales. It also results in much less control over simulation uncertainty.

Within this highly challenging context, SIMSMART positions itself as a mathematical and computational probability and statistics research team, dedicated to *Monte Carlo simulation* methods. Such methods include in particular particle Monte Carlo methods for rare event simulation, data assimilation and model reduction, with application to stochastic random dynamical physical models. The main objective of SIMSMART is to disrupt this now classical field by creating deeper mathematical frameworks adapted to the management of contemporary highly sophisticated physical models.

3 Research program

Introduction. Computer simulation of physical systems is becoming increasingly reliant on highly complex models, as the constant surge of computational power is nurturing scientists into simulating the most detailed features of reality – from complex molecular systems to climate/weather forecast.

Yet, when modeling physical reality, bottom-up approaches are stumbling over intrinsic difficulties. First, the timescale separation between the fastest simulated microscopic features, and the macroscopic effective slow behavior becomes huge, implying that the fully detailed and direct long time simulation of many interesting systems (*e.g.* large molecular systems) are out of reasonable computational reach. Second, the chaotic dynamical behaviors of the systems at stake, coupled with such multi-scale structures, exacerbate the intricate uncertainty of outcomes, which become highly dependent on intrinsic chaos, uncontrolled modeling, as well as numerical discretization. Finally, the massive increase of observational data addresses new challenges to classical data assimilation, such as dealing with high dimensional observations and/or extremely long time series of observations.

SIMSMART Identity. Within this highly challenging applicative context, SIMSMART positions itself as a computational probability and statistics research team, with a mathematical perspective. Our approach

is based on the use of *stochastic modeling* of complex physical systems, and on the use of *Monte Carlo simulation* methods, with a strong emphasis on dynamical models. The two main numerical tasks of interest to SIMSMART are the following: (i) simulating with pseudo-random number generators - a.k.a. *sampling* - dynamical models of random physical systems, (ii) sampling such random physical dynamical models given some real observations - a.k.a. *Bayesian data assimilation*. SIMSMART aims at providing an appropriate mathematical level of abstraction and generalization to a wide variety of Monte Carlo simulation algorithms in order to propose non-superficial answers to both *methodological and mathematical* challenges. The issues to be resolved include computational complexity reduction, statistical variance reduction, and uncertainty quantification.

SIMSMART Objectives. The main objective of SIMSMART is to disrupt this now classical field of particle Monte Carlo simulation by creating deeper mathematical frameworks adapted to the challenging world of complex (*e.g.* high dimensional and/or multi-scale), and massively observed systems, as described in the beginning of this introduction.

To be more specific, we will classify SIMSMART objectives using the following four intertwined topics:

- Objective 1: Rare events and random simulation.
- Objective 2: High dimensional and advanced particle filtering.
- Objective 3: Non-parametric approaches.
- Objective 4: Model reduction and sparsity.

Rare events Objective 1 are ubiquitous in random simulation, either to accelerate the occurrence of physically relevant random slow phenomena, or to estimate the effect of uncertain variables. Objective 1 will be mainly concerned with particle methods where *splitting* is used to enforce the occurrence of rare events.

The problem of high dimensional observations, the main topic in Objective 2, is a known bottleneck in filtering, especially in non-linear particle filtering, where linear data assimilation methods remain the state-of-the-art approaches.

The increasing size of recorded observational data and the increasing complexity of models also suggest to devote more effort into non-parametric data assimilation methods, the main issue of Objective 3.

In some contexts, for instance when one wants to compare solutions of a complex (*e.g.* high dimensional) dynamical systems depending on uncertain parameters, the construction of relevant reduced-order models becomes a key topic. Model reduction aims at proposing efficient algorithmic procedures for the resolution (to some reasonable accuracy) of high-dimensional systems of parametric equations. This overall objective entails many different subtasks: 1) the identification of low-dimensional surrogates of the target “solution” manifold, 2) The devise of efficient methodologies of resolution exploiting low-dimensional surrogates, 3) The theoretical validation of the accuracy achievable by the proposed procedures. This is the content of Objective 4.

With respect to volume of research activity, Objective 1, Objective 4 and the sum (Objective 2+Objective 3) are comparable.

Some new challenges in the simulation and data assimilation of random physical dynamical systems have become prominent in the last decade. A first issue (i) consists in the intertwined problems of simulating on large, macroscopic random times, and simulating *rare events* (see Objective 1). The link between both aspects stems from the fact that many effective, large times dynamics can be approximated by sequences of rare events. A second, obvious, issue (ii) consists in managing *very abundant observational data* (see Objective 2 and 3). A third issue (iii) consists in quantifying *uncertainty/sensitivity/variance* of outcomes with respect to models or noise. A fourth issue (iv) consists in managing *high dimensionality*, either when dealing with complex prior physical models, or with very large data sets. The related increase of complexity also requires, as a fifth issue (v), the construction of *reduced models* to speed-up comparative simulations (see Objective 4). In a context of very abundant data, this may be replaced by a sixth

issue (vi) where complexity constraints on modeling is replaced by the use of *non-parametric statistical inference* (see Objective 3).

Hindsight suggests that all the latter challenges are related. Indeed, the contemporary digital condition, made of a massive increase in computational power and in available data, is resulting in a demand for more complex and uncertain models, for more extreme regimes, and for using inductive approaches relying on abundant data. In particular, uncertainty quantification (item (iii)) and high dimensionality (item (iv)) are in fact present in all 4 Objectives considered in SimSmart.

4 Application domains

4.1 Domain 1 – Computational Physics

The development of large-scale computing facilities has enabled simulations of systems at the *atomistic scale* on a daily basis. The aim of these simulations is to bridge the time and space scales between the macroscopic properties of matter and the stochastic atomistic description. Typically, such simulations are based on the ordinary differential equations of classical mechanics supplemented with a random perturbation modeling temperature, or collisions between particles.

Let us give a few examples. In bio-chemistry, such simulations are key to predict the influence of a ligand on the behavior of a protein, with applications to drug design. The computer can thus be used as a *numerical microscope* in order to access data that would be very difficult and costly to obtain experimentally. In that case, a rare event (Objective 1) is given by a macroscopic system change such as a conformation change of the protein. In nuclear safety, such simulations are key to predict the transport of neutrons in nuclear plants, with application to assessing aging of concrete. In that case, a rare event is given by a high energy neutron impacting concrete containment structures.

A typical model used in molecular dynamics simulation of open systems at given temperature is a stochastic differential equation of Langevin type. The large time behavior of such systems is typically characterized by a hopping dynamics between 'metastable' configurations, usually defined by local minima of a potential energy. In order to bridge the time and space scales between the atomistic level and the macroscopic level, specific algorithms enforcing the realization of rare events have been developed. For instance, splitting particle methods (Objective 1) have become popular within the computational physics community only within the last few years, partially as a consequence of interactions between physicists and Inria mathematicians in ASPI (parent of SIMSMART) and MATHERIALS project-teams.

SIMSMART also focuses on various models described by partial differential equations (reaction-diffusion, conservation laws), with unknown parameters modeled by random variables.

4.2 Domain 2 – Meteorology

The traditional trend in data assimilation in geophysical sciences (climate, meteorology) is to use as prior information some very complex deterministic models formulated in terms of fluid dynamics and reflecting as much as possible the underlying physical phenomenon (*see e.g.*). Weather/climate forecasting can then be recast in terms of a Bayesian filtering problem (see Objective 2) using weather observations collected *in situ*.

The main issue is therefore to perform such Bayesian estimations with very expensive infinite dimensional prior models, and observations in large dimension. The use of some linear assumption in prior models (Kalman filtering) to filter non-linear hydrodynamical phenomena is the state-of-the-art approach, and a current field of research, but is plagued with intractable instabilities.

This context motivates two research trends: (i) the introduction of non-parametric, model-free prior dynamics constructed from a large amount of past, recorded real weather data; and (ii) the development of appropriate non-linear filtering approaches (Objective 2 and Objective 3).

SIMSMART will also test its new methods on multi-source data collected in North-Atlantic paying particular attention to coastal areas (*e.g.* within the inter-Labex SEACS).

4.3 Other Applicative Domains

SIMSMART also focuses on other applications including:

- Tracking and hidden Markov models.
- Robustness and certification in Machine Learning.

5 Social and environmental responsibility

5.1 Footprint of research activities

Members of SimSmart have avoided air traveling, with the notable exception of rare international conferences with publications for PhD students (this year Theo Guyard) which are considered important for their academic future.

6 New software, platforms, open data

6.1 New software

6.1.1 Screening4L0Problem

Keywords: Global optimization, Sparsity

Functional Description: This software contains "Branch and bound" optimization routines exploiting "screening" acceleration rules for solving sparse representation problems involving the L0 pseudo-norm.

URL: <https://gitlab.insa-rennes.fr/Theo.Guyard/bnb-screening>

Publication: hal-03462171

Contact: Cedric Herzet

Participants: Clément Elvira, Theo Guyard, Cedric Herzet

6.1.2 Screen&Relax

Keywords: Optimization, Sparsity

Functional Description: This software provides optimization routines to efficiently solve the "ElasticNet" problem.

URL: <https://gitlab.insa-rennes.fr/Theo.Guyard/screen-and-relax>

Publication: hal-03462191

Contact: Cedric Herzet

Participants: Clément Elvira, Theo Guyard, Cedric Herzet

6.1.3 npSEM

Name: Stochastic expectation-maximization algorithm for non-parametric state-space models

Keyword: Statistic analysis

Functional Description: npSEM is the combination of a non-parametric estimate of the dynamic using local linear regression (LLR), a conditional particle smoother and a stochastic Expectation-Maximization (SEM) algorithm. Further details of its construction and implementation are introduced in the article An algorithm for non-parametric estimation in state-space models of authors "T.T.T. Chau, P. Ailliot, V. Monbet", <https://doi.org/10.1016/j.csda.2020.107062>.

URL: <https://github.com/tchau218/npSEM>

Contact: Thi Tuyet Trang Chau

Participants: Valérie Monbet, Thi Tuyet Trang Chau

6.1.4 NHMSAR

Name: Non-Homogeneous Markov Switching Autoregressive Models

Keyword: Statistical learning

Functional Description: Calibration, simulation, validation of (non-)homogeneous Markov switching autoregressive models with Gaussian or von Mises innovations. Penalization methods are implemented for Markov Switching Vector Autoregressive Models of order 1 only. Most functions of the package handle missing values.

URL: <https://CRAN.R-project.org/package=NHMSAR>

Contact: Valérie Monbet

Participant: Valérie Monbet

6.1.5 3D Winds Fields Profiles

Functional Description: The algorithm computes 3D Atmospheric Motion Vectors (AMVs) vertical profiles, using incomplete maps of humidity, temperature and ozone concentration observed in a range of isobaric levels. The code is implemented for operational use with the Infrared Atmospheric Sounding Interferometer (IASI) carried on the MetOp satellite.

URL: https://www.esa.int/Applications/Observing_the_Earth/Meteorological_missions/MetOp/About_IASI

Contact: Patrick Heas

Participant: Patrick Heas

6.1.6 Screening4SLOPE

Keyword: Optimization

Functional Description: This software provides optimization routines to solve the SLOPE problem by exploiting "safe screening" reduction techniques.

URL: <https://gitlab-research.centralesupelec.fr/2020elvirac/slope-screening>

Publication: hal-03400322

Contact: Cedric Herzet

Participants: Clément Elvira, Cedric Herzet

7 New results

7.1 Objective 1 – Monte Carlo simulation and Stochastic analysis

Monte-Carlo simulation

Participants: Frédéric Cérou, Patrick Héas, Mathias Rousset, Mouad Ramil.

In [1], we obtained a rigorous general theorem for strong noise homogenisation, a recent problem where a strong (fast) noise coerces a Markov process near an effective sub-state space. Applications include quantum control and filtering.

In [6], we proposed a new rare event sampling methodology in a context where evaluations of the score function defining the rare event is amenable to reduced modeling with pointwise error bounds. The novelty is the use of an Importance Sampling cost criteria that automatically choose the level at which costly evaluation of the true model are performed.

In [7], we consider kinetic SDEs with low regularity coefficients and prove (among other things), under a Lyapunov condition, the existence and uniqueness (in a suitable class of measures) of a quasi-stationary distribution in cylindrical domains of the phase space.

7.2 Objective 2 and 3 – Data assimilation and statistics

Participants: Patrick Héas, Valérie Monbet.

In [3], we address the intricate challenge of reconciling environmental sustainability with economic viability within wastewater treatment plants (WWTPs). To address the stochastic and nonlinear nature of WWTP processes, we introduce a stochastic model and estimation method combining a Monte Carlo Sequential smoothing algorithm with a Stochastic Expectation Maximization method.

7.3 Objective 4 – Model Reduction and Sparsity

Participants: Patrick Héas, Théo Guyard.

In [2], we consider the resolution of learning problems involving l_0 -regularization via Branch-and-Bound (BnB) algorithms. We show through numerical simulations that our pruning strategy can improve the solving time of BnB procedures by several orders of magnitude for typical problems encountered in machine-learning applications.

8 Bilateral contracts and grants with industry

8.1 Bilateral contracts with industry

8.1.1 CIFRE grants

Participants: Valérie Monbet.

PhD project of Victor Bertret: *AI and stochastic control for automatic optimal driving of industrial systems* with company [Purecontrol](#).

8.1.2 Meteorological Satellite Data Processing

Participants: Patrick Héas.

Industrial Partner: EUMETSAT of Darmstadt.

Partner Contact: Regis.Borde@eumetsat.int

The transferred technology concerns an algorithm for the operational and real-time production of vertically resolved 3D atmospheric motion vector fields (AMVs) from measurements of new hyperspectral instruments: the infrared radiosounders on the third generation Meteosat satellites (MTG), developed by the European Space Agency (ESA) and the Infrared Atmospheric Sounding Interferometer (IASI) on MetOp-A and MetOp-B developed by the French Space Agency (CNES).

9 Partnerships and cooperations

9.1 National initiatives

9.1.1 ANR

ANR SINEQ (2021-2025).

Participants: Mathias Rousset, Frédéric Cérou.

Simulating non-equilibrium stochastic dynamics. The goal of the SINEQ project is, within a mathematical perspective, to extend various variance reduction techniques used in the Monte Carlo computation of equilibrium properties of statistical physics models.

The partners involved in the project are: CERMICS (PI: G. Stoltz), CEREMADE and Inria Rennes.

9.1.2 PEPR

Projet "PaRticules En interaction dédiées aux DynamIques ChaoTiques : un besoin pour la simulation d'évènements climatiques extrêmes (PREDICT)".

Participants: Mathias Rousset, Frédéric Cérou, Patrick Héas.

The goal of the present project is to stimulate interactions between i) physicists (Francesco Ragone, Univ. Louvain and J. Wouters, Univ. Reading) who have led recent works on numerical simulations of climate rare events, and ii) mathematicians and scientific computing experts (Mathias Rousset, Patrick Héas and Fred Cérou, IRMAR and Inria Univ Rennes) who have developed methodologies and the mathematical analysis of similar rare event Monte Carlo algorithms. The project will be led by Mathias ROUSSET (IRMAR and Inria, Rennes) and Francesco Ragone (Louvain, Belgium).

Financement (7.5 kEuros) Institut des Mathématiques pour la planète Terre IMPT. PI: Mathias Rousset et Francesco Ragone.

10 Dissemination

10.1 Promoting scientific activities

10.1.1 Scientific events: organisation

Valérie Monbet was part of the organization team of the following events.

- Organisation des **journées Innovation mathématique à Nantes**.
- Organisation de la **SEMES de Nantes**.

10.1.2 Invited talks

Excerpts:

Mathias Rousset

- Workshop "Mathématiques pour le nucléaire", RT Terre et Énergies, Jussieu, Février 2024.
- Workshop **MaThRad**, Warwick Uni, September 2024.
- Workshop "frugalité en IA et en statistique", SFdS, Jussieu, Octobre 2024.

Frédéric Cérou

- 2024 SIAM Conference on Uncertainty Quantification, Trieste.

Mouad Ramil

- Workshop "Recent progress in Mean-Field dynamics", ISFA Lyon, Décembre 2024.

Théo Guyard

- Journées SMAI MODE 2024 Lyon.

10.1.3 Scientific expertise

Mathias Rousset:

- was member of the Selection Committee that hired a Maître de Conférence in Probability (Ronan Herry) at IRMAR, Rennes Uni.

Valérie Monbet:

- author of a white paper on "Math algorithms and data assimilation" for **ECMWF** (through EU-mathin, co-author G. Louppe and Z. Horvath).

10.1.4 Research administration

Valérie Monbet is:

- Directrice de l'Agence Lebesgue
- Membre du bureau d'**AMIES**

10.2 Teaching - Supervision - Juries

10.2.1 Teaching

Mathias Rousset has given

- préparation à l'agrégation, modélisation option proba-stat.

Patrick Héas has given

- A course on "Algorithmique et Complexité", Ecole supérieure d'ingénieurs de Rennes (ESIR), 2-ième année, université de Rennes.
- A course on "Statistique Mathématique", travaux dirigés, parcours mathématiques fondamentales, Master 1-ère année, université de Rennes (24.h équivalent TD).

10.2.2 Supervision

PhD students:

- Valérie Monbet has been supervising the CIFRE PhD of Victor Bertret with company Purecontrol (Rennes), Apprentissage machine et contrôle stochastique pour un pilotage automatique optimisé de systèmes industriels. Starting sept. 2023.
- Valérie Monbet has been supervising the PhD thesis of David Martin. Thèse IRMAR-DIGISPORT, Performances sportives et microbiote intestinal, coencadrement F. Derbre, M2S, Univ Rennes 2.
- Théo Guyard has been supervised by Cédric Herzet (former SIMSMART member as of 2023). PhD: Screening methods for non-convex sparse representations. Funding by INSA, starting Sept. 2021, co-supervision James Ledoux.
- Mathias Rousset has been supervising the PhD of: Karim Tit: Rare event analysis of the Reliability of Deep Neural Networks, CIFRE Inria and Thalès, starting Jan. 2021, co-supervision: T.Furon. **PhD defended in 2024.**

PostDocs:

- Valérie Monbet has been supervising Pierre Houedry, (post doc passerelle de 9 mois). Development of deeplearning methods for environmental data.

10.2.3 Juries

PhD defenses:

- Valérie Monbet: rapporteur. Thèse de Robin Marcille (Université de Brest).
- Valérie Monbet: Membre du jury. Thèse d'Oliva Garcia (Bergen Uni, Norway).

11 Scientific production

11.1 Publications of the year

International journals

- [1] D. Faure and M. Rousset. 'A general martingale approach to large noise homogenization'. In: *Electronic Journal of Probability* 29 (Oct. 2024), pp. 1–49. DOI: [10.1214/24-EJP1177](https://hal.science/hal-04363393). URL: <https://hal.science/hal-04363393> (cit. on p. 7).
- [2] T. Guyard, C. Herzet, C. Elvira and A. N. Arslan. 'A New Branch-and-Bound Pruning Framework for ℓ_0 -Regularized Problems'. In: *Proceedings of Machine Learning Research* 235 (27th July 2024), pp. 48077–48096. URL: <https://hal.science/hal-04663577> (cit. on p. 7).

International peer-reviewed conferences

- [3] V. Bertret, R. Le Goff Latimier and V. Monbet. 'A stochastic expectation maximization algorithm for the estimation of wastewater treatment plant ammonium concentration'. In: ECC 2024 - 22nd European Control Conference. Stockholom, Sweden: IEEE, 2024, pp. 1–6. DOI: [10.23919/ECC64448.2024.10591038](https://hal.science/hal-04632445). URL: <https://hal.science/hal-04632445> (cit. on p. 7).

Conferences without proceedings

- [4] T. Guyard, C. Herzet and C. Elvira. 'Screen-and-Relax for Sparse Support Identification'. In: Journées SMAI MODE 2024. Lyon, France, 2024, pp. 1–1. URL: <https://hal.science/hal-04423101>.
- [5] T. Guyard, C. Herzet, C. Elvira and A. N. Arslan. 'A Generic Branch-and-Bound for L0-Penalized Problems'. In: Journées SMAI MODE 2024. Lyon, France, 2024, pp. 1–1. URL: <https://hal.science/hal-04423096>.

Reports & preprints

- [6] F. Cérou, P. Héas and M. Rousset. *Adaptive reduced tempering for bayesian inverse problems and rare event simulation*. 24th Oct. 2024. URL: <https://inria.hal.science/hal-04764656> (cit. on p. 7).
- [7] N. Champagnat, T. Lelièvre, M. Ramil, J. Reygner and D. Villemonais. *Quasi-stationary distribution for kinetic SDEs with low regularity coefficients*. 1st Oct. 2024. URL: <https://hal.science/hal-04720688> (cit. on p. 7).