

RESEARCH CENTRE

**Inria Center
at Université Grenoble Alpes**

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ACTIVITY REPORT

Project-Team

AIRSEA

**Mathematics and computing applied to
oceanic and atmospheric flows**

IN COLLABORATION WITH: Laboratoire Jean Kuntzmann (LJK)

DOMAIN

Digital Health, Biology and Earth

THEME

**Earth, Environmental and Energy
Sciences**

Inria

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Project-Team AIRSEA

Creation of the Project-Team: 2016 April 01

Keywords

Computer sciences and digital sciences

- A3.1.8. – Big data (production, storage, transfer)
- A3.4.1. – Supervised learning
- A3.4.2. – Unsupervised learning
- A3.4.5. – Bayesian methods
- A3.4.6. – Neural networks
- A3.4.7. – Kernel methods
- A3.4.8. – Deep learning
- A6.1.1. – Continuous Modeling (PDE, ODE)
- A6.1.2. – Stochastic Modeling
- A6.1.4. – Multiscale modeling
- A6.1.5. – Multiphysics modeling
- A6.2.1. – Numerical analysis of PDE and ODE
- A6.2.4. – Statistical methods
- A6.2.6. – Optimization
- A6.2.7. – High performance computing
- A6.3.1. – Inverse problems
- A6.3.2. – Data assimilation
- A6.3.4. – Model reduction
- A6.3.5. – Uncertainty Quantification
- A6.5.2. – Fluid mechanics
- A6.5.4. – Waves

Other research topics and application domains

- B3.2. – Climate and meteorology
- B3.3.2. – Water: sea & ocean, lake & river
- B3.3.4. – Atmosphere
- B3.4.1. – Natural risks
- B4.3.2. – Hydro-energy
- B4.3.3. – Wind energy
- B9.11.1. – Environmental risks

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2 Overall objectives

The general scope of the AIRSEA project-team is to develop *mathematical and computational methods for the modeling of oceanic and atmospheric flows*. The mathematical tools used involve both *deterministic and statistical approaches*. The main research topics cover a) modeling and coupling b) model reduction for sensitivity analysis, coupling and multiscale optimizations c) sensitivity analysis, parameter estimation and risk assessment d) algorithms for high performance computing. The range of application is from climate modeling to the prediction of extreme events.

3 Research program

Recent events have raised questions regarding the social and economic implications of anthropic alterations of the Earth system, i.e. climate change and the associated risks of increasing extreme events. Ocean and atmosphere, coupled with other components (continent and ice) are the building blocks of the Earth system. A better understanding of the ocean atmosphere system is a key ingredient for improving prediction of such events. Numerical models are essential tools to understand processes, and simulate and forecast events at various space and time scales. Geophysical flows generally have a number of characteristics that make it difficult to model them. This justifies the development of specifically adapted mathematical methods:

- Geophysical flows are strongly non-linear. Therefore, they exhibit interactions between different scales, and unresolved small scales (smaller than mesh size) of the flows have to be **parameterized** in the equations.
- Geophysical fluids are non closed systems. They are open-ended in their scope for including and dynamically coupling different physical processes (e.g., atmosphere, ocean, continental water, etc). **Coupling** algorithms are thus of primary importance to account for potentially significant feedback.
- Numerical models contain parameters which cannot be estimated accurately either because they are difficult to measure or because they represent some poorly known subgrid phenomena. There is thus a need for **dealing with uncertainties**. This is further complicated by the turbulent nature of geophysical fluids.
- The computational cost of geophysical flow simulations is huge, thus requiring the use of **reduced models, multiscale methods** and the design of algorithms ready for **high performance computing** platforms.

Our scientific objectives are divided into four major points. The first objective focuses on developing advanced mathematical methods for both the ocean and atmosphere, and the coupling of these two components. The second objective is to investigate the derivation and use of model reduction to face problems associated with the numerical cost of our applications. The third objective is directed toward the management of uncertainty in numerical simulations. The last objective deals with efficient numerical algorithms for new computing platforms. As mentioned above, the targeted applications cover oceanic and atmospheric modeling and related extreme events using a hierarchy of models of increasing complexity.

3.1 Modeling for oceanic and atmospheric flows

Current numerical oceanic and atmospheric models suffer from a number of well-identified problems. These problems are mainly related to lack of horizontal and vertical resolution, thus requiring the parameterization of unresolved (subgrid scale) processes and control of discretization errors in order to fulfill criteria related to the particular underlying physics of rotating and strongly stratified flows. Oceanic and atmospheric coupled models are increasingly used in a wide range of applications from global to regional scales. Assessment of the reliability of those coupled models is an emerging topic as the spread among the solutions of existing models (e.g., for climate change predictions) has not been reduced with the new generation models when compared to the older ones.

Advanced methods for modeling 3D rotating and stratified flows The continuous increase of computational power and the resulting finer grid resolutions have triggered a recent regain of interest in numerical methods and their relation to physical processes. Going beyond present knowledge requires a better understanding of numerical dispersion/dissipation ranges and their connection to model fine scales. Removing the leading order truncation error of numerical schemes is thus an active topic of research and each mathematical tool has to adapt to the characteristics of three dimensional stratified and rotating flows. Studying the link between discretization errors and subgrid scale parameterizations is also arguably one of the main challenges.

Complexity of the geometry, boundary layers, strong stratification and lack of resolution are the main sources of discretization errors in the numerical simulation of geophysical flows. This emphasizes the importance of the definition of the computational grids (and coordinate systems) both in horizontal and vertical directions, and the necessity of truly multi resolution approaches. At the same time, the role of the small scale dynamics on large scale circulation has to be taken into account. Such parameterizations may be of deterministic as well as stochastic nature and both approaches are taken by the AIRSEA team. The design of numerical schemes consistent with the parameterizations is also arguably one of the main challenges for the coming years. This work is complementary and linked to that on parameters estimation described in 3.3.

Ocean Atmosphere interactions and formulation of coupled models State-of-the-art climate models (CMs) are complex systems under continuous development. A fundamental aspect of climate modeling is the representation of air-sea interactions. This covers a large range of issues: parameterizations of atmospheric and oceanic boundary layers, estimation of air-sea fluxes, time-space numerical schemes, non conforming grids, coupling algorithms ... Many developments related to these different aspects were performed over the last 10-15 years, but were in general conducted independently of each other.

The aim of our work is to revisit and enrich several aspects of the representation of air-sea interactions in CMs, paying special attention to their overall consistency with appropriate mathematical tools. We intend to work consistently on the physics and numerics. Using the theoretical framework of global-in-time Schwarz methods, our aim is to analyze the mathematical formulation of the parameterizations in a coupling perspective. From this study, we expect improved predictability in coupled models (this aspect will be studied using techniques described in 3.3). Complementary work on space-time nonconformities and acceleration of convergence of Schwarz-like iterative methods (see 8.1.2) are also conducted.

3.2 Model reduction / multiscale algorithms

The high computational cost of the applications is a common and major concern to have in mind when deriving new methodological approaches. This cost increases dramatically with the use of sensitivity analysis or parameter estimation methods, and more generally with methods that require a potentially large number of model integrations.

A dimension reduction, using either stochastic or deterministic methods, is a way to reduce significantly the number of degrees of freedom, and therefore the calculation time, of a numerical model.

Model reduction Reduction methods can be deterministic (proper orthogonal decomposition, other reduced bases) or stochastic (polynomial chaos, Gaussian processes, kriging), and both fields of research are very active. Choosing one method over another strongly depends on the targeted application, which can be as varied as real-time computation, sensitivity analysis (see e.g., section 8.5) or optimisation for parameter estimation (see below).

Our goals are multiple, but they share a common need for certified error bounds on the output. Our team has a 4-year history of working on certified reduction methods and has a unique positioning at the interface between deterministic and stochastic approaches. Thus, it seems interesting to conduct a thorough comparison of the two alternatives in the context of sensitivity analysis. Efforts will also be directed toward the development of efficient greedy algorithms for the reduction, and the derivation of goal-oriented sharp error bounds for non linear models and/or non linear outputs of interest. This will be complementary to our work on the deterministic reduction of parametrized viscous Burgers and Shallow Water equations where the objective is to obtain sharp error bounds to provide confidence intervals for the estimation of sensitivity indices.

Reduced models for coupling applications Global and regional high-resolution oceanic models are either coupled to an atmospheric model or forced at the air-sea interface by fluxes computed empirically preventing proper physical feedback between the two media. Thanks to high-resolution observational studies, the existence of air-sea interactions at oceanic mesoscales (i.e., at $\mathcal{O}(1\text{ km})$ scales) have been unambiguously shown. Those interactions can be represented in coupled models only if the oceanic and atmospheric models are run on the same high-resolution computational grid, and are absent in a forced mode. Fully coupled models at high-resolution are seldom used because of their prohibitive computational cost. The derivation of a reduced model as an alternative between a forced mode and the use of a full atmospheric model is an open problem.

Multiphysics coupling often requires iterative methods to obtain a mathematically correct numerical solution. To mitigate the cost of the iterations, we will investigate the possibility of using reduced-order models for the iterative process. We will consider different ways of deriving a reduced model: coarsening of the resolution, degradation of the physics and/or numerical schemes, or simplification of the governing equations. At a mathematical level, we will strive to study the well-posedness and the convergence properties when reduced models are used. Indeed, running an atmospheric model at the same resolution as the ocean model is generally too expensive to be manageable, even for moderate resolution applications. To account for important fine-scale interactions in the computation of the air-sea boundary condition, the objective is to derive a simplified boundary layer model that is able to represent important 3D turbulent features in the marine atmospheric boundary layer.

Reduced models for multiscale optimization The field of multigrid methods for optimisation has known a tremendous development over the past few decades. However, it has not been applied to oceanic and atmospheric problems apart from some crude (non-converging) approximations or applications to simplified and low dimensional models. This is mainly due to the high complexity of such models and to the difficulty in handling several grids at the same time. Moreover, due to complex boundaries and physical phenomena, the grid interactions and transfer operators are not trivial to define.

Multigrid solvers (or multigrid preconditioners) are efficient methods for the solution of variational data assimilation problems. We would like to take advantage of these methods to tackle the optimization problem in high dimensional space. High dimensional control space is obtained when dealing with parameter fields estimation, or with control of the full 4D (space time) trajectory. It is important since it enables us to take into account model errors. In that case, multigrid methods can be used to solve the large scales of the problem at a lower cost, this being potentially coupled with a scale decomposition of the variables themselves.

3.3 Dealing with uncertainties

There are many sources of uncertainties in numerical models. They are due to imperfect external forcing, poorly known parameters, missing physics and discretization errors. Studying these uncertainties and their impact on the simulations is a challenge, mostly because of the high dimensionality and non-linear nature of the systems. To deal with these uncertainties we work on three axes of research, which are linked: sensitivity analysis, parameter estimation and risk assessment. They are based on either stochastic or deterministic methods.

Sensitivity analysis Sensitivity analysis (SA), which links uncertainty in the model inputs to uncertainty in the model outputs, is a powerful tool for model design and validation. First, it can be a pre-stage for parameter estimation (see 3.3), allowing for the selection of the more significant parameters. Second, SA permits understanding and quantifying (possibly non-linear) interactions induced by the different processes defining e.g., realistic ocean atmosphere models. Finally SA allows for validation of models, checking that the estimated sensitivities are consistent with what is expected by the theory. On ocean, atmosphere and coupled systems, only first order deterministic SA are performed, neglecting the initialization process (data assimilation). AIRSEA members and collaborators proposed to use second order information to provide consistent sensitivity measures, but so far it has only been applied to simple academic systems. Metamodels are now commonly used, due to the cost induced by each evaluation of complex numerical models: mostly Gaussian processes, whose probabilistic framework allows for the development of specific adaptive designs, and polynomial chaos not only in the context of intrusive Galerkin approaches but also in a black-box approach. Until recently, global SA was based primarily on a set of engineering practices. New mathematical and methodological developments have led to the numerical computation of Sobol' indices, with confidence intervals assessing for both metamodel and estimation errors. Approaches have also been extended to the case of dependent entries, functional inputs and/or output and stochastic numerical codes. Other types of indices and generalizations of Sobol' indices have also been introduced.

Concerning the stochastic approach to SA we plan to work with parameters that show spatio-temporal dependencies and to continue toward more realistic applications where the input space is of huge dimension with highly correlated components. Sensitivity analysis for dependent inputs also introduces new challenges. In our applicative context, it would seem prudent to carefully learn the spatio-temporal dependences before running a global SA. In the deterministic framework we focus on second order

approaches where the sought sensitivities are related to the optimality system rather than to the model; i.e., we consider the whole forecasting system (model plus initialization through data assimilation). All these methods allow for computing sensitivities and more importantly a posteriori error statistics.

Parameter estimation Advanced parameter estimation methods are barely used in ocean, atmosphere and coupled systems, mostly due to a difficulty of deriving adequate response functions, a lack of knowledge of these methods in the ocean-atmosphere community, and also to the huge associated computing costs. In the presence of strong uncertainties on the model but also on parameter values, simulation and inference are closely associated. Filtering for data assimilation and Approximate Bayesian Computation (ABC) are two examples of such association.

Stochastic approach can be compared with the deterministic approach, which allows to determine the sensitivity of the flow to parameters and optimize their values relying on data assimilation. This approach is already shown to be capable of selecting a reduced space of the most influent parameters in the local parameter space and to adapt their values in view of correcting errors committed by the numerical approximation. This approach assumes the use of automatic differentiation of the source code with respect to the model parameters, and optimization of the obtained raw code.

AIRSEA assembles all the required expertise to tackle these difficulties. As mentioned previously, the choice of parameterization schemes and their tuning has a significant impact on the result of model simulations. Our research will focus on parameter estimation for parameterized Partial Differential Equations (PDEs) and also for parameterized Stochastic Differential Equations (SDEs). Deterministic approaches are based on optimal control methods and are local in the parameter space (i.e., the result depends on the starting point of the estimation) but thanks to adjoint methods they can cope with a large number of unknowns that can also vary in space and time. Multiscale optimization techniques as described in 8.3 will be one of the tools used. This in turn can be used either to propose a better (and smaller) parameter set or as a criterion for discriminating parameterization schemes. Statistical methods are global in the parameter state but may suffer from the curse of dimensionality. However, the notion of parameter can also be extended to functional parameters. We may consider as parameter a functional entity such as a boundary condition on time, or a probability density function in a stationary regime. For these purposes, non-parametric estimation will also be considered as an alternative.

Risk assessment Risk assessment in the multivariate setting suffers from a lack of consensus on the choice of indicators. Moreover, once the indicators are designed, it still remains to develop estimation procedures, efficient even for high risk levels. Recent developments for the assessment of financial risk have to be considered with caution as methods may differ pertaining to general financial decisions or environmental risk assessment. Modeling and quantifying uncertainties related to extreme events is of central interest in environmental sciences. In relation to our scientific targets, risk assessment is very important in several areas: hydrological extreme events, cyclone intensity, storm surges... Environmental risks most of the time involve several aspects which are often correlated. Moreover, even in the ideal case where the focus is on a single risk source, we have to face the temporal and spatial nature of environmental extreme events. The study of extremes within a spatio-temporal framework remains an emerging field where the development of adapted statistical methods could lead to major progress in terms of geophysical understanding and risk assessment thus coupling data and model information for risk assessment.

Based on the above considerations we aim to answer the following scientific questions: how to measure risk in a multivariate/spatial framework? How to estimate risk in a non stationary context? How to reduce dimension (see 3.2) for a better estimation of spatial risk?

Extreme events are rare, which means there is little data available to make inferences of risk measures. Risk assessment based on observation therefore relies on multivariate extreme value theory. Interacting particle systems for the analysis of rare events is commonly used in the community of computer experiments. An open question is the pertinence of such tools for the evaluation of environmental risk. Most numerical models are unable to accurately reproduce extreme events. There is therefore a real need to develop efficient assimilation methods for the coupling of numerical models and extreme data.

3.4 High performance computing

Methods for sensitivity analysis, parameter estimation and risk assessment are extremely costly due to the necessary number of model evaluations. This number of simulations require considerable computational

resources, depends on the complexity of the application, the number of input variables and desired quality of approximations. To this aim, the AIRSEA team is an intensive user of HPC computing platforms, particularly grid computing platforms. The associated grid deployment has to take into account the scheduling of a huge number of computational requests and the links with data-management between these requests, all of these as automatically as possible. In addition, there is an increasing need to propose efficient numerical algorithms specifically designed for new (or future) computing architectures and this is part of our scientific objectives. According to the computational cost of our applications, the evolution of high performance computing platforms has to be taken into account for several reasons. While our applications are able to exploit space parallelism to its full extent (oceanic and atmospheric models are traditionally based on a spatial domain decomposition method), the spatial discretization step size limits the efficiency of traditional parallel methods. Thus the inherent parallelism is modest, particularly for the case of relative coarse resolution but with very long integration time (e.g., climate modeling). Paths toward new programming paradigms are thus needed. As a step in that direction, we plan to focus our research on parallel in time methods.

New numerical algorithms for high performance computing Parallel in time methods can be classified into three main groups. In the first group, we find methods using parallelism across the method, such as parallel integrators for ordinary differential equations. The second group considers parallelism across the problem. Falling into this category are methods such as waveform relaxation where the space-time system is decomposed into a set of subsystems which can then be solved independently using some form of relaxation techniques or multigrid reduction in time. The third group of methods focuses on parallelism across the steps. One of the best known algorithms in this family is parareal. Other methods combining the strengths of those listed above (e.g., PFASST) are currently under investigation in the community.

Parallel in time methods are iterative methods that may require a large number of iteration before convergence. Our first focus will be on the convergence analysis of parallel in time (Parareal / Schwarz) methods for the equation systems of oceanic and atmospheric models. Our second objective will be on the construction of fast (approximate) integrators for these systems. This part is naturally linked to the model reduction methods of section (8.3.1). Fast approximate integrators are required both in the Schwarz algorithm (where a first guess of the boundary conditions is required) and in the Parareal algorithm (where the fast integrator is used to connect the different time windows). Our main application of these methods will be on climate (i.e., very long time) simulations. Our second application of parallel in time methods will be in the context of optimization methods. In fact, one of the major drawbacks of the optimal control techniques used in 3.3 is a lack of intrinsic parallelism in comparison with ensemble methods. Here, parallel in time methods also offer ways to better efficiency. The mathematical key point is centered on how to efficiently couple two iterative methods (i.e., parallel in time and optimization methods).

4 Application domains

4.1 The Ocean-Atmosphere System

The evolution of natural systems, in the short, mid, or long term, has extremely important consequences for both the global Earth system and humanity. Forecasting this evolution is thus a major challenge from the scientific, economic, and human viewpoints.

Humanity has to face the problem of **global warming**, brought on by the emission of greenhouse gases from human activities. This warming will probably cause huge changes at global and regional scales, in terms of climate, vegetation and biodiversity, with major consequences for local populations. Research has therefore been conducted over the past 15 to 20 years in an effort to model the Earth's climate and forecast its evolution in the 21st century in response to anthropic action.

With regard to short-term forecasts, the best and oldest example is of course **weather forecasting**. Meteorological services have been providing daily short-term forecasts for several decades which are of crucial importance for numerous human activities.

Numerous other problems can also be mentioned, like **seasonal weather forecasting** (to enable powerful phenomena like an El Niño event or a drought period to be anticipated a few months in

advance), **operational oceanography** (short-term forecasts of the evolution of the ocean system to provide services for the fishing industry, ship routing, defense, or the fight against marine pollution) or the prediction of **floods**.

As mentioned previously, mathematical and numerical tools are omnipresent and play a fundamental role in these areas of research. In this context, the vocation of AIRSEA is not to carry out numerical prediction, but to address mathematical issues raised by the development of prediction systems for these application fields, in close collaboration with geophysicists.

5 Social and environmental responsibility

5.1 Impact of research results

Most of the research activities of the AIRSEA team are directed towards the improvement of numerical systems of the ocean and the atmosphere. This includes the development of appropriate numerical methods, model/parameter calibration using observational data and uncertainty quantification for decision making. The AIRSEA team members work in close collaboration with the researchers in the field of geophysical fluid and are partners of several interdisciplinary projects. They also strongly contribute to the development of state of the art numerical systems, like NEMO and CROCO in the ocean community.

6 Highlights of the year

- Clémentine Prieur was selected as one of the ambassadors for "La Science taille XX elles" in Grenoble xxlgrenoble.sciencesconf.org
- The MEDIATION (Methodological development for a robust and efficient digital twin of the ocean, see 10.4.1) project has been selected by the French Priority Program on Ocean and Climate. Coordinated by the AIRSEA team, the project will gather 2022-2027) 11 academic partners to work on the impact of climate change on coastal ecosystems.

7 New software and platforms

7.1 New software

7.1.1 AGRIF

Name: Adaptive Grid Refinement In Fortran

Keyword: Mesh refinement

Scientific Description: AGRIF is a Fortran 90 package for the integration of full adaptive mesh refinement (AMR) features within a multidimensional finite difference model written in Fortran. Its main objective is to simplify the integration of AMR functionalities within an existing model with minimal changes. Capabilities of this package include the management of an arbitrary number of grids, horizontal and/or vertical refinements, dynamic regridding, parallelization of the grids interactions on distributed memory computers. AGRIF requires the model to be discretized on a structured grid, like it is typically done in ocean or atmosphere modelling.

Functional Description: AGRIF is a Fortran 90 package for the integration of full adaptive mesh refinement (AMR) features within a multidimensional finite difference model written in Fortran. Its main objective is to simplify the integration of AMR functionalities within an existing model with minimal changes. Capabilities of this package include the management of an arbitrary number of grids, horizontal and/or vertical refinements, dynamic regridding, parallelization of the grids interactions on distributed memory computers. AGRIF requires the model to be discretized on a structured grid, like it is typically done in ocean or atmosphere modelling.

News of the Year: Within the framework of a European Copernicus contract, improvements have been made to the management of parallelization (assignment of processors to computational grids).

URL: <https://gitlab.inria.fr/ldebreu/agrif>

Publications: tel-01546328, hal-00387435

Contact: Laurent Debreu

Participant: Laurent Debreu

7.1.2 BALAISE

Name: Bibliothèque d'Assimilation Lagrangienne Adaptée aux Images Séquencées en Environnement

Keywords: Multi-scale analysis, Data assimilation, Optimal control

Functional Description: BALAISE (Bibliothèque d'Assimilation Lagrangienne Adaptée aux Images Séquencées en Environnement) is a test bed for image data assimilation. It includes a shallow water model, a multi-scale decomposition library and an assimilation suite.

Contact: Patrick Vidard

7.1.3 NEMOVAR

Name: Variational data assimilation for NEMO

Keywords: Oceanography, Data assimilation, Adjoint method, Optimal control

Functional Description: NEMOVAR is a state-of-the-art multi-incremental variational data assimilation system with both 3D and 4D var capabilities, and which is designed to work with NEMO on the native ORCA grids. The background error covariance matrix is modelled using balance operators for the multivariate component and a diffusion operator for the univariate component. It can also be formulated as a linear combination of covariance models to take into account multiple correlation length scales associated with ocean variability on different scales. NEMOVAR has recently been enhanced with the addition of ensemble data assimilation and multi-grid assimilation capabilities. It is used operationnaly in both ECMWF and the Met Office (UK)

Contact: Patrick Vidard

Partners: CERFACS, ECMWF, Met Office

7.1.4 SWEET

Name: Shallow Water Equation Environment for Tests, Awesome!

Keywords: High-Performance Computing, Time integration methods

Functional Description: SWEET supports periodic boundary conditions for * the bi-periodic plane (2D torus) * the sphere

Space discretization * PLANE: Spectral methods based on Fourier space * PLANE: Finite differences * SPHERE: Spherical Harmonics

Time discretization * Explicit RK * Implicit RK * Leapfrog * Crank-Nicolson * Semi-Lagrangian * Parallel-in-time ** Parareal ** PFASST ** Rational approximation of exponential Integrators (REXI) ...and many more time steppers...

Special features * Graphical user interface * Fast Helmholtz solver in spectral space * Easy-to-code in C++ ...

There's support for various applications * Shallow-water equations on plane/sphere * Advection * Burgers' ...

URL: <https://schreiberx.github.io/sweetsite/>

Contact: Martin Schreiber

Partners: University of São Paulo, Technical University of Munich (TUM)

8 New results

8.1 Modeling for Oceanic and Atmospheric flows

8.1.1 Numerical Schemes for Ocean Modelling

Participants: Eric Blayo, Laurent Debreu, Gabriel Derrida, Emilie Duval, Florian Lemarié, Gurvan Madec, Antoine Nasser, Sanal Parameswaran.

Dealing with complex geometries Accurate and stable implementation of bathymetry boundary conditions in ocean models remains a challenging problem. Generalized terrain-following coordinates are often used in ocean models, but they require smoothing the bathymetry to reduce pressure gradient errors. Geopotential z-coordinates are a common alternative that avoid pressure gradient and numerical diapycnal diffusion errors, but they generate spurious flow due to their “staircase” geometry. In [47], we introduce a new Brinkman volume penalization to approximate the no-slip boundary condition and complex geometry of bathymetry in ocean models. This approach corrects the staircase effect of z-coordinates, does not introduce any new stability constraints on the geometry of the bathymetry and is easy to implement in an existing ocean model. The porosity parameter allows modelling subgrid scale details of the geometry. As an illustration, through the use of penalization methods, the Gulf Stream detachment is correctly represented in a 1/8 degree simulation (see 1). These new results on realistic applications have been published in [7]. This opens the door to a clear improvement of climate models in which a good representation of this mechanism is essential. This work is currently extended to z coordinate ocean models through the PhD work of A. Nasser. We have also investigated the representation of coastlines and its sensitivity to the mesh orientation in [34].

Beyond the hydrostatic assumption With the increase of resolution, the hydrostatic assumption becomes less valid and the AIRSEA group also works on the development of non-hydrostatic ocean models. The treatment of non-hydrostatic incompressible flows leads to a 3D elliptic system for pressure that can be ill-conditioned, in particular with non geopotential vertical coordinates. That is why we favor the use of the non-hydrostatic compressible equations, that remove the need for a 3D resolution at the price of reincluding acoustic waves. For that purposes a detailed analysis of acoustic-gravity waves in a free-surface compressible and stratified ocean was carried out [41] in part in the PhD of E. Duval. The proposed numerical approach has been implemented in the CROCO ocean model and tested in various flow configurations [57], [13].

In the context of the French initiative CROCO (Coastal and Regional Ocean COMMunity model, www.croco-ocean.org) for the development of a new oceanic modeling system, Emilie Duval worked on the design of methods to couple local nonhydrostatic models to larger scale hydrostatic ones. Such a coupling is quite delicate from a mathematical point of view, due to the different nature of hydrostatic and nonhydrostatic equations (where the vertical velocity is either a diagnostic or a prognostic variable). A thorough analysis of the different families of waves that can be present in these equations was performed. Moreover a decomposition of the solutions into vertical modes, which is quite usual in the hydrostatic case, has been generalized in the nonhydrostatic case, which could be an interesting lead for coupling algorithms. A prototype has been implemented, which allows for analytical solutions in simplified configurations and makes it possible to test different numerical coupling approaches. Emilie Duval defended her PhD on 15 December 2022.

8.1.2 Coupling Methods for Oceanic and Atmospheric Models and Representation of the Air-Sea Interface

Participants: Eric Blayo, Florian Lemarié, Sophie Thery, Simon Clément.

The Airsea team is involved in the modeling and algorithmic aspects of ocean-atmosphere (OA) coupling. For the last few years we have been actively working on the analysis of such coupling both in terms of its continuous and numerical formulation [62], [63]. Our activities can be divided into three general topics

1. *Continuous and discrete analysis of Schwarz algorithms for OA coupling:* we have been developing coupling approaches for several years, based on so-called Schwarz algorithms. Schwarz-like domain decomposition methods are very popular in mathematics, computational sciences and engineering notably for the implementation of coupling strategies. However, for complex applications (like in OA coupling) it is challenging to have an a priori knowledge of the convergence properties of such methods. Indeed coupled problems arising in Earth system modeling often exhibit sharp turbulent boundary layers whose parameterizations lead to peculiar transmission conditions and diffusion coefficients. In the framework of S. Thery PhD (defended in February 2021) the well-posedness of the non-linear coupling problem including parameterizations has been addressed and a detailed continuous analysis of the convergence properties of the Schwarz methods has been pursued to entangle the impact of the different parameters at play in such coupling problem [78], [16]. In S. Clément PhD, a general framework has been proposed to study the convergence properties at a (semi)-discrete level to allow a systematic comparison with the results obtained from the continuous problem [5]. Such framework allows to study more complex coupling problems whose formulation is representative of the discretization used in realistic coupled models [46].

Within the COCOA project, a Schwarz-like iterative method has been applied in a state-of-the-art Earth-System model to evaluate the consequences of inaccuracies in the usual ad-hoc ocean-atmosphere coupling algorithms used in realistic models [68], [69]. Numerical results obtained with an iterative process show large differences at sunrise and sunset compared to usual ad-hoc algorithms thus showing that synchrony errors inherent to ad-hoc coupling methods can be significant. The objective now is to reduce the computational cost of Schwarz algorithms using deep learning techniques.

2. *Representation of the air-sea interface in coupled models:* During the PhD-thesis of Charles Pelletier the scope was on including the formulation of physical parameterizations in the theoretical analysis of the coupling, in particular the parameterization schemes to compute air-sea fluxes. Following this work, a novel and rigorous framework for a consistent two-sided modeling of the surface boundary layer has been proposed [72]. This framework allows for a more general representation of the vertical physics at the air-sea interface while improving the mathematical regularity of the numerical solutions. Moreover, it is flexible enough to include additional physical parameters for example to account for the effect of surface waves in the turbulent flux computation. This work is the first step toward more adequate discretization methods for the parameterization of surface and planetary boundary layers in coupled models.

At a more fundamental level, in collaboration with A. Wirth, we have studied turbulent fluctuations in a coupled Ekman layer problem with randomized drag coefficient [81].

3. *A simplified atmospheric boundary layer model for oceanic purposes:* Part of our activities within the IMMERSE and SHOM 19CP07 projects is dedicated to the development of a simplified model of the marine atmospheric boundary layer (called ABL1d) of intermediate complexity between a bulk parameterization and a full three-dimensional atmospheric model and to its integration to the NEMO general circulation model [65]. A constraint in the conception of such a simplified model is to allow an apt representation of the downward momentum mixing mechanism and partial

re-energization of the ocean by the atmosphere while keeping the computational efficiency and flexibility inherent to ocean only modeling. Realistic applications of the coupled NEMO-ABL1d modeling system have been carried out [44]. The next step is to find adequate ways to fill some gaps in the 1D approach either using multiple scales asymptotic techniques or by casting the equations in terms of perturbations around an ambient state given by a large-scale dataset.

These topics are addressed through strong collaborations between the applied mathematicians and the climate and operational community (Meteo-France, Ifremer, SHOM, Mercator-Ocean, LMD, and LOCEAN). Our work on ocean-atmosphere coupling has steadily matured over the last few years and has reached a point where it triggers interest from the physicists. Through the funding of the projects ANR COCOA (2017-2021, PI: E. Blayo) and SHOM 19CP07 (2020-2024, PI: F. Lemarié), Airsea team members play a major role in the structuration of a multi-disciplinary scientific community working on ocean-atmosphere coupling spanning a broad range from mathematical theory to practical implementations in climate and operational models.

8.1.3 Physics-Dynamics coupling: Consistent subgrid-scale modeling

Participants: Florian Lemarié, Manolis Perrot, Simon Clement.

Following the work started in 2021, the AIRSEA team continued to study new topics around physics-dynamics coupling [53]. Schematically, numerical models consist of two blocks generally identified as “physics” and “dynamics” which are often developed separately. The “Physics” represents unresolved or under-resolved processes with typical scales below model resolution while the “dynamics” corresponds to a discrete representation in space and time of resolved processes. Unresolved processes cannot be ignored because they directly influence the resolved part of the flow since energy is continuously transferred between scales. The interplay between resolved and unresolved scales is a large, incomplete and complex topic for which there is still much to do within the Earth system modeling community [64].

In current models, the scale separation between the resolved part of the flow and the unresolved part is carried out via the Reynolds decomposition which corresponds to a filtering of the Navier-Stokes equations. Such a filtering leads to an evolution equation for the large-scale flow containing unknown terms (often called Reynolds stress terms) which represent the average contribution of the small-scale processes. The system is closed by so-called parameterizations that arbitrarily relate the contribution of small-scale processes to large-scale variables. In this context, the AIRSEA team has started work on two aspects:

1. *Energetically consistent discretization of boundary layer parameterizations* Part of S. Clement’s thesis is about the discretization of boundary layer parameterizations. The problem of interest takes the form of a nonstationary nonlinear parabolic equation. The objective is to derive a discretization for which we could prove nonlinear stability criteria and show robustness to large variations in parabolic Courant number while being consistent with our knowledge of the underlying physical principles (e.g. the Monin-Obukhov theory in the surface layer).
2. *Representation of penetrative convection in oceanic models* Accounting for the mean effect of subgrid scale intermittent coherent structures like convective plumes is very challenging. Currently this is done very crudely in ocean models (vertical diffusion is locally increased to ‘mix’ unstable density profiles). A difficulty is that in convective conditions, turbulent fluxes are dominated by processes unrelated to local gradients thus invalidating the usual downgradient approach (a.k.a. Boussinesq Hypothesis). In the framework of the PhD of Manolis Perrot a first step is to study the derivation of mass-flux convection schemes, popular in atmospheric models, to extend them specifically to the oceanic context. This extension to the oceanic context will be carried out under certain “consistency” constraints: energetic considerations, scale-awareness and well-posedness of the resulting model. In a second step, reference LES simulations will be developed to guide the formulation of unknown/uncertain terms in the extended mass-flux scheme.

Those topics are addressed through collaborations with the climate and operational community (Meteo-France, SHOM, Mercator-Ocean, and IGE). Two projects are currently funded, one on the energetically consistent discretization aspect (SHOM 19CP07, 2020-2024, PI: F. Lemarié) and one on the convection parameterization (Institut des Mathématiques pour la Planète Terre, 2021-2024, PIs: F. Lemarié and G. Madec).

8.1.4 Machine learning for reconstruction of model parameters.

Participants: Laurent Debreu, Eugene Kazantsev, Arthur Vidard, Olivier Zahm.

Artificial intelligence and machine learning may be considered as a potential way to address unresolved model scales and to approximate poorly known processes such as dissipation that occurs essentially at small scales. In order to understand the possibility to combine numerical model and neural network learned with the aid of external data, we develop a network generation and learning algorithm and use it to approximate nonlinear model operators.

A potential way to reconstruct subgrid scales consists in application the Image Super-Resolution methods that refer to the process of recovering high-resolution images from low-resolution image in computer vision and image processing. Recent years have shown remarkable progress of image super-resolution using machine learning techniques [80]. We try to use this methodology in order to identify fine structure of the chaotic turbulent solution of a simple barotropic ocean model. After the learning the flow patterns obtained by the high resolution model, the neuron net can identify fine structure in the low-resolution model solution with better precision than bicubic interpolation.

Different techniques of neuron net construction have been analyzed. Full-connected networks, basic convolutional and encoder-decoder processes [60] as well as mixed architectures were compared with each other and with the classical interpolation of model solution on a low-resolution grid.

8.2 Assimilation of spatially dense observations

Participant: Elise Arnaud, Arthur Vidard, Emilie Rouzies, Aurélien Prat.

8.2.1 Direct assimilation of image sequences

At the present time the observation of Earth from space is done by more than thirty satellites. These platforms provide two kinds of observational information:

- Eulerian information as radiance measurements: the radiative properties of the earth and its fluid envelops. These data can be plugged into numerical models by solving some inverse problems.
- Lagrangian information: the movement of fronts and vortices give information on the dynamics of the fluid. Presently this information is scarcely used in meteorology by following small cumulus clouds and using them as Lagrangian tracers, but the selection of these clouds must be done by hand and the altitude of the selected clouds must be known. This is done by using the temperature of the top of the cloud.

Our current developments are targeted at the use of learning methods methods to describe the evolution of the images. This approach has been applied to the tracking of oceanic oil spills in the framework of a Long Li's Phd in co-supervision with Jianwei Ma. It led to the publication of [12].

8.2.2 Observation error representation

Accounting for realistic observations errors is a known bottleneck in data assimilation, because dealing with error correlations is complex. Following a previous study on this subject, we propose to use multi-scale modelling, more precisely wavelet transform, to address this question. In [45] we investigate the problem further by addressing two issues arising in real-life data assimilation: how to deal with partially missing data (e.g., concealed by an obstacle between the sensor and the observed system); how to solve convergence issues associated to complex observation error covariance matrices? Two adjustments relying on wavelets modelling are proposed to deal with those, and offer significant improvements. The first one consists in adjusting the variance coefficients in the frequency domain to account for masked information. The second one consists in a gradual assimilation of frequencies. Both of these fully rely on the multiscale properties associated with wavelet covariance modelling.

This kind of work was put to application in STORM, a collaborative project with Université de La Réunion ended this year. Our role was to prepare for the assimilation of data collected by sea turtles., and in particular work on the description of observation error statistics.

8.3 Model reduction / multiscale algorithms

8.3.1 Parameter space dimension reduction and Model order reduction

Participants: Youssef Marzouk, Clémentine Prieur, Arthur Macherey, Ricardo Baptista, Tong Xin, Cui Tiangang, Olivier Zahm.

The high computational cost of complex numerical simulations is a common and major concern when deriving new methodological approaches. This cost increases dramatically with the use of sensitivity analysis or parameter estimation methods, and more generally with any method requiring numerous model integrations. Model reduction, using either stochastic or deterministic methods, is a way to reduce significantly the computing time of a numerical model. Over the past year, our team focused on different reduction aspects, emphasized and described below.

In the paper [29], we address the problem of the parametrization and the learning of monotone triangular transport maps. Transportation of measure provides a versatile approach for modeling complex probability distributions, with applications in density estimation, Bayesian inference, generative modeling, and beyond. Monotone triangular transport maps—approximations of the Knothe–Rosenblatt (KR) rearrangement are a canonical choice for these tasks. Yet the representation and parameterization of such maps have a significant impact on their generality and expressiveness, and on properties of the optimization problem that arises in learning a map from data (e.g., via maximum likelihood estimation). We present a general framework for representing monotone triangular maps via invertible transformations of smooth functions. We establish conditions on the transformation such that the associated infinite-dimensional minimization problem has no spurious local minima, i.e., all local minima are global minima; and we show for target distributions satisfying certain tail conditions that the unique global minimizer corresponds to the KR map. Given a sample from the target, we then propose an adaptive algorithm that estimates a sparse semi-parametric approximation of the underlying KR map. We demonstrate how this framework can be applied to joint and conditional density estimation, likelihood-free inference, and structure learning of directed graphical models, with stable generalization performance across a range of sample sizes.

In the paper [28], we consider the problem of reducing the dimensions of parameters and data in non-Gaussian Bayesian inference problems. Our goal is to identify an “informed” subspace of the parameters and an “informative” subspace of the data so that a high-dimensional inference problem can be approximately reformulated in low-to-moderate dimensions, thereby improving the computational efficiency of many inference techniques. To do so, we exploit gradient evaluations of the log-likelihood function. Furthermore, we use an information-theoretic analysis to derive a bound on the posterior error due to parameter and data dimension reduction. This bound relies on logarithmic Sobolev inequalities,

and it reveals the appropriate dimensions of the reduced variables. We compare our method with classical dimension reduction techniques, such as principal component analysis and canonical correlation analysis, on applications ranging from mechanics to image processing.

Markov chain Monte Carlo (MCMC) methods form one of the algorithmic foundations of Bayesian inverse problems. The recent development of likelihood-informed subspace (LIS) methods offers a viable route to designing efficient MCMC methods for exploring high-dimensional posterior distributions via exploiting the intrinsic low-dimensional structure of the underlying inverse problem. However, existing LIS methods and the associated performance analysis often assume that the prior distribution is Gaussian. This assumption is limited for inverse problems aiming to promote sparsity in the parameter estimation, as heavy-tailed priors, e.g., Laplace distribution or the elastic net commonly used in Bayesian LASSO, are often needed in this case. To overcome this limitation, we consider in the paper [6] a prior normalization technique that transforms any non-Gaussian (e.g. heavy-tailed) priors into standard Gaussian distributions, which makes it possible to implement LIS methods to accelerate MCMC sampling via such transformations. We also rigorously investigate the integration of such transformations with several MCMC methods for high-dimensional problems. Finally, we demonstrate various aspects of our theoretical claims on two nonlinear inverse problems.

In a joint work [14] with Didier Georges (GIPSA Lab, Grenoble) and Mathieu Oliver (internship student), we proposed a spatialized extension of a SIR model that accounts for undetected infections and recoveries as well as the load on hospital services. The spatialized compartmental model we introduced is governed by a set of partial differential equations (PDEs) defined on a spatial domain with complex boundary. We proposed to solve the set of PDEs defining our model by using a meshless numerical method based on a finite difference scheme in which the spatial operators were approximated by using radial basis functions. Then we calibrated our model on the French department of Isère during the first period of lockdown, using daily reports of hospital occupancy in France. Our methodology allowed to simulate the spread of Covid-19 pandemic at a departmental level, and for each compartment. However, the simulation cost prevented from online short-term forecast. Therefore, we proposed to rely on reduced order modeling tools to compute short-term forecasts of infection number. The strategy consisted in learning a time-dependent reduced order model with few compartments from a collection of evaluations of our spatialized detailed model, varying initial conditions and parameter values. A set of reduced bases was learnt in an offline phase while the projection on each reduced basis and the selection of the best projection was performed online, allowing short-term forecast of the global number of infected individuals in the department. This work is going on in the framework of Robin Vaudry's PhD (co-supervised with Didier Georges). We are investigating the more complex setting of spatialized models taking into account the vaccination and the loss of immunity.

In the framework of Arthur Macherey's PhD (defended in June 2021), in collaboration with Anthony Nouy and Marie Billaud-Friess (Ecole Centrale Nantes), we have proposed algorithms for solving high-dimensional Partial Differential Equations (PDEs) that combine a probabilistic interpretation of PDEs, through Feynman-Kac representation, with sparse interpolation [43]. Monte-Carlo methods and time-integration schemes are used to estimate pointwise evaluations of the solution of a PDE. We use a sequential control variates algorithm, where control variates are constructed based on successive approximations of the solution of the PDE. We are now interested in solving parametrized PDE with stochastic algorithms in the framework of potentially high dimensional parameter space. A preliminary step was the development of a PAC algorithm in relative precision for bandit problem with costly sampling [3].

8.4 Parameter estimation and robust inversion

Reduced models are also developed in the framework of robust inversion. In [48], we have combined a new greedy algorithm for functional quantization with a Stepwise Uncertainty Reduction strategy to solve a robust inversion problem under functional uncertainties. In a more recent work, we further reduced the number of simulations required to solve the same robust inversion problem, based on Gaussian process meta-modeling on the joint input space of deterministic control parameters and functional uncertain variable [49]. These results are applied to automotive depollution. This research axis was conducted in the framework of the Chair OQUAIDO. This research axis is still active in the team through Clément Duhamel's PhD, in collaboration with Céline Helbert (Ecole Centrale Lyon) and Miguel Munoz Zuniga, Delphine Sinoquet (IFPEN, Rueil Malmaison) [32].

8.5 Sensitivity analysis

Participants: Elise Arnaud, Eric Blayo, Laurent Gilquin, Maria Belén Heredia, Adrien Hirvoas, Henri Mermoz Kouye, Clémentine Prieur.

Scientific context Forecasting geophysical systems require complex models, which sometimes need to be coupled, and which make use of data assimilation. The objective of this project is, for a given output of such a system, to identify the most influential parameters, and to evaluate the effect of uncertainty in input parameters on model output. Existing stochastic tools are not well suited for high dimension problems (in particular time-dependent problems), while deterministic tools are fully applicable but only provide limited information. So the challenge is to gather expertise on one hand on numerical approximation and control of Partial Differential Equations, and on the other hand on stochastic methods for sensitivity analysis, in order to develop and design innovative stochastic solutions to study high dimension models and to propose new hybrid approaches combining the stochastic and deterministic methods. We took part to the writing of a position paper on the future of sensitivity analysis [75].

8.5.1 Global sensitivity analysis with dependent inputs

Participants: Elise Arnaud, Eric Blayo, Laurent Gilquin, Maria Belén Heredia, Adrien Hirvoas, Alexandre Janon, Henri Mermoz Kouye, Clémentine Prieur, Arthur Vidard, Emilie Rouzies.

An important challenge for stochastic sensitivity analysis is to develop methodologies which work for dependent inputs. Recently, the Shapley value, from econometrics, was proposed as an alternative to quantify the importance of random input variables to a function. Owen [70] derived Shapley value importance for independent inputs and showed that it is bracketed between two different Sobol' indices. Song et al. [76] recently advocated the use of Shapley value for the case of dependent inputs. In a recent work [71], in collaboration with Art Owen (Stanford's University), we showed that Shapley value removes the conceptual problems of functional ANOVA for dependent inputs. We also investigated further the properties of Shapley effects in [59]. By the end of 2021, Clémentine Prieur started a collaboration with Elmar Plischke (TU Clausthal, Germany) and Emanuele Borgonovo (Bocconi University, Milan, Italy) to estimate total Sobol' indices as a measure for variable selection even in the framework of dependent inputs. In particular, it allows to estimate total Sobol' indices for inputs defined on a non rectangular domain. This setting is of particular interest for applications where the input space is reduced due to physical constraints on the quantity of interest. This last setting was encountered, e.g., in Maria Belén Heredia's PhD thesis (defended in december, 2020), and analyzed by estimating Shapley effects with a nonparametric procedure based on nearest neighbors [1] (see Section 8.5.2 for more details). In October 2021, Ri Wang has started a PhD, cosupervised by Clémentine Prieur and Véronique Maume-Deschamps (ICJ, Lyon 1) on the estimation of quantile oriented sensitivity indices in the framework of dependent inputs, by means of random forests or other machine learning tools. Ri Wang has received a funding from the Chinese Scientific Council.

8.5.2 Green sensitivity for multivariate and functional outputs

Participants: María Belén Heredia, Clémentine Prieur.

Another research direction for global SA algorithm starts with the report that most of the algorithms to compute sensitivity measures require special sampling schemes or additional model evaluations so that

available data from previous model runs (e.g., from an uncertainty analysis based on Latin Hypercube Sampling) cannot be reused. One challenging task for estimating global sensitivity measures consists in recycling an available finite set of input/output data. Green sensitivity, by recycling, avoids wasting. These given data have been discussed, e.g., in [73], [74]. Most of the given data procedures depend on parameters (number of bins, truncation argument...) not easy to calibrate with a bias-variance compromise perspective. Adaptive selection of these parameters remains a challenging issue for most of these given-data algorithms. In the context of María Belén Heredia's PhD thesis, we have proposed [42] a non-parametric given data estimator for aggregated Sobol' indices, introduced in [61] and further developed in [51] for multivariate or functional outputs. We also introduced aggregated Shapley effects and we have extended a nearest neighbor estimation procedure to estimate these indices [1]. We also started a collaboration with Sébastien Da Veiga (Safran Tech), Agnès Lagnoux, Thierry Klein and Fabrice Gamboa (Institut de Mathématiques de Toulouse) on a new nonparametric estimation procedure for closed Sobol' indices of any order based on degenerate U-statistics.

8.5.3 Global sensitivity analysis for parametrized stochastic differential equations

Participants: Henri Mermoz Kouye, Clémentine Prieur.

Many models are stochastic in nature, and some of them may be driven by parametrized stochastic differential equations (SDE). It is important for applications to propose a strategy to perform global sensitivity analysis (GSA) for such models, in presence of uncertainties on the parameters. In collaboration with Pierre Etoré (DATA department in Grenoble), Clémentine Prieur proposed an approach based on Feynman-Kac formulas [50]. The research on GSA for stochastic simulators is still ongoing, first in the context of the MATH-AmSud project FANTASTIC (Statistical inFERENCE and sensitivity ANalysis for models described by sTochASTIC differential equations) with Chile and Uruguay, secondly through the PhD thesis of Henri Mermoz Kouye, co-supervised by Clémentine Prieur, in collaboration with Gildas Mazo and Eliza Vergu (INRAE, département MIA, Jouy). Note that our recent developments with P. Etoré on GSA for parametrized SDEs and are strongly related to reduced order modeling (see Section 8.3), as GSA requires intensive computations of the quantity of interest. In collaboration with Pierre Etoré and Joël Andrepont (master internship started in spring 2021), Clémentine Prieur is working on GSA for parametrized SDEs based on Fokker-Planck equation and kernel based sensitivity indices. Note that a joint work between Pierre Etoré, Clémentine Prieur and Jose R. Leon has been submitted, related to exact or approximated computation of Kolmogorov hypoelliptic equations (KHE). Even if not dealing with GSA, it could be a starting point for analyzing sensitivity for models described by a parametrized version of KHE. Concerning Henri Mermoz Kouye's PhD thesis, the approach is different. We are interested in GSA for compartmental stochastic models. Our methodology relies on a deterministic representation of continuous time Markov chains stochastic compartmental models [33]. Henri Mermoz Kouye defended in December, 2022.

8.5.4 Sensitivity analysis in pesticide transfer models

Participants: Arthur Vidard, Emilie Rouzies, Katarina Radisic.

Pesticide transfer models are valuable tools to predict and prevent pollution of water bodies. However, using such models in operational contexts requires a strong knowledge of their structure including influential parameters. This project aims at performing global sensitivity analysis (GSA) of the PESHMELBA model (pesticide and hydrology: modelling at the catchment scale). This work is made hard due to the modular, complex structure of the model that couples different physical processes. It results in a large input space dimension and a high computational cost that limits the number of available runs. Using classical GSA tools such as Sobol' indices is thus not feasible. In order to circumvent those limitations, we

also explored alternative techniques such as HSIC dependence measure or Random Forest metamodel. The use of such methods in the specific context of spatially distributed output was submitted in a journal paper [36]. We extended this work to spatiotemporal output, as presented in [15].

To conclude Section 8.5, let us mention that Clémentine Prieur took part to the writing on a monography on recent trends in sensitivity analysis, which appeared by the end of 2021 [79].

8.6 Model calibration and statistical inference

Participants: Maria Belén Heredia, Adrien Hirvoas, Clémentine Prieur, Victor Trappier, Arthur Vidard, Elise Arnaud, Laurent Debreu.

8.6.1 Bayesian calibration

Physically-based avalanche propagation models must still be locally calibrated to provide robust predictions, e.g. in long-term forecasting and subsequent risk assessment. Friction parameters cannot be measured directly and need to be estimated from observations. Rich and diverse data is now increasingly available from test-sites, but for measurements made along ow propagation, potential autocorrelation should be explicitly accounted for. In the context of María Belén Heredia's PhD, in collaboration with IRSTEA Grenoble, we have proposed in [56] a comprehensive Bayesian calibration and statistical model selection framework with application to an avalanche sliding block model with the standard Voellmy friction law and high rate photogrammetric images. An avalanche released at the Lautaret test-site and a synthetic data set based on the avalanche were used to test the approach. Results have demonstrated i) the efficiency of the proposed calibration scheme, and ii) that including autocorrelation in the statistical modelling definitely improves the accuracy of both parameter estimation and velocity predictions. In the context of the energy transition, wind power generation is developing rapidly in France and worldwide. Research and innovation on wind resource characterisation, turbin control, coupled mechanical modelling of wind systems or technological development of offshore wind turbines floaters are current research topics. In particular, the monitoring and the maintenance of wind turbine is becoming a major issue. Current solutions do not take full advantage of the large amount of data provided by sensors placed on modern wind turbines in production. These data could be advantageously used in order to refine the predictions of production, the life of the structure, the control strategies and the planning of maintenance. In this context, it is interesting to optimally combine production data and numerical models in order to obtain highly reliable models of wind turbines. This process is of interest to many industrial and academic groups and is known in many fields of the industry, including the wind industry, as "digital twin". The objective of Adrien Hirvoas's PhD work is to develop of data assimilation methodology to build the "digital twin" of an onshore wind turbine. Based on measurements, the data assimilation should allow to reduce the uncertainties of the physical parameters of the numerical model developed during the design phase to obtain a highly reliable model. Various ensemble data assimilation approaches are currently under consideration to address the problem. In the context of this work, it is necessary to develop algorithms of identification quantifying and ranking all the uncertainty sources. This work is done in collaboration with IFPEN [8], [58].

8.6.2 Simulation & Estimation of EPIdemics with Algorithms

Participants: Clémentine Prieur.

Due to the sanitary context, Clémentine Prieur decided to join a working group, SEEPIA Simulation & Estimation of EPIdemics with Algorithms, animated by Didier Georges (Gipsa-lab). A first work has been published [54]. An extension of the classical pandemic SIRD model was considered for the regional spread of COVID-19 in France under lockdown strategies. This compartment model divides the infected

and the recovered individuals into undetected and detected compartments respectively. By fitting the extended model to the real detected data during the lockdown, an optimization algorithm was used to derive the optimal parameters, the initial condition and the epidemics start date of regions in France. Considering all the age classes together, a network model of the pandemic transport between regions in France was presented on the basis of the regional extended model and was simulated to reveal the transport effect of COVID-19 pandemic after lockdown. Using the the measured values of displacement of people mobilizing between each city, the pandemic network of all cities in France was simulated by using the same model and method as the pandemic network of regions. Finally, a discussion on an integro-differential equation was given and a new model for the network pandemic model of each age was provided. As already mentioned in Section 8.3, Clémentine Prieur went on working on the pandemic, in collaboration with Didier Georges (GIPSA Lab, Grenoble). Both of them supervised the internship of Matthieu Oliver, submitting a work proposing time-dependent reduced order modeling for short-term forecast from a spatialized SIR model [14]. Robin Vaudry started in October 2021 a PhD, funded by the CNR research platform MODCOV19, and cosupervised by Clémentine Prieur and Didier Georges. The objective of this PhD is to solve inverse problems related to spatialized and ages structured compartmental models of COVID19 pandemic.

8.7 Modeling and inference for extremes

Participants: Philomène Le Gall, Clémentine Prieur, Patricia Tencaliec.

In [77], we are considering the modeling of precipitation amount with semi-parametric models, modeling both the bulk of the distribution and the tails, but avoiding the arbitrary choice of a threshold. We work in collaboration with Anne-Catherine Favre (LGGE-Lab in Grenoble) and Philippe Naveau (LSCE, Paris).

In the context of Philomène Le Gall's PhD thesis, we are applying the aforementioned modeling of extreme precipitation with the aim of regionalizing extreme precipitation [11].

8.8 High performance computing

Participants: Rishabh Bhatt, Matthieu Brachet, Laurent Debreu, Martin Schreiber, Arthur Vidard.

8.8.1 Dynamic compute-resource utilization

The way how applications are executed on supercomputers still follows a traditional static resource allocation pattern: Computing resources are allocated at the start of a job which executes the application and are only released at the end of the job's runtime. This still follows the way of running jobs since decades where a dynamic resource allocation over the application's runtime would lead to several benefits: higher utilization of the computing resources, ad-hoc allocation of AI accelerator cards, less energy consumption, faster response for interactive jobs, improved data locality and I/O over the full runtime, support of urgent computing without necessarily killing running jobs, etc. Various attempts have been conducted under different terminologies used such as “evolving” jobs (application-driven dynamic resource changes) and “malleability” (system-driven dynamic resource changes) where we see a hybridization of them required for reaching optimal results.

We currently investigate possibilities to extend the MPI parallel programming model (which is the de-facto standard in HPC) and also models beyond MPI with such interfaces. As part of that, we participate in regular MPI Session working group meetings where certain effort has been done to investigate such interfaces. This also resulted in some prototype implementations with an emulator [20] as well as an implementation based on PMIx [18].

8.8.2 Hardware-aware numerics

We started investigating Domain Specific Languages (DSL) for ocean simulation models targeting to close the increasing gap between the numerics and HPC with a separation of concerns: A DSL allows on the one hand applied mathematicians to express their model equations and on the other hand also HPC experts to develop tools to automatically transform this into highly performing code on the target programming model and corresponding architecture. As part of this, we started working with the PsyIR development (package of PsyClone) and successfully applied it to parsing the entire CROCO ocean model. This forms the basis for currently undergoing work to support different HPC programming models and architectures in a sustainable way for the CROCO model.

8.8.3 New time-integration methods

We investigate new time-integration methods by also taking HPC requirements into account, hence targeting a better wallclocktime vs. error ratio. These numerical methods include different forms of exponential, semi-Lagrangian as well as parallel-in-time integration methods. Our team and collaborators made significant progress on this over the last years, however, publishable results have not yet been generated or are currently in production.

As part of a collaboration with the University of São Paulo (USP), we investigated exponential integration methods based on Faber polynomials. with a preprint available [35]. Although this paper's main focus is on seismic wave propagation, these results can be also applied to the linearized fast modes in atmospheric models, e.g., as part of time splitting methods. Theoretical as well as numerical results have been deeply investigated for a variety of wave propagation problems. In [4], we have also studied in detail the application of Runge Kutta exponential integrators and its variants to shallow water equations.

In a previous work, we have been able to show significant speedups using the Parallel Full Approximation Scheme in Space and Time (PFASST) parallel-in-time method for the shallow-water equations on the rotating sphere with an IMEX-SDC scheme using benchmarks which are used for the development of dynamical cores [55]. Motivated by this work, we started to investigate this in collaboration with USP using the MGRIT parallel-in-time method where we expect to have even better results in combination with exponential time integration methods.

On variational data assimilation and parallel-in-time integration methods: Rishabh Bhatt started his PhD in December 2019. Under the supervision of Laurent Debreu and Arthur Vidard, he studies the application of time parallelization algorithms to variational data assimilation methods. Thus, at each step of the optimization algorithm, the direct model is integrated by a time-parallel method (here the Parareal algorithm [67]). One of the main difficulties lies in the choice of the stopping criterion of the Parareal algorithm. To do so, we rely on theoretical results on the convergence of conjugate gradient methods in the presence of approximate gradient calculations [52]. The first results are encouraging and show the possibility to optimally tune the stopping criterion of the Parareal algorithm (and thus the number of iterations) without affecting the convergence of the conjugate gradient. These results are reported in ([30]).

8.8.4 Variational data assimilation and parallel in time methods

Rishabh Bhatt started his PhD in December 2019. Under the supervision of Laurent Debreu and Arthur Vidard, he studies the application of time parallelization algorithms to variational data assimilation methods. Thus, at each step of the optimization algorithm, the direct model is integrated by a time-parallel method (here the Parareal algorithm [66]). One of the main difficulties lies in the choice of the stopping criterion of the Parareal algorithm. To do so, we rely on theoretical results on the convergence of conjugate gradient methods in the presence of approximate gradient calculations [52]. The first results are encouraging and show the possibility to optimally tune the stopping criterion of the Parareal algorithm (and thus the number of iterations) without affecting the convergence of the conjugate gradient. These results are reported in ([30]). We are now working on taking better advantage of the coupling of these two iterative methods (conjugate gradient and Parareal), in particular by optimally reusing the Krylov bases of the Krylov Enhanced version of the Parareal algorithm.

9 Bilateral contracts and grants with industry

9.1 Bilateral contracts with industry

- A 5-year contract (started in January 2020) 19CP07 with the Oceanographic and Hydrographic Service of the French Navy (SHOM) on the topic « Analyse numérique pour la réconciliation en espace et en temps des discrétisations des échanges air-mer et leur paramétrisation. Application à des cas simplifiés et réalistes couplés. » (PI: F. Lemarié).
- Consortium CIROQUO – Consortium Industrie Recherche pour l’Optimisation et la QUantification d’incertitude pour les données Onéreuses – gathers academical and technological partners to work on problems related to the exploitation of numerical simulators. This Consortium, created in January 2021, is the continuation of the projects DICE, ReDICE and OQUAIDO which respectively covered the periods 2006-2009, 2011-2015 and 2015-2020.
- ATOS. In the context of the French recovery plan, a collaboration with the ATOS group has been launched late 2021. This collaboration allows to have a total of 5 people working full time on topics related to the application of learning methods for ocean atmosphere problems.

9.2 Bilateral grants with industry

- Funding of Clément Duhamel’s PhD by IFP Energies nouvelles (IFPEN) within the framework of IFPEN and Inria strategic partnership. PhD subject: Robust inversion of a computer code under functional uncertainties. Application to the design of floating wind turbines.

10 Partnerships and cooperations

10.1 International initiatives

10.1.1 Inria associate team not involved in an IIL or an international program

UNQUESTIONABLE

Title: UNQUESTIONABLE

Duration: 2018 - 2020 (due to COVID 19 pandemic, the duration was extended until 2022)

Coordinator: Clémentine Prieur

Partners:

- Aerospace Computational Design Laboratory, Massachusetts Institute of Technology (United States)

Inria contact: Olivier Zahm

Summary: The ability to understand and predict the behavior of geophysical flows is of greatest importance, due to its strong societal impact. Numerical models are essential to describe the evolution of the system (ocean + atmosphere), and involve a large number of parameters, whose knowledge is sometimes really poor. The reliability of the numerical predictions thus requires a step of parameter identification. The Inria-AIRSEA team has a strong expertise in variational approaches for inverse problems. An alternative is the use of particle filters, whose main advantage is their ability to tackle non-gaussian frameworks. However, particle filters suffer from the curse of dimensionality. The main objective of the collaboration we propose between the Inria-AIRSEA team and the MIT UQ group is the understanding of potential low-dimensional structure underlying geophysical applications, then the exploitation of such structures to extend particle filter to high-dimensional applications. See also team.inria.fr/unquestionable/

10.1.2 STIC/MATH/CLIMAT AmSud projects

FANTASTIC

Title: Statistical inFerence and sensitivity ANalysis for models described by sTochASTIC differential equations

Program: MATH-AmSud

Duration: January 1, 2020 – 2022

Local supervisor: Clémentine Prieur

Partners:

- Karine Bertin (Chili)
- Jose R. Leon (Uruguay)

Inria contact: Clémentine Prieur

Summary: The general aim of our research project is to tackle probabilistic and statistical issues driven by applications. It is divided in four axes. The first one deals with sensitivity analysis for parametrized stochastic differential equations (SDE), with an application to models arising in neurosciences. The aim is to rank uncertain parameters with respect to their influence on the variability of a quantity of interest, related to the solution of the SDE. The second one is concerned with the emergence of collective behaviors in particle systems with mean field interaction. The aim for this second axis is to enlarge the class of stochastic models with collective organization features for which a mathematical analysis is possible. The two last axes are more focused to statistical issues, namely non-parametric regression estimation with Poisson and Wiener covariates and the estimation of autoregressive random processes with random sampling times. Regression estimation with Poisson covariates arises e.g., in speech recording analysis. That axis will make use of concentration inequalities for suprema of integral functionals of Poisson processes, as far hypercontractivity properties. Concerning the last axis, it seems a natural issue to be studied, as deterministic sampling is not always a reasonable assumption. Specific random times have been treated in the literature. The aim on this axis is to handle more general classes of random designs.

10.2 International research visitors

10.2.1 Visits of international scientists

Other international visits to the team

Fernando Valdes RAVELO

Status PhD Candidate

Institution of origin: University of Sao Paulo

Country: Brazil

Dates: From 2022-02-01 until 2022-07-31.

Context of the visit: Collaboration on the topic of exponential time integration method

Mobility program/type of mobility: research stay

Martin SCHULZ**Status** Full Professor**Institution of origin:** Technical University of Munich**Country:** Germany**Dates:** From 2022-10-07 until 2022-10-09.**Context of the visit:** Collaboration on the topic of exponential time integration method**Mobility program/type of mobility:** short research stay**10.2.2 Visits to international teams**

- Olivier Zahm was invited for 2 weeks at DTU in Copenhagen. This visit is part of a collaboration with the CUQI-group at DTU which support the PhD thesis of Rafael Flock, co-supervised with Yiqiu DONG and Olivier ZAHM.

10.3 European initiatives**10.3.1 H2020 projects****IMMERSE** [IMMERSE project on cordis.europa.eu](https://cordis.europa.eu)**Title:** Improving Models for Marine EnviRonment Services**Duration:** From December 1, 2018 to November 30, 2022**Partners:**

- INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET AUTOMATIQUE (INRIA), France
- PLYMOUTH MARINE LABORATORY LIMITED (PML), United Kingdom
- MET OFFICE, United Kingdom
- Puertos del Estado (EPPE), Spain
- HELMHOLTZ-ZENTRUM HEREON GMBH (HEREON), Germany
- CENTRE EUROPEEN DE RECHERCHE ET DEFORMATION AVANCEE EN CALCUL SCIENTIFIQUE (CERFACS), France
- UNITED KINGDOM RESEARCH AND INNOVATION (UKRI), United Kingdom
- OCEAN NEXT (OCEAN NEXT), France
- ALMA MATER STUDIORUM - UNIVERSITA DI BOLOGNA (UNIBO), Italy
- UNIVERSITEIT UTRECHT (UU), Netherlands
- FONDAZIONE CENTRO EURO-MEDITERRANEOSUI CAMBIAMENTI CLIMATICI (FONDAZIONE CMCC), Italy
- HELMHOLTZ-ZENTRUM FUR OZEANFORSCHUNG KIEL (GEOMAR), Germany
- INSTITUT DE RECHERCHE POUR LE DEVELOPPEMENT (IRD), France
- CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS (CNRS), France
- MERCATOR OCEAN (MERCATOR OCEAN 2), France
- BARCELONA SUPERCOMPUTING CENTER CENTRO NACIONAL DE SUPERCOMPUTACION (BSC CNS), Spain
- SORBONNE UNIVERSITE, France

Inria contact: Florian LEMARIE

Coordinator: CNRS

Summary: The overarching goal of IMMERSE project is to ensure that the Copernicus Marine Environment Monitoring Service (CMEMS) will have continuing access to world-class marine modelling tools for its next generation systems while leveraging advances in space and information technologies, therefore allowing it to address the ever-increasing and evolving demands for marine monitoring and prediction in the 2020s and beyond.

In response to the future priorities for CMEMS, IMMERSE will develop new capabilities to:

- enable the production of ocean forecasts and analyses that exploit upcoming high resolution satellite datasets,
- deliver ocean analyses and forecasts with the higher spatial resolution and additional process complexity demanded by users,
- exploit the opportunities of new high performance computing (HPC) technology
- allow easy interfacing of CMEMS products with detailed local coastal models.

These developments will be delivered in the NEMO ocean model, an established, world-class ocean modelling system that already forms the basis of the majority of CMEMS analysis and forecast products. Hence the pathway from the research in IMMERSE to implementation in CMEMS will be simple and seamless, as the model code developed will be directly applicable in CMEMS models. NEMO has a long track record of producing and maintaining a stable, robustly engineered code base of the type that is needed for operational applications, including CMEMS.

The IMMERSE consortium combines world-class expertise in ocean modelling, applied mathematics and HPC, established software engineering processes and infrastructure, and in-depth knowledge of the CMEMS systems and downstream CMEMS systems. Thus IMMERSE is exceptionally well placed to deliver the operational-quality model code required to meet the emerging needs of CMEMS, and maintain it into the future.

10.3.2 Other european programs/initiatives

- Program: C3S2
- Project acronym: ERGO2
- Project title: Advancing ocean data assimilation methodology for climate applications
- Duration: August 2022 - July 2025
- Coordinator: Arthur Vidard
- Other partners: Cerfacs (France), CNR (Italy)
- Abstract: The scope of this contract is to improve ocean data assimilation capabilities at ECMWF, used in both initialization of seasonal forecasts and generation of coupled Earth System reanalyses. In particular it shall focus on i) improving ensemble capabilities in NEMO and NEMOVAR and the use of their information to represent background error statistics; ii) extend NEMOVAR capabilities to allow for multiple resolution in multi-incremental 3D-Var; iii) make better use of ocean surface observations. It shall also involve performing scout experiments and providing relevant diagnostics to evaluate the benefit coming from the proposed developments.

10.3.3 Collaborations with Major European Organizations

- Partner : SAMO-board
- SAMO board is in charge of the organization of the SAMO (sensitivity analysis of model outputs) conferences, every three years. It is strongly supported by the Joint Research Center of the European Commission.

In 2019, Clémentine Prieur, which is part of this board, as also co-chair of a satellite event on the future of sensitivity analysis. A position paper [75] has been published in 2021, as a synthesis of the discussions hold in Barcelona (autumn 2019).

10.3.4 EuroHPC

- Martin Schreiber is a member of the TIME-X EuroHPC-01-2019 project where he's leading the research on runtime-varying computing resources to optimize the energy and resource efficiency of iterative parallel-in-time methods: time-x.eu.

10.4 National initiatives

10.4.1 ANR

- A 4-year contract: ANR MODENA, "Model and data reduction for efficient assimilation", PI: Olivier ZAHM The reliability of numerical predictions strongly rely on our ability to calibrate the unknown model parameters using observable data. Data assimilation is a particularly challenging task in ocean modelling because of the complexity of the computational models and because of the high-dimension of both the parameters and the data. The objective of this project is to explore novel methodologies to improve the probabilistic description of the Bayesian solution to inverse problem while, at the same time, taking into consideration the computational limitations imposed by large scale applications. This project relies on three building blocks and on their interplay:

1. transport maps as a novel approximation tool of complex probability densities,
2. reduced order models to alleviate the computational burden of expensive models and
3. dimension reduction to concentrate the computational efforts onto the most relevant directions.

In addition, the proposed methodology addresses key challenges present in many real-world applications and therefore we expect that they can find applications in other domains.

- A 4-year contract: ANR ADOM (Asynchronous Domain decomposition methods) anr.fr/Projet-ANR-18-CE46-0008
- A 5-year contract: ANR MELODY (Bridging geophysics and Machine Learning for the modeling, simulation and reconstruction of Ocean Dynamic) anr.fr/Projet-ANR-19-CE46-0011
- A 5-year contract with the French Navy (SHOM) on the improvement of the CROCO ocean model www.croco-ocean.org.
- **Title:** MEDIATION. Methodological developments for a robust and efficient digital twin of the ocean.

Duration: 2022-2027

Funding: French priority research program (PPR) "Ocean and Climate"

Partners: – Inria (DATAMOVE and ODYSSEY teams)

- CNRS
- IFREMER
- IMT-Atlantique
- IRD
- Météo-France
- SHOM
- Univ. Grenoble Alpes
- Univ. Aix-Marseille.

Inria contact: Laurent Debreu

Coordinator: Laurent Debreu

Summary: The MEDIATION project targets two questions: how will global change impact the functioning of regional marine ecosystems, and how to evaluate the effect of measures to preserve the environment? With two main demonstrators on the French coasts (Atlantic and Mediterranean), MEDIATION combines methodological developments in numerical sciences (taking into account uncertainties, high performance computing and artificial intelligence) with advances in the modeling of physical, biogeochemical and biological processes in the ocean. It aims at setting up a modeling chain, integrating data and allowing to significantly increase the number of scenarios (climate change, human activities) evaluated. The digital tools developed will also contribute to a better science-society-policy interaction

10.4.2 Inria Challenge

- Sea Uncertainty Representation and Forecast (SURF),
- Coord : Airsea (A. Vidard),
- Partenaires Inria : Ange, Cardamom, Fluminance, Lemon, Mingus, Defi
- Partenaires extérieurs: BRGM, Ifremer, SHOM

10.4.3 Other Initiatives

- A 3-year contract (started in Sept 2021) funded by the *Institut des Mathématiques pour la Planète Terre* (IMPT) on the topic "Modélisation cohérente des échelles sous-maille pour les modèles océaniques de climat" (PI: F. Lemarié).
- E. Blayo is co-advising the PhD thesis of Valentin Bellemin-Laponnaz with IGE Lab, in the framework of the NASA-CNES working group on the SWOT satellite.
- C. Prieur is co-advising the PhD thesis of Henri Mermoz Kouye, in the framework of the Inria-INRA partnership.
- C. Prieur chaired GdR MASCOT NUM 2010-2017, in which are also involved M. Nodet, E. Blayo, C. Helbert, E. Arnaud, L. Viry, S. Nanty, L. Gilquin. She is still strong involved in the group (co-chair). In particular, she will co-chair next GdR annual meeting in Aussois (May 2020, reported to April 2021).

11 Dissemination

Participants: Elise Arnaud, Eric Blayo, Laurent Debreu, Christine Kazantsev, Florian Lemarie, Clémentine Prieur, Martin Schreiber, Arthur Vidard, Olivier Zahm.

11.1 Promoting scientific activities

11.1.1 Scientific events: organisation

- Martin Schreiber organized the "1st EuroHPC Workshop on Malleability in HPC"

11.1.2 Scientific events: selection

Member of the conference program committees

- Martin Schreiber, International Conference on Computational Science (ICCS)
- Martin Schreiber, Euro-Par Conference (EUROPAR)

- Martin Schreiber, International Workshop on OpenCL (IWOCL)
- Clémentine Prieur is a member of the scientific committee of the international SAMO conference.
- Clémentine Prieur is a member of the scientific committee of the next international MASCOT NUM conference (to be held in Le Croisic).

Reviewer

- Martin Schreiber, International Conference on Computational Science (ICCS)
- Martin Schreiber, Workshop on “Malleability Techniques Applications in High-Performance Computing” (HPCMALL)

11.1.3 Journal

Member of the editorial boards

- F. Lemarié is associate editor of the Journal of Advances in Modeling Earth Systems (JAMES)
- Clémentine Prieur is associate editor for Computational and Applied Mathematics journal.
- Clémentine Prieur is associate editor for SIAM/ASA Journal of Uncertainty Quantification journal.
- Clémentine Prieur is a member of the reading committee of Annales Mathématiques Blaise Pascal.

Reviewer - reviewing activities

- Martin Schreiber: Journal of High-Performance Computing Applications, Journal of Computational Science.
- Olivier Zahm: Statistics and Computing (STCO), Mathematics of Computation (Math Comp), SIAM Journal of Scientific Computing (SISC), SIAM/ASA Journal on Uncertainty Quantification (JUQ).
- Other permanent members of the Airsea team are also regular reviewers for numerous international journals.

11.1.4 Invited talks

- Eric Blayo was invited as plenary speaker of the workshop "Coastal flow models and boundary conditions" , Toulouse, October 24-27, 2022.
- Elise Arnaud : "Parameter control in the presence of uncertainties", workshop Machine learning and uncertainties in climate simulations, centre Henri Lebesgue, Mon, 06/06/2022 - 06/09/2022 - Logonna-Daoulas, Finistère, France
- Martin Schreiber: Nov. 2022, Enabling I/O and Computation Malleability in High-Performance Computing: Application perspective on dynamic resources, Birds of Feather, Supercomputing 2022, Dallas, Texas, USA
- Martin Schreiber: Oct. 2022, Invasive Computing - Part IX: Return of the Jedi, InvasIC Colloquium, Erlangen, Germany
- Martin Schreiber: Nov. 2022, A Brief Glimpse on Emerging (Parallel-in-)Time Integration Methods for Weather and Climate Simulations, Seminar, University of Colorado Boulder, USA
- Martin Schreiber: Jul. 2022, A Brief Glimpse on Some Emerging (Parallel-in-)Time Integration Methods for Weather and Climate Simulations, International Conference on Scientific Computation and Differential Equations (SciCADE), Reykjavík, Iceland, Minisymposium

- Martin Schreiber: Jun. 2022, A Brief Glimpse on Emerging Time Integration Methods for Weather and Climate Simulations, Seminar series, Université de Pau, France
- Martin Schreiber: May 2022, Using Artificial Neural Network to solve PDEs? International Supercomputing Conference, Panel discussion, Hamburg, Germany, presentation as panel member
- Clémentine Prieur was invited as plenary speaker SAMO 2022 (Florida, US).
- Clémentine Prieur was invited as plenary speaker at SFdS annual conference in Lyon, 2022, France.
- Clémentine Prieur was invited as plenary speaker of the conference in honor of Marc Lavielle and Jose R. León (Montevideo, Uruguay, 2022).

11.1.5 Leadership within the scientific community

- L. Debreu is the chair of the CNRS-INSU research program LEFE-MANU on mathematical and numerical methods for ocean and atmosphere https://programmes.insu.cnrs.fr/lefe/cs_actions/manu since April 2018.
- F. Lemarié is the co-leader with Mike Bell (UK Met Office) of the NEMO (www.nemo-ocean.eu) Working Group on numerical kernel development.

11.1.6 Scientific expertise

- L. Debreu is a member of the steering committee of the CROCO ocean model www.croco-ocean.org
- L. Debreu is a member of the evaluation committee of the axis Interfaces: mathematics, numerical sciences - earth and and environmental sciences of the French National Research Agency.
- E. Blayo is a member of the ANR selection committee CE40
- F. Lemarié is a member of the CROCO (www.croco-ocean.org) scientific committee in charge of the "numerical methods" topic.
- Martin Schreiber is a member of the MPI Forum (representing the Université Grenoble Alpes) and in particular active in the MPI Session workgroup.
- As part of the TIME-X project, Martin Schreiber is responsible for organizing and determining possible collaboration topics with other EuroHPC-19 projects.
- Martin Schreiber was an external reviewer of the “Neue Methoden und Technologien für das Exascale-Höchstleistungsrechnen” (SCALEXA) funding program from Germany: www.bmbf.de

11.1.7 Research administration

- E. Blayo is a deputy director of the Jean Kuntzmann Lab.
- C. Prieur is local correspondent in Grenoble for the Mathematical Society of France (SMF).
- C. Prieur is a member of the MSTIC pole council of UGA.
- C. Prieur is responsible for the applied math speciality for doctoral school MSTII edinstii.univ-grenoble-alpes.fr

11.2 Teaching - Supervision - Juries

11.2.1 Teaching

- Licence (ou équivalent) : E. Arnaud, Mathematics for engineers, 50h, L2, UGA, France
- Licence (ou équivalent) : E. Arnaud, Statistics, 20h, L2, UGA, France
- Licence (ou équivalent) : E. Blayo, analysis and algebra, 145h, L1, University Grenoble Alpes, France
- Licence (ou équivalent) : C. Kazantsev, Mathématiques approfondies pour l'ingénieur, 72h, L2, UGA, France
- Licence (ou équivalent) : C. Kazantsev, Mathématiques pour les sciences de l'ingénieur, 45h, L2, UGA, France
- Licence (ou équivalent) : Martin Schreiber, Advanced Analysis & Algebra, L1, 67.5h, UGA, France
- Licence (ou équivalent) : Martin Schreiber, Analysis, L1, 37h, UGA, France
- Master (ou équivalent) : E. Arnaud, Statistics, 30h, M1, UGA, France
- Master (ou équivalent) : E. Arnaud, Supervision of student in apprenticeship, 30h, M2, UGA, France
- Master (ou équivalent) : E. Blayo, Partial Differential Equations, 18h, M1, University Grenoble Alpes, France
- Master (ou équivalent) : Martin Schreiber, High-Performance Computing, M1, 31.1h, UGA, France
- Master (ou équivalent) : Martin Schreiber, Object oriented programming with C++, M1, 18h, UGA, France
- Master (ou équivalent) : Martin Schreiber, Partial differential equations, M1, 34.5h, UGA, France
- Master (ou équivalent) : Olivier ZAHM, PDE for finance and Geostatistics , 4h, Ensimag, France
- E-learning : E. Arnaud is in charge of the pedagogic platform math@uga : implementation of a collaborative moodle platform math.u-ga.fr to share pedagogical resources within teachers and towards students.
- E. Blayo is in charge of the Ecole des Mathématiques Appliquées: organization and coordination of pedagogical and administrative aspects related to teaching for the applied maths department.

11.2.2 Supervision

- Master 2 internship : Exaucé Luweh Adjim Ngarti (supervision : Elise Arnaud and Arthur Vidard)
- Engineer : Aurélien Prat, Multi-resolution techniques for ocean data assimilation, July 2021, December 2022, A. Vidard
- PhD in progress: Manolis Perrot, Consistent subgrid scale modeling for oceanic climate models. October 2021, E. Blayo and F. Lemarié.
- PhD in progress: Pierre Lozano, Coupling hydrostatic and nonhydrostatic ocean circulation models. October 2022, E. Blayo and L. Debreu
- PhD in progress : Qiao CHEN, Low-dimensional structure of ocean data assimilation problems via gradient information, Octobre 2021, Olivier ZAHM and Élise Arnaud.
- PhD in progress: Benjamin Zanger, Compositional surrogates for reduced order modeling, Septembre 2022, M. Schreiber, O. Zahm

- PhD in progress: Dominik Huber, “Dynamic Resource Management with MPI Sessions and PMIX” (preliminary title), PhD candidate at the Technical University of Munich (TUM), M. Schulz (TUM), M. Schreiber
- PhD in progress: Fernando V. Ravelo, PhD candidate at the University of Sao Paulo (USP), P. Peixoto (USP), M. Schreiber
- PhD in progress : Ri Wang, Apprentissage statistique pour l’analyse de sensibilité globale avec entrées dépendantes, October 2021, V. Maume-Deschamps (Université Lyon 1), C. Prieur.
- PhD in progress : Robin Vaudry, Analyse de Sensibilité, quantification d’incertitudes et calibration pour des modèles épidémiologiques structurés, October 2021, D. Georges (Grenoble INP), C. Prieur.
- PhD in progress : Clément Duhamel, Inversion robuste d’un code de calcul prenant en entrée des données de nature fonctionnelle. Application à la conception d’éoliennes, October 2020, C. Helbert (Ecole Centrale Lyon), C. Prieur, promoted by M. Munoz Zuniga, D. Sinoquet (IFPEN)
- PhD in progress : Rafael Floch, Dimension reduction of large-scale linear Bayesian inverse problems, Octobre 2021, Olivier ZAHM et Yiqiu DONG.
- PhD in progress : Romain Verdière, Nonlinear dimension reduction for uncertainty quantification problems, Septembre 2022, Olivier ZAHM et Clémentine PRIEUR
- PhD in progress : Antoine Nasser, Volume penalization methods for the representation of flows along topography in 3D ocean models, October 2019, L. Debreu and G. Madec.
- PhD in progress : Rishabh Bhatt, Asynchronous parallel in time schemes for data assimilation, December 2019, L. Debreu and A. Vidard.
- PhD in progress: Emilie Rouziès, Assimilation of multi-source data in a pesticide transfer model in a small agricultural watershed, Université Grenoble-Alpes, December 2019, C. Lauvernet (Inrae) and A. Vidard.
- PhD in progress: Katarina Radisic, Prise en compte d’incertitudes externes dans l’estimation de paramètres d’un modèle de transfert d’eau et de pesticides à l’échelle du bassin versant, Université Grenoble-Alpes December 2021, C. Lauvernet (Inrae) and A. Vidard.
- PhD : Emilie Duval, Coupling hydrostatic and nonhydrostatic ocean circulation models. October 2018 - December 2022, L. Debreu and E. Blayo.
- PhD : Henri Mermoz Kouye, Analyse de sensibilité basée sur les indices de Sobol’ pour modèles à sorties stochastiques et fonctionnelles, [26] Octobre 2019, G. Mazo, E. Vergu (INRAE, MIA, Jouy), C. Prieur. Defended in December, 2022.
- PhD: Simon Clément, Numerical analysis for reconciling in space and time the air-sea exchanges and their parameterization, [25] Université Grenoble-Alpes, defended on 23 November 2022, E. Blayo and F. Lemarié.

11.2.3 Juries

- E. Blayo:
 - Oct. 4, 2022: HDR thesis of Pierre Jolivet, Institut National Polytechnique de Toulouse (president)
 - Dec. 9, 2022: PhD thesis of Hugo Frezat, University Grenoble Alpes (president)
- Martin Schreiber:
 - July 1st 2022: PhD thesis of Sebastian FRIEDEMANN, Université Grenoble Alpes (president)
 - Nov. 23rd 2022: PhD thesis of Simon CLEMENT, Université Grenoble Alpes (president)

- Dec. 15th 2022: PhD thesis of Emilie DUVAL, Université Grenoble Alpes (president)
- E. Arnaud, Dec.14, 2022: PhD thesis of Francois-Remi Mazy, UGA.
- C. Prieur is jury president of Prix de thèse AMIES (2020-2022).

11.3 Popularization

11.3.1 Internal or external Inria responsibilities

- F. Lemarié is a member of the local "comité des emplois scientifiques" (CES) (since Sept 2019)
- F. Lemarié is the local scientific correspondent for national calls for projects (since July 2020)
- E. Arnaud : member of Inria PhD recruitment committee CORDI-S
- E. Arnaud : in charge of the parity commission at Jean Kuntzmann Lab

11.3.2 Articles and contents

- Clémentine Prieur took part to a webcast on [The Future of Sensitivity Analysis for Systems Modelling and Policy Support](#)
- Clémentine Prieur gave interviews as a CNRS expert (Figaro, Hoffpost, RCF) on the evolution of COVID19 pandemic.
- C. Prieur was placed on a list of experts who could answer questions on various aspects of the news related to the ongoing Covid-19 epidemic by the CNRS press office. This list is made available to journalists in order to direct them to the appropriate interlocutors according to the angle of their questions.

11.3.3 Education

- Ch. Kazantsev and E. Blayo are strongly involved in the creation and dissemination of pedagogic suitcases with mathematical activities designed for primary and secondary schools, as well as an escape game. These activities were used by more than 12,000 pupils in 2021-2022, despite the sanitary crisis. This is done in collaboration with the Rectorat de Grenoble.
- C. Kazantsev is a member of an IREM group for creation of scientific activities for professional development of secondary schools teachers.
- C. Kazantsev is a member of an International Inter-IREM commission, which work on the multi-languages problem for children in the mathematical learning. Three meetings take place in Paris during the year, the first was on October 1.

11.3.4 Creation of media or tools for science outreach

- C.Kazantsev participated in the edition of the Teachers notebooks which explain and advise how to use the "La Grange Suitcases" (sets of mathematical games, problems and animations) destined for primary and secondary schools teachers as well as for the general public.
- C.Kazantsev participated in the creation of mathematical activities that can be autonomously used by schoolchildren of primary and secondary schools and by the general public.
- C.Kazantsev participated in the creation of a mathematical serious game that can be played by schoolchildren of secondary schools and by the general public. See www.la-grange-des-maths.fr/mission-exoplanetes/

- C.Kazantsev participated in the creation of a mathematical exposition on Johannes Kepler : "Kepler, les maths pour décrire le monde", in collaboration with Jean-Louis Hodeau, a cristallographer of the Neel Institut and CNRS (Grenoble, France). This exposition was visited on the fête de la science by schoolchildren of secondary schools and by the general public.
- C.Kazantsev had encadred for 3 months a L3 student who participates to the creation of a mathematical activity for secondary schools children.

11.3.5 Interventions

- E. Blayo gave several outreach talks, in particular for middle school and high school students, and for more general audiences.
- E. Arnaud has given a seminar "(se) tromper avec les chiffres", for secondary school students

12 Scientific production

12.1 Publications of the year

International journals

- [1] M. Belén Heredia, C. Prieur and N. Eckert. 'Global sensitivity analysis with aggregated Shapley effects, application to avalanche hazard assessment'. In: *Reliability Engineering and System Safety* 222.108420 (June 2022), pp. 1–11. DOI: [10.1016/j.ress.2022.108420](https://doi.org/10.1016/j.ress.2022.108420). URL: <https://hal.archives-ouvertes.fr/hal-02908480>.
- [2] D. Bigoni, Y. Marzouk, C. Prieur and O. Zahm. 'Nonlinear dimension reduction for surrogate modeling using gradient information'. In: *Information and Inference* (14th May 2022). URL: <https://hal.inria.fr/hal-03146362>.
- [3] M. Billaud-Friess, A. Macherey, A. Nouy and C. Prieur. 'A PAC algorithm in relative precision for bandit problem with costly sampling'. In: *Mathematical Methods of Operations Research* 96 (2022), pp. 161–185. DOI: [10.1007/s00186-022-00769-x](https://doi.org/10.1007/s00186-022-00769-x). URL: <https://hal.archives-ouvertes.fr/hal-03139679>.
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- [26] H. M. Kouye. ‘Sensitivity analysis approaches for stochastic models. Application to compartmental models in epidemiology’. Université Paris - Saclay, 2nd Dec. 2022. URL: <https://theses.hal.science/tel-03883271>.

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- [28] R. Baptista, Y. Marzouk and O. Zahm. *Gradient-based data and parameter dimension reduction for Bayesian models: an information theoretic perspective*. 29th Nov. 2022. URL: <https://hal.inria.fr/hal-03877649>.
- [29] R. Baptista, Y. Marzouk and O. Zahm. *On the representation and learning of monotone triangular transport maps*. 30th Jan. 2023. URL: <https://hal.inria.fr/hal-03060198>.
- [30] R. Bhatt, L. Debreu and A. Vidard. *Introducing time parallelisation within data assimilation using parareal method*. 6th Apr. 2022. URL: <https://hal.inria.fr/hal-03540480>.
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- [32] C. Duhamel, C. Helbert, M. M. Zuniga, C. Prieur and D. Sinoquet. *A SUR version of the Bichon criterion for excursion set estimation*. 19th Sept. 2022. URL: <https://hal.archives-ouvertes.fr/hal-03780559>.
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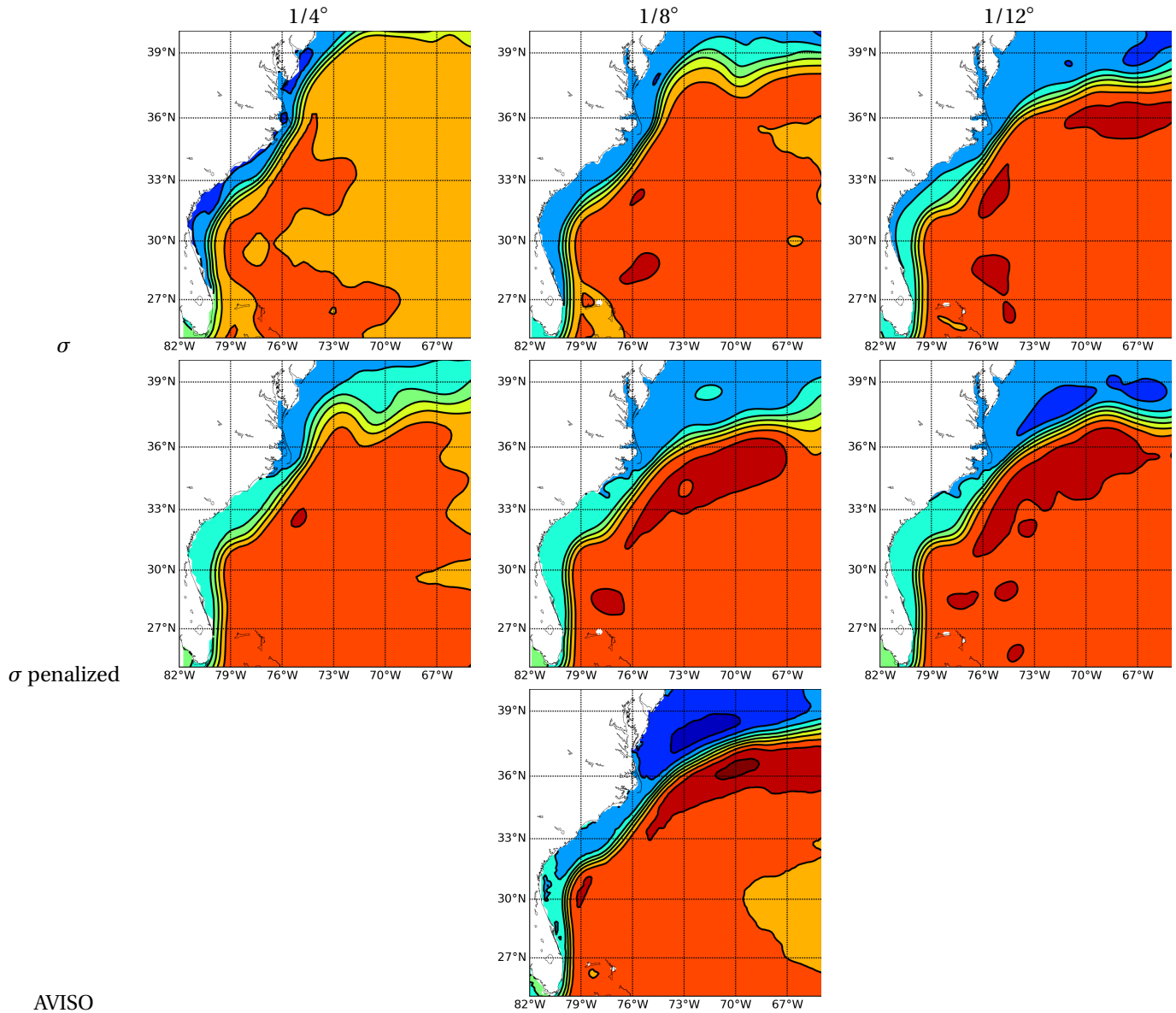


Figure 1: Mean sea surface height in CROCO simulations at different resolutions for the standard case with terrain-following (σ) coordinates (top) and penalization (below). The third row shows the AVISO product for comparison