Alexandre Hoffmann

Postdoctoral Research Scientist

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Date of Birth: 11th July 1990

General presentation

Education

2018 **PhD thesis in applied mathematics**, *Docking Flexible Proteins using Polynomial Expansions*, supervised by Valérie Perrier and Sergei Grudinin, Grenoble Alpes University, Laboratoire Jean Kuntzmann, INRIA, Grenoble, France.

2014 **Master 2 Mathematics, Informatics and Applications**, *Specialization: Modeling and scientific calculus*, Joseph Fourier University, Grenoble, France.

2013 **Master 1 Applied and Industrial Mathematics**, *Joseph Fourier University*, Grenoble, France.

2012 **Bachelor in Mathematics and Computer science**, *Joseph Fourier University*, Grenoble, France.

Work Experience

2022-now **Post-doc position**, *Studying the impact of numerical precision on Krylov methods*, supervised by Yves Durand, CEA-List, Grenoble, France, CEA, Grenoble, France.

2020-2022 **Post-doc position**, *Full waveform inversion (FWI) uncertity quantification*, supervised by Ludovic Métivier and Romain Brossier, Grenoble Alpes University, Institut des Sciences de la Terre, UGA, Grenoble, France.

2018-2020 **Post-doc position**, *Developping new methods for the FWI problem*, supervised by Dimitri Komatitsch, Vadim Monteiller and Cédric Bellis, Aix Marseille Univesity, Laboratoire de Mécanique et d'Acoustique, CNRS, Marseille, France.

April 2014 **Research internship**, *ISTerre (Institute of Earth Sciences)*, Grenoble, France.
August 2014 We improved a high-performance computing code that computes the mass redistribution of the earth in a 3D sphere. The final goal was to use this code during the simulation of seismic waves. We used the spectral element method and implemented our code in Fortran with the MPI library. This internship was supervised by Emmanuel Chaljub.

April 2013 **Research internship**, *INRIA*, Grenoble, France.
August 2013 We carried out the research on how to use Hermite functions in cryo-electron microscopy reconstruction and fitting algorithm. The code was implemented in Matlab and C++. This internship was supervised by Sergei Grudinin.

Mai 2012 **Research internship**, *Laboratoire Jean Kunzmann*, Grenoble, France.
July 2012 We implemented several 2D interpolation methods and studied their impact on the advection/diffusion of a passive plotter. The internship was supervised by Vincent Chabot, Maëlle Nodet, and Arthur Vidard. The code was implemented in Fortran and Matlab.

Honors & Awards

May 2017 **Cover for a scientific journal**, *Journal of Chemical Theory and Computation*, Volume 13, Number 5, Pages 1867-2366.

August 2017 **Cover for a scientific journal** , *Journal of Applied Crystallography*, Volume 50, Number 4, Pages 1036-1047.

Language skills

French Native

English Fluent

Spanish Basic

Computer skills

Languages C, C++, C#, Java, Fortran, Python, Matlab, Scilab

Libraries MPI(C), OpenMP(C), Gtk+(C), QT(C++), Eigen(C++), Armadillo(C++)

Research

PhD project

2014-2018 I worked with Nano-D research team. Nano-D is a laboratoire Jean Kuntzmann and INRIA research team, which develops algorithms for Modelling and Simulation of Nanosystems. My doctoral thesis focused on algorithm designs for system modelling for Proteins and Macromolecular assemblies. My research consisted of two main parts.

Fast Fourier transform accelerated exhaustive search.

Our goal was to extend the fast Fourier transform-based exhaustive search method, applied so far to 6D rigid bodies degrees of freedom (DOFs), to the off-grid rigid and flexible DOFs. We started by exhaustively sampling the rigid off-grid DOFs and later implemented flexible global DOFs, which were obtained using the normal mode analysis (NMA). The first part has been presented in [C6, C7] and published in [A7]. The later part has been presented in [C5, C4, C3].

Large scale global molecular motions.

We proposed a method for nonlinear NMA called NOLB [A6], which relies on the theoretical basis of the rotations-translations of blocks method. Overall, our method produces better structures compared with the standard approach, especially at large deformation amplitudes. To the best of our knowledge, this was the first work on non-linear normal mode extrapolation in the Cartesian space. This work has been presented and published in [C2, C5, A6]. And later applied to root-mean-square deviation computation [A5], flexible fitting [A4], functional motions prediction [A3]

Post-doctoral research

2018-now My post-doctoral research was focused on working on two aspects the full waveform inversion (FWI) inverse problem.

The optimization part of the FWI.

I first worked on the optimization part of the problem within the Laboratoire de Mécanique et d'Acoustique under the supervision of Dimitri Komatitsch, Vadim Monteiller and Cédric Bellis. We first proposed a robust FWI algorithm [A2]. The method produced excellent results on difficult synthetic problems with strong contrasts, even when low frequency data were not available. The standard method was unable to solve this problem du to cycle-skipping. We are currently working on another optimization algorithm that uses both a trust region method and tools from image processing to regularize the FWI.

Uncertainty quantification for FWI.

I then worked on the uncertainty quantification for the FWI within the Institut des Sciences de la Terre under the supervision of Ludovic Métivier and Romain Brossier. We worked on a time domain ensemble-FWI scheme that uses an ensemble transform Kalman filter to estimate the uncertainty of a FWI scheme. Our work was applied to a North Sea ocean-bottom-cable data-set [A1, P2].

Extended precision for numerical methods.

I'm currently working on the impact of numerical precision on Krylov solvers CEA-List under the supervision of Yves Durand. We first showed how numerical precision can speedup the convergence of both bi-conjugate gradient and quasi-minimal residual solvers for the wave equation, especially when it is discretized with high-order spectral element method [P1]. We are currently working on a FWI inspired exampled with block and global Krylov methods.

International Collaboration

Research Collaboration between the NANO-D team (INRIA, Grenoble, France) and ABC team (Stony Brook University, New York,USA). The aim of this project was to evaluate the poses given by a docking algorithm based on this energy transfer between binding sites.

Participation in scientific challenges

January 2016 – 17 June 2016 **EMDataBank Model Challenge**, `http://challenges.emdatabank.org/`.
This challenge was organized by a comity from the three-dimensional electron microscopy community, which aims to highlight the need for tools of validation during the study by electron microscopy. We participated in the model challenge, which consists in generating models using the provided densities.

Other research activities

SMAI Conference, *8-12 juin 2015*, Azureva Les Karellis, France.

Winter School, Algorithm in Structural Bioinformatics, *8-12 December 2014*, Inria Sophia Antipolis, France.

Publications and scientific presentations

Journals

[A1] L. Metivier et al. "Anisotropic diffusion filter for 3D full waveform inversion: application to a North Sea dataset". In: 2023.1 (2023), pp. 1–5.

[A2] Alexandre Hoffmann, Vadim Monteiller, and Cédric Bellis. "A penatly-free approach to PDE constrained optimization: Application to an inverse wave problem". In: *Inverse Problems* (Feb. 2021).

[A3] Sergei Grudinin, Elodie Laine, and Alexandre Hoffmann. "Predicting Protein Functional Motions: an Old Recipe with a New Twist". In: *Biophysical Journal* 118.10 (May 2020), pp. 2513–2525.

[A4] Sergei Grudinin et al. "Flexible fitting of macromolecular structures into small-angle scattering (SAXS and SANS) profiles". In: *Acta Crystallographica Section A Foundations and Advances* 74.a2 (Aug. 2018), e180–e180.

[A5] Emilie Neveu et al. "RapidRMSD: rapid determination of RMSDs corresponding to motions of flexible molecules". In: *Bioinformatics* 34.16 (Mar. 2018). Ed. by Alfonso Valencia, pp. 2757–2765.

[A6] Alexandre Hoffmann and Sergei Grudinin. "NOLB: Nonlinear Rigid Block Normal-Mode Analysis Method". In: *Journal of Chemical Theory and Computation* 13.5 (Apr. 2017). (cover publication), pp. 2123–2134.

[A7] Alexandre Hoffmann, Valérie Perrier, and Sergei Grudinin. "A novel fast Fourier transform accelerated off-grid exhaustive search method for cryo-electron microscopy fitting". In: *Journal of Applied Crystallography* 50.4 (June 2017). (cover publication), pp. 1036–1047.

In preparation

[P1] A. Hoffmann, Y. Durand, and J. Fereyre. "Accelerating Spectral Elements Method with Extended Precision: A Case Study". In: *International Journal of Applied Physics and Mathematics* (To be published).

[P2] Alexandre Hoffmann et al. "Uncertainty quantification for 3D time-domain full waveform inversion with ensemble Kalman filters: application to a North sea OBC dataset". In: *Geophysical Journal International* (Submited).

Distributed software

[S1] Alexandre Hoffmann. *LightFEM*. `https://github.com/alexandrehoffmann/LightFEM`. 2022.

[S2] Alexandre Hoffmann and Sergei Grudinin. *NOLB Normal Modes*. `https://team.inria.fr/nano-d/software/nolb-normal-modes/`. 2017.

[S3] Alexandre Hoffmann and Sergei Grudinin. *OffGridFit*. `https://team.inria.fr/nano-d/software/offgridfit/`. 2017.

Scientific presentations

[C1] Alexandre Hoffmann. *Some work on FWI.* Oral presentation at Avignon Université - UMR EMMAH. Avignon, France, Nov. 2021.

[C2] Sergei Grudinin. *On the non-linear normal mode analysis and its applications.* Oral presentation at the GGMM conference. Reims, France, May 2017.

[C3] Alexandre Hoffmann. *On FFT-Accelerated Flexible Exhaustive Search for Cryo-EM Fitting.* Oral presentation at the CryoEM Structure Challenges Workshop. Stanford University, USA, Oct. 2017.

[C4] Alexandre Hoffmann and Sergei Grudinin. *FFT-accelerated exhaustive flexible fitting method.* Poster presentation at the GGMM conference. Reims, France, May 2017.

[C5] Alexandre Hoffmann and Sergei Grudinin. *FFT-accelerated exhaustive flexible fitting method.* Oral presentation at the MAPPING Conference. Lyon, France, Apr. 2017.

[C6] Alexandre Hoffmann and Sergei Grudinin. *Towards FFT-accelerated off-grid search with applications to structural bioinformatics.* Poster presentation at the JOBIM Conference. Lyon, France, June 2016.

[C7] Alexandre Hoffmann and Sergei Grudinin. *Towards FFT-accelerated off-grid search with applications to structural bioinformaticss.* Poster presentation at the CAPRI Conference. Tel-Aviv, Israel, Apr. 2016.

Teaching

2016-2017 **teaching undergraduate tutorial classes (TC) and practical work (PW) (54-hour of teaching per year).**, *Grenoble Alpes university*, national school of computer science and Applied Mathematics (ENSIMAG) and the département licence sciences et technologies (DLST), Grenoble, France.

2023 **teaching undergraduate TC and PW (33-hour).**, *Grenoble Alpes university*, DLST, Grenoble, France.

Courses	Chain	TC	PW
Basic numerical methods	first year ENSIMAG	33	
Analysis [Scilab]	first year ENSIMAG		12
Analysis remedial	first year ENSIMAG	33	
Modeling and programming [C++]	second year ENSIMAG		9
Introduction to applied math [Scilab]	first year DLST		21
Algorithmics and imperative programming [C]	second year DLST	16.5	16.5

Hobbies

2022-now Initiateur snowboard-alpi au Club Alpin Français

2022-2024 Responsable activité pour la section snowboard-alpi au Club Alpin Français