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).

Large scale global molecular motions.

We proposed a method for nonlinear NMA called NOLB [**?**], 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 was applied to root-mean-square deviation computation, flexible fitting, functional motions prediction.

Post-doctoral research

2018-2020 **The optimization part of the FWI**.

I first worked on the optimization part of full waveform inversion (FWI) 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. 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.

2020-2022 **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.

2022-now **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 [**?**]. 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 **EMDataBank Model Challenge**, `http://challenges.emdatabank.org/`.

17 June 2016 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

Publications under review

[R1] **Hoffmann, A., Durand, Y. & Fereyre (Submited)**, *Stabilizing the Block Bi-Conjugate Gradient Solver with Extended Precision: A Case Study*, EEE International Symposium on Computer Arithmetic.

[R2] **Hoffmann, A., Durand, Y. & Fereyre (Accepted)**, *Accelerating Spectral Elements Method with Extended Precision: A Case Study.*, International Journal of Applied Physics and Mathematics.

International journals

[J1] **Hoffmann, A., Brossier, R., Métivier, L., & Tarayoun, A. (2024)**, *Local uncertainty quantification for 3D time-domain full waveform inversion with ensemble Kalman filters: application to a North sea OBC dataset*, Geophysical Journal International, ggae114.

[J2] **Métivier, L., Brossier, R., Hoffmann, A., Mirebeau, J. M., Provenzano, G., Tarayoun, A., & Yong, P. (2024)**, *Coherence-enhancing anisotropic diffusion filter for 3D high-resolution reconstruction of P-wave velocity and density using full-waveform inversion: Application to a North Sea ocean bottom cable data set*, Geophysics, 89(1), R33-R58.

[J3] **Hoffmann, A., Monteiller, V., & Bellis, C. (2021)**, *A penalty-free approach to PDE constrained optimization: application to an inverse wave problem*, Inverse Problems, 37(5), 055002.

[J4] **Grudinin, S., Laine, E., & Hoffmann, A. (2020)**, *Predicting protein functional motions: an old recipe with a new twist*, Biophysical journal, 118(10), 2513-2525.

[J5] **Grudinin, S., Hoffmann, A., Martel, A. & Prevost, S. (2018)**, *Flexible fitting of macromolecular structures into small-angle scattering (SAXS and SANS) profiles*, Acta Crystallographica Section A Foundations and Advances, 74(a2):e180–e180.

[J6] **Neveu, E., Popov, P., Hoffmann, A., Migliosi, A., Besseron, X., Danoy, G., ... & Grudinin, S. (2018)**, *RapidRMSD: Rapid determination of RMSDs corresponding to motions of flexible molecules*, Bioinformatics, 34(16), 2757-2765.

[J7] **Hoffmann, A., & Grudinin, S. (2017)**, *NOLB: Nonlinear rigid block normal-mode analysis method*, Journal of chemical theory and computation, 13(5), 2123-2134.

[J8] **Hoffmann, A., Perrier, V., & Grudinin, S. (2017)**, *A novel fast Fourier transform accelerated off-grid exhaustive search method for cryo-electron microscopy fitting*, Journal of Applied Crystallography, 50(4), 1036-1047.

Reviewed international conferences

[C1] **Metivier, L., Brossier, R., Hoffmann, A., Mirebeau, J., Provenzano, G., Tarayoun, A., & Yong, P. (2023, June)**, *Anisotropic diffusion filter for 3D full waveform inversion: application to a North Sea dataset*, In 84th EAGE Annual Conference & Exhibition (Vol. 2023, No. 1, pp. 1-5), European Association of Geoscientists & Engineers.

Other international publications

[O1] **Hoffmann, A. & Grudinin, S. (2017 May)**, *FFT-accelerated exhaustive flexible fitting method*, Poster presentation at the GGMM conference, Reims, France.

[O2] **Hoffmann, A. & Grudinin, S. (2016 April)**, *Towards FFT-accelerated off-grid search with applications to structural bioinformaticss*, Poster presentation at the CAPRI Conference, Tel-Aviv, Israel.

Distributed software

[S1] **Hoffmann, A.**, *LightFEM*, Light weight expression template based high order finite element library, `github.com/alexandrehoffmann/LightFEM`.

[S2] **Hoffmann, A. & Grudinin, S.**, *NOLB Normal Modes*, NOn-Linear rigid Block NMA approach (NOLB) a new conceptually simple and computationally efficient method for non-linear normal mode analysis., `githubhttps://team.inria.fr/nano-d/software/nolb-normal-modes/`.

[S3] **Hoffmann, A. & Grudinin, S.**, *OffGridFit*, OffGridFit is a novel FFT-based exhaustive search method extended to off-grid translational and rotational degrees of freedom, `https://team.inria.fr/nano-d/software/offgridfit/`.

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