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POST - DOCTORATE IN
COMPUTATIONAL SCIENCE
DRIVEN BY
NATURAL SCIENCE APPLICATIONS
AND SCIENCE FOSTERING

Motivations and Expertises

to enrich natural science by learning from data and physics laws

numerics	*Learning* - inverse problems, data assimilation, machine learning, non convex optimisation, cross-validation tests
	Big Data - complex physics, large amount of physical information and observations, statistics of errors
	Accuracy - convergence analysis, discretisation schemes to solve partial differential equations, frequency analysis, data analysis
	Numerical Efficiency - parsimony, linear algebra, multigrids, Fast Fourier transform, polynomial expansion
	Algorithmic Development - programming, object-oriented, code optimisation, distributed revision control, multi-threaded computing, tests
structural biology	Structural docking predictions, protein-protein interactions, clustering of conformations, rigid body mechanics, collective motions, sequence alignments, pose similarities, molecular modeling, cristallographic data
ocean-atmosphere	Operational models parameterisation, data assimilation, strong non linearities and multiresolution, fluid dynamics equation, processing of large amount of physical observations, correlation and variability analysis

to promote and share science

professionaly	Teaching, supervision of interns, co-coordination of a research thinktank about mathematics and the environment for the French National Research Agency
volunteering	Creation and animation of a scientific web-blog *Sens et sensations des sciences,* elected member of *Café des Sciences* the French science blog community, organisation of public scientific round tables, scientific volunteer at the *Monterey Bay Marine Sanctuary*, active on social networks

Experiences

Since 2014 **Research assistant, post-doctorate** - Referee: Sergei Grudinin
ANR PEPSI, INRIA Grenoble-Minatec, LJK, Université de Grenoble
To predict protein structures and their interactions

2013 - 2014 **Research think-tank scientific coordinator** - Referee: Didier Bresch
ANR Think-Tank MathsinTerre, Institut Henri Poincaré, CNRS, Université de Savoie
To help better fund research in applied mathematics

2011 - 2013 **Research assistant, post-doctorate** - Referee: Andrew Moore
NSF project, University of California of Santa Cruz, USA
To analyse the variability of the California Current Circulation

2007 - 2011 **Doctorate -** Referee: Laurent Debreu
Fundings Région Rhône-Alpes, INRIA, LJK, Université de Grenoble
***6-months scholarship Explora'Doc* to work with CICESE (oceanographic research center), MEXICO**
To apply multigrid technics to data assimilation in geophysics models

Teaching assistant
180h in mathematics, ESISAR, Grenoble-INP, Valence

$\mathcal{E}$ducation

2011	**PhD. in applied mathematics**
	Université de Grenoble
2007	**Master degree of applied mathematics**
	Université de Grenoble
2006	**Computer science and applied mathematics master degree, ENSIMAG**
	Grenoble-INP
	9-months Student international scholarship, Universidad de Concepción, **CHILE**

$\mathcal{R}$esearch

Protein structures prediction and their interactions

Post-Doctorate, since 2014
Fundings
Agence Nationale de la Recherche PEPSI Project
Direction
Sergei Grudinin CNRS, Nano-D INRIA-team, Laboratoire Jean Kuntzmann

To help biologists understand and predict molecular complex behaviours, we develop numerical methods that analyse and extract knowledge from biological data using image processing and machine learning technics. Docking predictions are particularly challenging for large proteins but will improve structure-based virtual drug screening. We work on an algorithm, derived from Support Vector Machine methods, that defines protein-protein interactions using only descriptions of the contact interfaces observed in cristallographic data of protein complexes. This algorithm is among the most efficient ones in CSAR and CASP/CAPRI experiments [1,2].

Contribution - Improve docking prediction for large proteins, without using prior knowledge of binding sites

› Adaptation of the machine learning algorithm so that the potentials can be used for docking predictions on the spherical grid and integration into the exhaustive 3D search of Hex code [4]. First results give a fair prediction rate but suffer from the non regular size of the discretised search grid [5].

› Initiation of a collaboration with a team of the University of Luxembourg. Co-supervision of an intern who studies the use of evolutionary-based algorithms to make affordable docking predictions allowing for flexibility.

› Adaption of a previous rapid computation of deviations between rigid bodies [3] adding flexibility modeled as collective motions.

All of these results are going to be published.

REFERENCES

1. Grudinin S, Popov P, Neveu E, Cheremovskiy G. *Predicting binding poses and affinities in the CSAR 2013-2014 docking exercises using the knowledge-based Convex-PL potential.* J. Chem. Inf. Model., 2015.
2. Lensink, M. Grudinin S., Ritchie D., Neveu E. *et al. Prediction of homo- and hetero-protein complexes by ab-initio and template-based docking: a CASP-CAPRI experiment.* PROTEINS: Structure, Function, and Bioinformatics, 2015.
3. Grudinin S, Popov P. *Rapid determination of RMSDs corresponding to macromolecular rigid body motions.* Journal of Computational Chemistry, Wiley-Blackwell, 2014, 35 (12), pp.950-956.
4. Ritchie D.W, Kemp G.J.L. *Protein Docking Using Spherical Polar Fourier Correlations*, PROTEINS: Struct. Funct. Genet. 39, 178-194, 2000
5. Grudinin S., Neveu E., Popov P., Ritchie D.W, *PEPSI-DOCK: a detailed data-driven protein-protein interaction potential using Polar Fourier Correlation.* Basel Computational Biology Conference. Poster: **PDF-link**

Historical analysis and variability of the California Current Circulation using an operational regional high resolution ocean model

Post-Doctorate 2011-2013
Fundings
National Science Foundation
Direction
Andrew Moore Ocean Sciences Department, UCSC

To better understand the energy exchanges between the global ocean circulation and the *upwelling* - cold deep current coming up to the surface - appearing every spring along the California Coast, we computed a historical analysis of the California Current Circulation using the data assimilation system ROMS-4DVAR (Regional Oceanic Model System - 4D Variational) [Moore et al., 2013]. We produced a high resolution current circulation simulation from 1980 to 2010, using all the satellites data available to fit the parameters of the models.

Contribution - Development of algorithms to process data and analyse the simulation results

› Pre-processing of the observations and physical validation of the simulation, programming algorithms capable of treating large amount of data (10^7 variables for each time step with 30.000 time steps over 30 years) [1,3]

› Co-supervion of a master and a PhD student in studying the variability of the regional circulation and its interactions with the global circulation.

First qualitative results using wavelet analysis [Torrence et al., 98] showed a significant correlation between the ENSO (El Niño Southern Oscillation) and the sea surface temperature anomalies appearing during the upwelling events [2].

REFERENCES

1. Neveu E, Moore A M, Edwards C A, Fiechter J, Drake P, Jacoxand M G, Nuss E. *A Historical analysis of the California Current Circulation using ROMS 4D-Var. Part I: System Configuration and Diagnostics.* Ocean Modelling 2015.
2. Crawford W J, Moore A M, Jacox M G, Neveu E, Fiechter J, Edwards, C A. *A Historical analysis of the California Current Circulation using ROMS 4D-Var Part II: Climate Variability.* Ocean Modelling, 2015.
3. Moore A, Edwards C, Fiechter J, Drake P, Neveu E, Arango H G, Gürol S, Weaver A T. *A 4D-Var Analysis System for the California Current: A Prototype for an Operational Regional Ocean Data Assimilation System.* in *Data Assimilation for Atmospheric, Oceanic and Hydrological Applicvations: Vol. II*, Edition: 2013 ed., Chapter: 14, Publisher: Springer-Verlag Berlin and Heidelberg GmbH & Co. KG, Editors: Seon K. Park, Lian Xu, pp.345-366.

Multigrids and variational data assimilation

Variational data assimilation methods are aimed to combine all the information available (physics laws, numerical equations, observations, statistics of errors) in order to improve numerical simulations. Rigorous and powerful (they rely on the optimal control theory), they nevertheless suffer from a high computational cost that prevents an accurate use in operational geophysics applications where each time step of simulation handles millions of variables.

Contribution - Study of the effects of multigrid technics, subtle algorithms that use coarser grid discretisation models to accelerate the data assimilation system solution.

› Creation of two algorithms, the first solving the non-convex optimisation system, and the second being the multigrids applied on the Gauss-Newton approximation - a local linearisation technic.

› Definition of the conditions to be satisfied by the models and the statistics of errors so that the algorithms converge. Implementation of both algorithms and verification of the convergence acceleration on simplified models such as 2-D Shallow water equations [4,5,6].

The Gauss-Newton multigrid is being implemented on a realistic ocean model by Arthur Vidard [2,3] while we are developing a multigrid preconditioner as a variant algorithm with a more robust behavior for the non-convex case [1].

REFERENCES

1. Debreu L, Neveu E, Simon E, Le Dimet F-X, Vidard A. *Multigrid solvers and multigrid preconditioners for the solution of variational data assimilation problems*. Quaterly Journal of the Royal Meteorological Society, 2015.

2. Vidard A, Debreu L, Neveu E. *Multi Resolution Variational Data Assimilation Schemes With Application to a Realistic Ocean Model*. Sixth WMO Symposium on Data Assimilation, Oct 2013, College Park, United States. 2013.

3. Vidard A, Debreu L, Neveu E. *Multi resolution variational data assimilation system for the ocean*. EGU 2013 - European Geosciences Union General Assembly 2013, Apr 2013, Vienne, Austria. 2013.

4. Debreu L, Neveu E, Le Dimet F-X, Simon E. *Multigrid algorithms and local mesh refinement methods in the context of variational data assimilation*. Eric Blayo; Marc Bocquet; Emmanuel Cosme; F. Cugliandolo Leticia. *Lecture notes of Les Houches summer school* 2012, Oxford University Press, pp.576, 2014, 9780198723844.

5. Neveu E, Debreu L, Le Dimet F-X. *Multigrid methods and data assimilation - Convergence study and first experiments on non-linear equations*. Revue Africaine de la Recherche en Informatique et Mathématiques Appliquées, Le Chesnay : INRIA, 2011, 14, pp.63-80.

6. Neveu E, Debreu L, Le Dimet F-X. *Méthodes multigrilles pour le 4D-VAR*. Colloque National sur l'Assimilation de Données, Dec 2010, Grenoble, France. 2010.

$\mathcal{P}$romoting

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Project coordination

Research think-tank « Mathematics and the complexity of the Earth system », French National Research Agency (Agence Nationale de la Recherche)

The 'MathsInTerre' Research Thinktank is a project launched in January 2013 for one year with the aim of making a contribution to a more systemic and integrated vision of the subject. Related to the initiative entitled MPE2013 (Mathematics of Planet Earth), the Thinktank goal was to

› synthesise the actual researches in mathematics applied to the Earth system

› promote interactions with social and human sciences on environment and societal issues ;

› increase the interactions with natural sciences ;

› establish a global and strategical view of the research project to support.

Contribution - Science coordination of the project to achieve the writing of final reports

› Investigation and collection of texts from researchers of applied mathematics, human and natural science communities, learned societies in mathematics, universities and research institutes

› Organisation of conferences and round-tables to make researchers meet and discuss about science and institutions action plans

› Management of the writing and the structuration of the reports, including a 10 pages summary in English. All the results are available on mathsmonde.math.cnrs.fr, a website that I have designed.

I am proud to have been part of this project that highlighted french institutional issues in promoting, hiring and training multidisciplinary researchers and proposed for structural action plans that are aimed at encouraging scientific interactions.

REFERENCES

Bresch D., Neveu E., *Summary of the MathsInTerre ResearchThinktank - The current state and future of French research into mathematics and the environment*, 2014. available in mathsmonde.math.cnrs.fr

$\mathcal{S}$upervision

2015 **Angelo Migliosi, with Xavier Besseron - Faculty of Science, Technology and Communication, University of Luxembourg, and Sergei Grudinin - CNRS, INRIA NanoD Team project**
Master project and Internship: Evolutionary algorithms for the prediction of structures of large proteins accounting for flexibility with normal mode analysis.

2012 **Emma Nuss, with Andrew Moore - University of California, Santa Cruz**
Internship: Wavelets for the analysis of the variability of the California Current Circulation
William Crawford, with Andrew Moore - University of California, Santa Cruz
PhD: Analysis of the correlation between temperature variability of the California Current Circulation and the global ocean circulation

$\mathcal{P}$ublications

Articles in international peer-reviewed journals

A1 Grudinin S, Popov P, Neveu E, Cheremovskiy G. *Predicting binding poses and affinities in the CSAR 2013-2014 docking exercises using the knowledge-based Convex-PL potential.* doi: 10.1021/acs.jcim.5b00339, J. Chem. Inf. Model., 2015.

A2 Neveu E, Moore A M, Edwards C A, Fiechter J, Drake P, Jacoxand M G, Nuss E. *An Historical analysis of the California Current Circulation using ROMS 4D-Var. Part I: System Configuration and Diagnostics.* doi: 10.1016/j.ocemod.2015.11.012, Ocean Modelling 2015.

A3 Debreu L, Neveu E, Simon E, Le Dimet F-X, Vidard A. *Multigrid solvers and multigrid preconditioners for the solution of variational data assimilation problems.* doi: 10.1002/qj.2676, Quaterly Journal of the Royal Meteorological Society, 2015.

A4 Neveu E, Debreu L, Le Dimet F-X. *Multigrid methods and data assimilation - Convergence study and first experiments on non-linear equations.* hal-00658106, Revue Africaine de la Recherche en Informatique et Mathématiques Appliquées, Le Chesnay : INRIA, 2011, 14, pp.63-80.

Book chapters

C1 Moore A, Edwards C, Fiechter J, Drake P, Neveu E, Arango H G, Gürol S, Weaver A T. *A 4D-Var Analysis System for the California Current: A Prototype for an Operational Regional Ocean Data Assimilation System.* in *Data Assimilation for Atmospheric, Oceanic and Hydrological Applicvations: Vol. II*, Edition: 2013 ed., Chapter: 14, Publisher: Springer-Verlag Berlin and Heidelberg GmbH & Co. KG, Editors: Seon K. Park, Lian Xu, pp.345-366

C2 Debreu L, Neveu E, Le Dimet F-X, Simon E. *Multigrid algorithms and local mesh refinement methods in the context of variational data assimilation.* Eric Blayo; Marc Bocquet; Emmanuel Cosme; F. Cugliandolo Leticia. *Lecture notes of Les Houches summer school* 2012, Oxford University Press, pp.576, 2014, 9780198723844.

Proceedings

P1 Vidard A, Debreu L, Neveu E. *Multi Resolution Variational Data Assimilation Schemes With Application to a Realistic Ocean Model.* Sixth WMO Symposium on Data Assimilation, Oct 2013, College Park, United States. 2013.

P2 Vidard A, Debreu L, Neveu E. *Multi resolution variational data assimilation system for the ocean.* EGU 2013 - European Geosciences Union General Assembly 2013, Apr 2013, Vienne, Austria. 2013.

P3 Neveu E, Debreu L, Le Dimet F-X. *Méthodes multigrilles pour le 4D-VAR.* Colloque National sur l'Assimilation de Données, Dec 2010, Grenoble, France. 2010.

P4 Neveu E, Debreu L, Le Dimet F-X. *Multigrid methods and data assimilation applied to a linear advection equation.* CARI'10 - African Conference on Research in Computer Science and Applied Mathematics, Oct 2010, Yamoussoukro, Côte d'Ivoire. 2010.

Articles submitted

S1 Lensink, M. *et al. Prediction of homo- and hetero-protein complexes by ab-initio and template-based docking: a CASP-CAPRI experiment.* PROTEINS: Structure, Function, and Bioinformatics, 2015. **Major revisions requested**

S2 Crawford W J, Moore A M, Jacox M G, Neveu E, Fiechter J, Edwards, C A. *An Historical analysis of the California Current Circulation using ROMS 4D-Var. Part II: Climate Variability.* Ocean Modelling, 2015.

Conferences

Communications in international conferences

2015   *PEPSI-DOCK: a detailed data-driven protein-protein interaction potential using Polar Fourier Correlation.* Basel Computational Biology Conference, Bâle, Switzerland. **Poster**

2012   *A faster variational non-convex data assimilation solver using multigrid methods. Experiments on a high resolution Shallow-Water model.* TOS/ASLO/AGU Ocean Sciences Meeting, Salt Lake City, USA. **Poster**

2010   *Multigrid methods and data assimilation applied to a linear advection equation.* 10th African Conference on Research in Computer Science and Applied Mathematics, Yamoussoukro, Côte d'Ivoire. **Oral presentation**

2009   *Variational data assimilation methods for multiresolution models.* 3rd International Meeting of Students in Physical Oceanography, IMSPO, CICESE, Ensenada, Mexico. **Oral presentation**

Communications in national (french) conferences

2015   *PEPSI-DOCK: a detailed data-driven protein-protein interaction potential using Polar Fourier Correlation.* Graphisme et Modélisation Moléculaire, Sète. **Oral presentation**

2012   *An historical analysis of the California Current using ROMS 4D-Var : 1980-2010.* Colloque National en Assimilation de données, Nice. **Poster**

2010   *Multigrid methods and variational data assimilation.* Colloque National en Assimilation de données, Grenoble. **Oral presentation**

Seminar and workshops

2015   *Searching for the structures of complexes of proteins: combining machine learning and 3D protein geometry.* Seminar TIMC, Biologie Computationnelle et Mathématiques team. **Oral presentation**

2010   *Méthodes multigrilles et assimilation de données : Applications sur des modèles 1D.* Workshop, research project ANR MSDAG, Paris. **Oral presentation**

2010   *Multigrid methods applied to variational data assimilation.* Seminar: Advanced methods and perspectives in non-linear optimization and control, STAE, Toulouse. **Poster**

2009   *Los metodos multirejas para la assimilacion de datos multiresolucion.* Workshop, research-team CANEK, CICESE, Ensenada, Mexico. **Oral presentation**

2009   *Assimilation multirésolution d'images pour les modèles géophysiques.* Workshop, cluster Environment, Région Rhône Alpes. **Poster**

Teaching

Teaching assistant, Fellowship CIES, Grenoble-INP- ESISAR, Valence

2007 - 2009   **Complex analysis**
92h - Bachelor students: 6 classes of 20 - holomorphic function, Cauchy-Riemann equations, curvilinear numerical integration, calculating residues, Cauchy's theorems, Jordan's lemma

Mathematics
56h (tutorials) - First years students: 4 classes of 30 - Taylor series, parametric surfaces, algebra (group, division ring, ring), arithmetic, polynomial, rational numbers

Probability
61h - Bachelor students: 1 classe of 30 + 2 classes of 15 apprenticeship - combinatorics, random variable, law of large numbers, central limit theorem

Science fostering

Since 2013 **Blog Sense The Science, sens et sensations des sciences**
Creation, animation, writing and graphic design. Interactions between science and society, enlight research through examples of art, technology, culture, governance, education using science.
Elected member of the non-profit organisation Café des Sciences, the french community of science communication

Since 2014 **Cafés Sciences et Citoyens de l'Agglomération Grenobloise**
Public round-tables organisation

2014 **Publication Brèves de Maths**, Mathématiques de la Planète Terre, Nouveau Monde Editions
Writing of « Ignorer la météo d'hier, c'est aussi louper celle de demain »

2012 **Scientific docent**, Monterey Bay National Marine Sanctuary, Santa Cruz, USA

2009 **Fête de la Science,** Lyon

2008 **Festival Remue-Méninges,** for primary schools children

Volunteerism

08-10 **Food and clothes supply for homeless people during winter**
Red cross, Grenoble

06-10 **Social secretary**
Grenoble Alpes Canoë Kayak - 100 members (Regional team in canoe polo, white-water)

Skills

Programming

languages
C, C++, Fortran, Python, SVN-Git, LaTeX, web, NCL

softwares
Matlab, Scilab, Ferret, CMS

DTP-Graphic design
Inkscape, Photoshop, InDesign

Languages

French
mother tongue

English
Spanish
fluent

Italian
Portuguese
Russian
basics