

MARIO FERNÁNDEZ PENDÁS

PERSONAL INFORMATION

date of birth 7 October 1988
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EDUCATION

*PhD in
Mathematics and
Statistics*

2014-2018 University of the Basque Country

Thesis: *Adapting Hybrid Monte Carlo methods for solving complex problems in Life and Materials sciences*

Description: The aim of this project is to develop novel algorithms for modelling and simulating different phenomena in chemistry and biology more efficiently and accurately. All the methodologies are implemented in the parallel software code aiming to the high performance computers.

Advisor: Prof. Elena AKHMATSKAYA · akhmatskaya@bcamath.org

*Masters in
Mathematics and
Computation*

2011-2012 University of Cantabria

Thesis: *Some Metric Aspects in Algebraic Geometry, on the average*

Description: This thesis contains some highly technical results of "interdisciplinary mathematics". The main motivation of this research is the Design and Analysis of Efficient Numerical Algorithms in Algebraic Geometry. Thus, the motivation comes at least from three usually distant mathematical frameworks: Computational Complexity, Numerical Analysis and Algebraic Geometry. Most of these results focus on questions related to Smale's Seventeenth Problem.

Advisor: Prof. Luis M. PARDO · luis.pardo@unican.es

*Bachelor in
Mathematics*

2006-2011 University of Oviedo

Thesis: *An approach to the P vs NP problem*

Description: In this thesis techniques and theoretical results in complexity theory such as Cook's Theorem are introduced and explained. The main goal is to introduce and explain the P vs NP problem and show some techniques to attack different kinds of NP-complete problems.

Advisor: Prof. Elías FERNÁNDEZ-COMBARRO · efernandezca@uniovi.es

EMPLOYMENT

BCAM

2018-2019 Postdoctoral Fellow, BASQUE CENTER FOR APPLIED MATHEMATICS (BCAM)

Postdoctoral Fellow in the MSLMS group under the supervision of Professor Elena Akhmatskaya. My research is dedicated to the study and development of hybrid Monte Carlo methods applied to the simulation of complex physical systems. I am interested in the theoretical formulation and implementation of Generalized Shadow Hybrid Monte Carlo (GSHMC) methods in different statistical ensembles, and also in the development and testing of efficient symplectic integrators for molecular dynamics simulations.

Reference: Elena AKHMATSKAYA · akhmatskaya@bcamath.org

BCAM

2014-2018 PhD Student, BASQUE CENTER FOR APPLIED MATHEMATICS (BCAM)

PhD student in the MSLMS group under the supervision of Professor Elena Akhmatskaya. My research was dedicated to the study and development of hybrid Monte Carlo methods for molecular simulations. I am interested in the theoretical formulation and implementation of generalized shadow hybrid Monte Carlo (GSHMC) methods in different statistical ensembles. The development and testing of new symplectic integrators for molecular dynamics is another field of my interest.

Reference: Elena AKHMATSKAYA · akhmatskaya@bcamath.org

BCAM

2013-2014 Internship Student, BASQUE CENTER FOR APPLIED MATHEMATICS (BCAM)

I worked in the MSLMS group under the supervision of Professor Elena Akhmatskaya and Dr. Bruno Escribano. We developed and implemented (in the GROMACS software package of molecular dynamics) new ideas for performing simulations in the framework of hybrid Monte Carlo methods.

Reference: Bruno ESCRIBANO · bescribano@bcamath.org

PUBLICATIONS

Journal of Computational Physics, 373, 900-916

2018 Multi-stage splitting integrators for sampling with modified Hamiltonian Monte Carlo methods

Authors: Tijana RADIVOJEVIĆ, Mario **Fernández-Pendás**, Jesús María SANZ-SERNA, Elena AKHMATSKAYA

Proceedings of the 115th European Study Group with Industry

2018 Synthesis of Monodisperse Spherical Nanocrystals

Authors: Vincent CREGAN, Revathi BACSA, Marc CALVO SCHWARZWÄLDER, Mario **Fernández-Pendás**, Brendan FLORIO, Antonio MARQUINA, Iain MOYLES, Tim MYERS, Helena RIBERA PONSÁ, Simone RUSCONI, Susana SERNA

Langmuir, 33(42), 11530-11542

2017 Adaptive Splitting Integrators for Enhancing Sampling Efficiency of Modified Hamiltonian Monte Carlo Methods in Molecular Simulation

Authors: Elena AKHMATSKAYA, Mario **Fernández-Pendás**, Tijana RADIVOJEVIĆ, Jesús María SANZ-SERNA

Theoretical Chemistry Accounts, 136(43), 43

2017 Enhancing sampling in atomistic simulations of solid state materials for batteries: a focus on olivine NaFePO₄

Authors: Bruno ESCRIBANO, Ariel LOZANO, Tijana RADIVOJEVIĆ, Mario **Fernández-Pendás**, Javier CARRASCO, Elena AKHMATSKAYA

Journal of Computational Physics, 327, 434-449

2016 Adaptive multi-stage integrators for optimal energy conservation in molecular simulations

Authors: Mario **Fernández-Pendás**, Elena AKHMATSKAYA, Jesús María SANZ-SERNA

Journal of Molecular Modeling, 20, 2487

2014 Constant pressure hybrid Monte Carlo simulations in GROMACS

Authors: Mario **Fernández-Pendás**, Bruno ESCRIBANO, Tijana RADIVOJEVIĆ, Elena AKHMATSKAYA

Confidential

2014 Technical Report for the industrial project led by Math-in

Description: Math-in collaborative project "Demanda de sampling y optimización".

Authors: Tijana RADIVOJEVIĆ, Mario **Fernández-Pendás**, Elena AKHMATSKAYA

*Journal of
Complexity, 29,
323-350*

2013 An Arithmetic Poisson Formula for the multi-variate resultant

Authors: Mario **Fernández-Pendás**, Luis M. PARDO

INVITED PRESENTATIONS

*BCAM, Bilbao
(Spain)*

April 12, 2018 Hybrid Monte Carlo methods for sampling in complex physical systems

LIGHT Seminar.

Authors: Mario **Fernández-Pendás**

*Universidad de
Valladolid,
Valladolid (Spain)*

January 26, 2017 Adaptive splitting integrators for enhancing sampling efficiency of shadow Hamiltonian Monte Carlo methods

IMUVA Seminar.

Authors: Mario **Fernández-Pendás**, Tijana RADIVOJEVIĆ, Jesús María SANZ-SERNA, Elena AKHMATSKAYA

*ICERM, Brown
University,
Providence (USA)*

July 21, 2016 Adaptive two-stage integrators for sampling algorithms based on Hamiltonian dynamics

Stochastic numerical algorithms, multiscale modeling and high-dimensional data analytics.

Authors: Elena **Akhmatskaya**, Mario FERNÁNDEZ-PENDÁS, Tijana RADIVOJEVIĆ, Jesús María SANZ-SERNA

*University of
Potsdam, Potsdam
(Germany)*

September 15, 2015 Adaptive multi-stage integrators with optimal energy conservation

SciCADE Potsdam 2015.

Authors: Mario **Fernández-Pendás**, Elena AKHMATSKAYA, Jesús María SANZ-SERNA

*ITQB, Lisboa
(Portugal)*

December 4, 2014 Enhanced Sampling hybrid Monte Carlo Methods in GROMACS Package: MultiHMC-GROMACS

Invited Seminar.

Authors: Elena **Akhmatskaya**, Bruno ESCRIBANO, Mario FERNÁNDEZ-PENDÁS, Ivan TERTEROV

*Repsol
Technological
Center, Madrid
(Spain)*

June 25, 2014 Improving the Efficiency in Sampling of the Posterior PDF for Reservoirmodel Parameters

Technological meeting for the analysis of the Brugge model using mathematical technology.

Authors: Tijana **Radivojević**, Mario **Fernández-Pendás**, Elena AKHMATSKAYA

*Universidad de
Valladolid,
Valladolid (Spain)*

January 22, 2014 Momentum Flips in Generalized Hybrid/Hamiltonian Monte Carlo Methods

Invited Seminar.

Authors: Tijana **Radivojević**, Elena AKHMATSKAYA, Bruno ESCRIBANO, Mario FERNÁNDEZ-PENDÁS

*BCAM, Bilbao
(Spain)*

October 18, 2013 Enabling Constant Pressure Hybrid Monte Carlo Simulations Using the GROMACS Molecular Simulation Package

The Second BCAM Workshop on Computational Mathematics.

Authors: Mario **Fernández-Pendás**, Bruno ESCRIBANO, Elena AKHMATSKAYA

CONTRIBUTED PRESENTATIONS

- DIPC, Donostia
(Spain)* *September 29, 2016* Adaptive multi-stage integrators for optimal energy conservation in molecular simulations (poster)
DIPC summer school on computational methods for biological molecules.
Authors: Mario **Fernández-Pendás**, Elena AKHMATSKAYA, Jesús María SANZ-SERNA
- CECAM-HQ-EPFL, Lausanne
(Switzerland)* *February 15, 2016* Adaptive multi-stage integrators for optimal energy conservation in molecular simulations (poster)
CECAM workshop on Models for Protein Dynamics 1976-2016.
Authors: Mario **Fernández-Pendás**, Elena AKHMATSKAYA, Jesús María SANZ-SERNA
- Manchester University,
Manchester
(United Kingdom)* *July 16, 2014* Constant Pressure hybrid Monte Carlo simulations in GROMACS (poster)
CCP5 Summer School 2014 - Methods in Molecular Simulations.
Authors: Mario **Fernández-Pendás**, Bruno ESCRIBANO, Elena AKHMATSKAYA, Tijana RADIVOJEVIĆ
- Manchester University,
Manchester
(United Kingdom)* *July 24, 2013* New Hybrid Monte Carlo methods for sampling in Biology, Material Sciences and Statistics (poster)
CCP5 Summer School 2014 - Methods in Molecular Simulations.
Authors: Tijana **Radivojević**, Elena AKHMATSKAYA, Bruno ESCRIBANO, Mario FERNÁNDEZ-PENDÁS, Ivan TERTEROV
- BCAM, Bilbao
(Spain)* *June 24, 2013* NPT GSHMC and its implementation in the GROMACS software package (oral presentation)
MSBMS Working Group activity.
Authors: Mario **Fernández-Pendás**, Bruno ESCRIBANO, Elena AKHMATSKAYA
- BCAM, Bilbao
(Spain)* *May 28, 2013* Advanced GSHMC methods (oral presentation)
MSBMS Working Group activity.
Authors: Mario **Fernández-Pendás**, Bruno ESCRIBANO, Elena AKHMATSKAYA

RESEARCH VISITS

- Universidad de Valladolid,
Valladolid (Spain)* *January 26-27, 2017* Visit to Universidad de Valladolid on invitation of Prof. J.M. Sanz-Serna
Description: Research visit to Professor J.M. Sanz-Serna to work on a collaborative project
- ITQB, Oeiras
(Portugal)* *September 1- November 30, 2016* Visit to ITQB on invitation of Prof. Antonio M. Baptista
Description: Research visit to Professor Antonio M. Baptista, head of the Molecular Simulation Laboratory at ITQB, to work on a collaborative project
- ITQB, Oeiras
(Portugal)* *December 3-5, 2014* Visit to ITQB on invitation of Prof. Antonio M. Baptista
Description: Research visit to Professor Antonio M. Baptista, head of the Molecular Simulation Laboratory at ITQB, to start a collaboration

ATTENDED CONFERENCES, WORKSHOPS AND SCHOOLS

<i>summer school</i>	<i>May 28-31, 2018</i>	Summer School on Fractional and Other Non-Local Models BCAM, Bilbao (Spain)
<i>summer school</i>	<i>September 25-30, 2016</i>	DYNAPEUTICS DIPC, Donostia (Spain)
<i>summer school</i>	<i>July 4-7, 2016</i>	BCAM-IMUVA Summer School on Uncertainty Quantification for Applied Problems Universidad de Deusto, Bilbao (Spain)
<i>workshop</i>	<i>April 6-7, 2016</i>	Energy Based Modeling, Simulation, and Control of Complex Physical Systems Technische Universität, Berlin (Germany)
<i>summer school</i>	<i>April 4-5, 2016</i>	Energy Based Modeling, Simulation, and Control of Complex Physical Systems Technische Universität, Berlin (Germany)
<i>workshop</i>	<i>February 15-18, 2016</i>	Models for Protein Dynamics 1976-2016 CECAM-HQ-EPFL, Lausanne (Switzerland)
<i>school</i>	<i>January 25-29, 2016</i>	European Study group with Industry: ESGI 2016 Centre de Recerca Matemàtica, Barcelona (Spain)
<i>conference</i>	<i>September 14-18, 2015</i>	SciCADE 2015 University of Potsdam, Potsdam (Germany)
<i>workshop</i>	<i>July 12-14, 2015</i>	The 5-th Workshop Quantum Days in Bilbao BCAM, Bilbao (Spain)
<i>summer school</i>	<i>June 8-12, 2015</i>	New Perspectives in Markov Chain Monte Carlo Universidad de Valladolid, Valladolid (Spain)
<i>conference</i>	<i>September 23, 2014</i>	8th RES Users' Conference University of Cantabria, Santander (Spain)
<i>summer school</i>	<i>July 13-22, 2014</i>	CCP5 Summer School 2014 - Methods in Molecular Simulations Manchester University, Manchester (United Kingdom)
<i>conference</i>	<i>July 10-11, 2014</i>	The 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications University Autónoma, Madrid (Spain)
<i>workshop</i>	<i>June 25-26, 2014</i>	Technological meeting for the analysis of the Brugge model using mathematical technology Repsol Technological Center, Madrid (Spain)

- workshop* *January 13-15, 2014* HPC-GA 3rd Workshop
Inria, Bordeaux (France)
- workshop* *December 10-11, 2013* Workshop on Dynamical Systems and
Applications
BCAM, Bilbao (Spain)
- workshop* *October 17-18, 2013* The Second BCAM Workshop on
Computational Mathematics
BCAM, Bilbao (Spain)
- workshop* *March 11-15, 2013* HPC-GA 2nd Workshop
BCAM, Bilbao (Spain)
- summer school* *July 16-20, 2012* Santaló Summer School - Recent Advances in
Real Complexity and Computation
UIMP, Santander (Spain)

DISSEMINATION ACTIVITIES

- Pint of Science,
Bilbao (Spain)* *May 25, 2016* ¿Qué aprendimos del Proyecto Manhattan?
(outreach talk)
Pint of Science dissemination event.
Author: Mario FERNÁNDEZ-PENDÁS

SCIENTIFIC PROJECTS

- working team* *January 1, 2017 -
December 31, 2019* Member of the working team of the project
*Electromagnetic Imaging of the Earth's Subsurface using Advanced
Galerkin Methods*, Spanish Ministry of Economy and
Competitiveness MINECO
Project Reference: MTM2016-76329-R. Electromagnetic Imaging of the Earth's
Subsurface using Advanced Galerkin Methods. Basque Center for Applied
Mathematics (BCAM) and University of the Basque Country (UPV/EHU),
Bilbao (Spain)
PI: David PARDO

AWARDS AND GRANTS

- Postdoc fellowship* *May 2018-2019* Grant BES-2014-068640, postdoctoral
fellowship, Spanish Ministry of Economy and Competitiveness
MINECO
Project Reference: MTM2013-46553-C3-1-P. Retos en Integración Numérica: de
las Estructuras Algebraicas a Simulaciones Monte Carlo. University of
Valladolid, Valladolid (Spain)
PI: Jesús María SANZ-SERNA
- award nomination* *May 11, 2018* Nomination for the *Premio Extraordinario de
Doctorado*
University of the Basque Country (Spain)

<i>scientific visit grant</i>	September 1 - November 30, 2016	Traveling grant associated to the predoctoral student fellowship BES-2014-068640, Spanish Ministry of Economy and Competitiveness MINECO ITQB, Oeiras (Portugal)
<i>travel grant</i>	April 4-8, 2016	Registration and local expenses grant for the school and the workshop Energy Based Modeling, Simulation, and Control of Complex Physical Systems Technische Universitt Berlin, Berlin (Germany)
<i>travel grant</i>	January 25-29, 2016	Accommodation grant for the school European Study group with Industry: ESGI 2016 Centre de Recerca Matemàtica, Barcelona (Spain)
<i>travel grant</i>	June 8-12, 2015	Accommodation and local expenses grant for the school New Perspectives in Markov Chain Monte Carlo Universidad de Valladolid, Valladolid (Spain)
<i>PhD fellowship</i>	May 2015-2018	Grant BES-2014-068640, predoctoral student fellowship, Spanish Ministry of Economy and Competitiveness MINECO Project Reference: MTM2013-46553-C3-1-P. Retos en Integración Numérica: de las Estructuras Algebraicas a Simulaciones Monte Carlo. University of Valladolid, Valladolid (Spain) PI: Jesús María SANZ-SERNA

COMPUTER SKILLS

<i>Programming languages</i>	C, C++, JAVA, MATLAB/OCTAVE, FORTRAN, PYTHON, R
<i>Operating systems</i>	GNU/Linux distributions: Ubuntu, Debian
<i>Symbolic computation</i>	Wolfram Mathematica
<i>Parallel computing</i>	OpenMP, MPI
<i>Molecular dynamics software</i>	GROMACS
<i>Text processing</i>	L ^A T _E X

LANGUAGES

<i>Basic</i>	French, Basque
<i>Fluent</i>	English
<i>Mother tongue</i>	Spanish

September 13, 2018