Marta Garcia Martinez
Principal Project Specialist - Computational Science

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Curriculum Vitae
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Research Interests

My current research focuses on applying business and leadership principles to the management and execution of complex and challenging projects with multidisciplinary teams. Based on experiences from projects managed since 2013, I have particular interest in cross-functional, cross-organizational relationships and in understanding human dynamics between teams to build social capital. In addition, my research in the past years has been focused on topics related to high-performance computing (HPC) in the computational fluid dynamics (CFD) field, and most recently in the field of neuroscience.

Education

PhD in Fluid Mechanics, National Polytechnic Institute of Toulouse (INPT) 2009
Carried out at the European Centre for Research and Advanced Training in Scientific Computation (CERFACS), Toulouse, France

Dissertation: "Development and Validation of the Euler-Lagrange Formulation on a Parallel and Unstructured Solver for Large-Eddy Simulation"

Advisor: Dr. Thierry Poinsot

Master's Degree in Mechanical Engineering, Centro Politécnico Superior, Zaragoza, Spain, 2001
Final Project: "Numerical Simulation of the Effects of Components Deterioration in Gas Turbine Systems."

Carried out at the Aerospace and Mechanical Engineering Department, Sapienza University of Rome under a Socrates/Erasmus Grant.

Major: Energy and Technology of Heat and Fluid

Relevant courses: Fluid Dynamics, Mechanics, Thermodynamics, Mathematical Analysis, Machines, Propulsion Systems, Numerical Methods, Structures, Elasticity, Automatic and Electronic Systems, Circuits, Chemistry, Economy, Materials, Statistical Methods, Industrial Design and Organisation, Norms and Quality, Environment, Renewable Energies.

Employment

Principal Project Specialist - Computational Science, Argonne National Laboratory   **2018-present**
Computational Science Division (CPS)
- Senior Institute Fellow, Northwestern-Argonne Institute of Science and Engineering (NAISE) focused on expanding collaborations between neuroscientist from the Feinberg School of Medicine at Northwestern University and Argonne scientists.
- Program Director of the Argonne Training Program on Extreme-Scale Computing (ATPESC) 2016-2019.
- Committee Chair: 2019 and 2020 Exascale Computing Project Annual Meeting

- Member of Review Committees: SC18, SC19, SC20, IPDPS 2019 and INCITE CR 2011-present
- 2020-2021 INCITE Computational Readiness Review Deputy
- Part of the staff involved in conversations and working groups for the Intel-Cray exascale system Aurora.
- Catalyst and single point of contact for INCITE projects and Director's Discretionary allocations.
- Member of the Advisory Committee for University Partnership Program

Principal Project Specialist - Computational Science, Argonne National Laboratory   **2016-2018**
Catalyst Team, Argonne Leadership Computing Facility (ALCF)
- Part of the ALCF staff involved in conversations, working groups and acceptance tests group for future Intel-Cray systems (Theta and Aurora).
- Team member of an Early Science Program project on Theta (early production system based on Intel's second-generation Xeon Phi processor)
- Program Director of the Argonne Training Program on Extreme-Scale Computing 2017.
- Participation in review committees, division and laboratory activities

Assistant Computational Scientist, Argonne National Laboratory   **2010 – 2016**
Catalyst Team, Argonne Leadership Computing Facility (ALCF)
- Program Director of the Argonne Training Program on Extreme-Scale Computing 2016
- Serve as single point of contact for key research initiatives and provide full project lifecycle assistance on more than 20 INCITE projects and more than 20 Director's Discretionary allocations.
- Help with algorithm development, debugging, profiling, scaling efforts, and collaboration with Leadership Science Project Teams to enable breakthrough science and engineering research at the ALCF.
- Report at internal meetings on the use of ALCF resources to advance research goals.
- Member of the support team that monitors project progress and helps forestall user problems with ALCF resources (BG/P & BG/Q systems and visualization clusters).

Participant in division activities:
- User support ticketing system, internal meetings to formulate and implement ALCF plans, development of website technical content and internal documentation, and preparation of weekly communications to users.
- Prepare training material, speak at workshops and videoconferences to educate users of the ALCF.
- Build relationships with other supercomputer centers to address common challenges of computational science.
- Install and maintain software on BG/P and BG/Q systems.
- Actively participate on external, Laboratory and division review committees: SBIR Phase I, INCITE, ESP, AURORA reviews.
- Principal Author – CY2016 Operational Assessment Review Strategic Results Section
- Participate in Laboratory activities/events: tour guide for the Interim Supercomputer Support Facility, mentor of middle-school girls at Introducing a Girl to Engineering Day, guide at Science Careers in Search of Women Day.

Researcher, CERFACS, Toulouse, France   **2009 – 2010**
- Analyze dynamic load balancing and implementation of parallel partitioning algorithms (from ParMETIS library) for unstructured 3D CFD codes.
- Provide code and user support of the Lagrangian module developed during the Ph.D. and memory modules of the CFD code AVBP.

Study Engineer, CERFACS, Toulouse, France   **2002 – 2005**
- Implement partitioning algorithms (from METIS library) for CFD computations.
- Support parallelism development, code debugging, profiling, and memory optimisation of the CFD unstructured solver AVBP.
- Redact technical reports and code documentation of partitioning and parallel library.

Project Manager, INGEMETAL S.A., Zaragoza, Spain   **2001**

- Construct the *Burke Brise Soleil* cover for the Milwaukee Art Museum addition (designed by Santiago Calatrava).
- Responsible for communication, work supervision, and interactions between American and Spanish working teams.

Honors and Awards

Two (2) Argonne Core Values Shout-Out – Teamwork (10/17/2019 & 12/19/2019)

ANL Pacesetter Award February 2018, for extraordinary effort in supporting and leading preparation efforts for the DOE Exascale Computing Project's Second Annual Meeting

ANL Pacesetter Award September 2016, for extraordinary effort and leadership skills for the Argonne Training Program on Extreme-Scale Computing

ISC Research Poster Award 2015, "Performance Enhancement of an Internal Combustion Engine CFD Simulation on IBM BG/Q," J. Kodavasal, K. Harms, P. Srivastava, S. Som, S. Quan, K. Richards, and **M. García**. *ISC High Performance*, July 12-16, 2015, Frankfurt, Germany

Strategic Laboratory Leadership Program (SLLP) – (2013)
- Non-degree Executive Leadership Program developed by the University of Chicago Booth School of Business, and sponsored by UChicago Argonne, LLC.
- Participants selected by the Argonne National Laboratory Director because of their leadership abilities, exceptional work ethic, collaborative thinking skills, rigorous scholarship aptitude, and innovative and creative problem solving capabilities.

Label C3I - Certificat de Compétences en Calcul Intensif – (2009)

This certificate is granted by the CPU (Conférence des Présidents d'Universités), GENCI and the *Maison de la Simulation*. Label awarded to Ph.D. holders who developed and applied during their Ph.D. skills in High-Performance Computing.

Professional Development

The University of Chicago Booth School of Business – Executive Education:

- "*Engagement, Performance and Execution*" (2018)
- "*Essentials of Effective Management: The Psychology of Management*" (2015)
- "*Negotiation and Decision Making Strategies*" (2013)

Argonne – Managerial Skills Series (FY18)
- **ALI100:** Inclusive Leadership
- **ALI203:** Providing Performance Feedback
- **ALI207:** Skillful Conversations
- **ALI209:** Resolving Conflicts Within Your Team

Professional Activities

Member, SC20 Technical Papers Committee of the State of the Practice area (2020)

CoChair, Program Committee Exascale Computing Project 2020 Annual Meeting (2019-2020)

Program Director, Argonne Training Program on Extreme-Scale Computing (2016-2019)

Chair, Program Committee Exascale Computing Project 2019 Annual Meeting (2018-2019)

Member, IPDPS 2019 Program Committee (2018)

Member, SC18 Technical Papers Committee of the State of the Practice area (2018)

Member, Steering Committee Exascale Computing Project 2018 Annual Meeting (2017-2018)

Member, Organizing Committee Scaling to Petascale Institute 2017 (2017)

Member, Technical Advisor Committee ANL University Partnerships Program (2017)

Member, ANL Laboratory Directed Research and Development for the Director's Competitive Grants (2013–2015)

    Vice-Chair (2014)

    Chair (2015)

Member, Margaret Butler Symposium Speaker and Planning Committee (2014–2016)

Member, Programming Environment' Committee for ANL internal (CORAL) proposal evaluations (February–March 2014)

Member, ALCF Computational Readiness Committee for INCITE Reviews (2011–present)

Mentor, Avanthi Lalitha Mantrala (2012), Preeti Malakar (2015-2016), Gina Magnotti (2017-2019)

Professional Skills

- Knowledge of high-performance computational science in the CFD field. Code portability on different architectures, parallelism and partitioning strategies, use of versioning tools, scalability, profiling and debugging analysis.

- Development, maintenance, and utilization of high-performance massively parallel unstructured CFD codes for industrial applications.

- Considerable communications skills, both verbal and written: Spanish, English, French, and Italian.

- Strong collaborative skills, including the ability to work well with other laboratories, universities, supercomputer centers, and industry in an interdisciplinary framework.

- Experience in the creation and maintenance of websites.

Workshops and other

Argonne Training Program on Extreme-Scale Computing 2016-2019

- Program Director in charge of the organization of the training in collaboration with close to 150 people (reviewers, lecturers, administration, support teams, etc).

Petascale Computing Institute 2019

- ANL representative in the organizing team composed by the different institutions.
- Responsible for organizing the ANL Host Site.

Northwestern-Argonne Workshop on Computational Neuroscience 2018

- Responsible for organizing the workshop at ANL in collaboration with the Director of Research at NAISE and the Director of the NUIN Program.

Scaling to Petascale Institute 2017

- ALCF representative in the organizing team composed by the different institutions.
- Responsible for organizing the ANL Host Site.

VERIFI Workshop: Hands-on Session, November 2014 and June 2016

- ALCF point of contact and responsible for the hands-on session on Mira (BG/Q at ALCF) organized at the Workshop for High-Performance Computing-Enabled Engine Simulations for the Virtual Engine Research Institute and Fuels Initiative (VERIFI).
- Supported the setup and optimization of the test case for the hands-on session. Coordinated other ALCF staff with workshop organizers for different tasks: allocation creation, guidelines for ALCF accounts, reservation request, presentation for the workshop, etc.

Grants and Proposals

Laboratory Computing Resource Center (LCRC) Computing Award (PI):

- "Machine Learning for Semantic Segmentation of feline spinal cord images"
  NAISE_Segment_ML: 599,999 core-hours on Bebop (LCRC), 1/2/2020 - 6/30/2020

- "Modeling of motorpool output with respect to excitation and inhibition inputs", NAISE_MN_AVrate_2: 599,999 core-hours on Bebop (LCRC), 1/2/2020 - 6/30/2020
- "Modeling of motorpool output with respect to excitation and inhibition inputs", NAISE_MN_AVrate, 750,000 core-hours on Bebop (LCRC), 2/13/2019 - 9/30/2019
- "Segmentation algorithms and pipeline for feline spinal cord studies", NAISE_SI19_Segment: 600,00 core-hours on Bebop (LCRC), 5/30/2019 - 9/30/2019
- "Parameter tuning and analysis of motoneurons", NAISE_SI19_Tuning: 600,000 core-hours on Bebop (LCRC), 5/30/2019 - 9/30/2019

Advanced Photon Source (APS) User Proposal for beamtime (Co-PI)
- GUP-64547: "Large volume feline spinal cord microtomography", 2-BM-A,B, 2020-1 (2020-02-27 – 2020-03-02

Argonne Leadership Computing Facility (ALCF) Computing Award:
- "Segmentation algorithms and pipeline for feline spinal cord studies", NAISE_SI19_Segment: 8,000 core-hours on Cooley (ALCF), 6/14/2019 - 10/01/2019

LDRD Strategic Initiative Grant, FY13–FY15
Co-Principal Investigator in a Strategic Initiative LDRD proposal (Applied Energy and Sustainable Transportation) in collaboration with other scientists from Argonne's Energy Systems Division and the Chemical Sciences and Engineering Division.

> **Project Number:** 09229-00-147
> **Title:** "Development of Predictive Multi-dimensional Combustion Modeling Capability with Detailed Chemistry"

INCITE Awards
Co-Principal Investigator with Alexei Khokhlov, University of Chicago: "First-Principles Simulations of High-Speed Combustion and Detonation" (2014–2016)

ALCC Awards
Co-Principal Investigator with Sibendu Som, Argonne National Laboratory: "Advancing Internal Combustion Engine Simulations using Sensitivity Analysis" (2015)

Main Collaborations

Northwestern University (2017-present)

Collaborating with Northwestern neuroscientists from The Heckman Laboratory (Dept. of Physiology, Northwestern Univ.) to use computational resources to develop a model of a motoneuron pool to study the mechanisms underlying spinal cord stimulation. In addition, collaboration with the Director of Science from NAISE and the Director of the Northwestern University Interdepartmental Neuroscience (NUIN) program to organize events and workshop to boost neuroscience collaborations between both institutions.

Convergent Science, Inc. (2011–2017)
Collaborating with Convergent Science, Inc., a world leader in CFD software, to use supercomputers to conduct engine simulations. My work focuses on improving CFD solver CONVERGE™ to run efficiently on HPC systems like Mira.

Publications and Presentations

[1]   R. Paoli, O. Thouron, D. Cariolle, **M. García** and J. Escobar, "*Three-dimensional large-eddy simulations of the early phase of contrail-to-cirrus transition: effects of atmospheric turbulence and radiative transfer*", Meteorologische Zeirschrift, 26:597-620 (2017)

[2]   J. Kodavasal, Y. Pei, K. Harms, S. Ciatti, A. Wagner, P.K. Senecal, **M. García** and S. Som, "*Global Sensitivity Analysis of a Gasoline Compression Ignition Engine Simulation with Multiple Targets on an IBM Blue Gene/Q Supercomputer*", SAE technical paper offer/number 16PFL-0871, SAE 2016 World Congress & Exhibition, 12-14 April 2016, Detroit, Michigan, USA.

[3]   J. Kodavasal, K. Harms, P. Srivastava, S. Som, S. Quan, K. Richards and **M. García**, "*Development of a Stiffness-Based Chemistry Load Balancing Scheme, and Optimization of Input/Output and Communication, to Enable Massively Parallel High-Fidelity Internal Combustion Engine Simulations*", Journal of Energy Resources Technology, 138(5), 052203 (Feb 23, 2016) (11 pages)

[4]   A. Insley, J. Kodavasal, X. Chai, K. Harms, **M. García** and S. Som, "Gasoline Compression Ignition: Optimizing Start of Injection Time", SC 15 Visualization Showcase presentation, Nov. 18, 2015, Austin, TX, USA.

[5]   J. Kodavasal, K. Harms, P. Srivastava, S. Som, S, Quan, K. Richards and **M. García**, "Scaling up a high-fidelity internal combustion engine simulation on an IBM Blue Gene/Q supercomputer." *Proceedings of the ASME 2015 Internal Combustion Engine Division Fall Technical Conference*, ICEF2015-1035, November 8-11, Houston (2015).

[6]   J. A. Insley, J. Kodavasal, Xiaochuan Chai, K. Harms, **M. García** and S. Som, "Gasoline Compression Ignition: Optimizing Start of Injection Time" presented as an interactive kiosk at the National Science Bowl, April/May 2015, Washington, DC.

[7]   R. Paoli, O. Thouron, J. Picot, D. Cariolle, **M. García**, "Large-eddy simulations of contrail-to-cirrus transition in the atmosphere." Abstract for American Society of Mechanical Engineers (ASME) 4th Joint US-Europe Fluids Engineering Division Summer Meeting, August 3-7, Chicago (2014).

[8]   S. Som, D. E. Longman, S. M. Aithal, R. Bair, **M. García**. S. P. Quan, K.J. Richards, P.K. Senecal, T. Shethaji and M. Weber. "A Numerical Investigation on Scalability and Grid Convergence of Internal Combustion Engine Simulations." SAE 2013 World Congress & Exhibition, 13PFL-0587 / 2013-01-1095, April 16 (2013).

[9]   T. Poinsot, **M. García**, J.-M. Senoner, L. Gicquel, G. Staffelbach and O. Vermorel. "Numerical and Physical Instabilities in Massively Parallel LES of Reacting Flows." *Journal of Scientific Computing*, 49:78-93 (2011).

[10] F. Jaegle, J.-M. Senoner, **M. García**, F. Bismes, R. Lecourt, B. Cuenot and T. Poinsot. "Eulerian and Lagrangian spray simulations of an aeronautical multipoint injector." *Proc. of the Combustion Institute,* 33:2099–2107 (2011)

[11] N. Gourdain, L.Y.M. Gicquel, M. Montagnac, O. Vermorel, M. Gazaix, G. Staffelbach, **M. García**, J.-F. Boussuge and T. Poinsot. "High performance parallel computing of flows in complex geometries: I. Methods." *Computational Science & Discovery* **2** (November) 015003 (26pp) (2009).

[12] N. Gourdain, L.Y.M. Gicquel, M. Montagnac, O. Vermorel, M. Gazaix, G. Staffelbach, **M. García**, J.-F. Boussuge and T. Poinsot. "High performance computing of industrial flows: Application to aeronautic and propulsion challenges – invited conference." In *VKI Lecture Series on High Performance Computing of Industrial Flows*, Von Kármán Institute, Brussels (2009).

[13] F. Jaegle, J.-M. Senoner, **M. García**, C. Jiménez, B.Cuenot, and T. Poinsot. "Evaluation of simulation strategies for multipoint injection systems in aero-engines on the example of a liquid jet in a gaseous crossflow." In *11th Triennial International Conference on Liquid Atomization and Spray Systems,* Paper Number 042, Vail, Colorado (2009).

[14] J.-M. Senoner, M. Sanjosé, T. Lederlin, F. Jaegle, **M. García**, E. Riber, B. Cuenot, L.Y.M. Gicquel, H. Pitsch and T. Poinsot. "Eulerian and lagrangian large-eddy simulations of an evaporating two-phase flow." *Comptes Rendus Mécanique*, 337(6-7), 458-468 (2009).

[15] E. Riber, V. Moureau, **M. García**, T. Poinsot and O. Simonin. "Evaluation of numerical strategies for LES of two-phase recirculating flows". *Journal of Computational Physics*, 228(2), 539-564 (2009).

[16] J. M. Senoner, **M. García**, S. Mendez, G. Staffelbach, O. Vermorel and T. Poinsot. "Growth of Rounding Errors and Repetitivity of Large-Eddy Simulations." *AIAA Journal*, 46(7), 1773-1781 (2008).

[17] **M. García**, E. Riber, O. Simonin and T. Poinsot. "Comparison between Euler/Euler and Euler/Lagrange LES approaches for confined bluff-body gas-solid flow." *Proceedings of the 6th International Conference on Multiphase Flow*, CD-Rom - S3_Fri_A_62 - Leipzig (2007).

[18] E. Riber, **M. García**, V. Moureau, H. Pitsch, O. Simonin and T. Poinsot. "Evaluation of numerical strategies for LES of two-phase reacting flows." In *Proceedings of the Summer Program 2006,* 197-211 (2006).

[19] **M. García**, Y. Sommerer, T. Schönfeld and T. Poinsot. "Evaluation of Euler/Euler and Euler/Lagrange strategies for large-eddy simulations of turbulent reacting flows." In *ECCOMAS Thematic Conference on Computational Combustion*. Lisbon (2005).

Presentations

- Argonne Outloud, "Catch a Rising Science Star" (2015).
- Women in Computing Panel in Science Careers in Search of Women (SCSW) Conference, Argonne (2015).
- VERIFI Workshop: Hands-on Session (step-by-step), Argonne (2014 and 2016).
- Panelist at the First Friday WIST Forum, Argonne (2014).
- ALCF Getting Started Videoconference (speaker, 2013-present).
- SCSW 2012, Argonne (2012).
- DOE CSGF Conference: HPC Workshop, Arlington (2011).