GIANNI DE FABRITIIS

CEO Acellera
ICREA Researcher
Associate Professor UPF
PhD

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SUMMARY

CEO/ and CSO of Acellera and ICREA research professor at Universitat Pompeu Fabra where I lead the Computational Science Laboratory .

I hold a bachelor degree with honors in applied mathematics (1997) from the Univ. of Bologna and a PhD from Univ. of London (2002). In 2008 I won the tenure-track Ramon y Cajal research position and later the national I3-tenured program. In 2014 I became a research professor by winning the prestigious ICREA research tenured position. I have performed research stays as visiting professor at Stanford University and at UCLA.

My research interests are rooted in the applications of computation to science, in particular for molecular simulation, machine learning and machine intelligence. I have published over a hundred and twenty articles in high-ranking international journals such as PNAS, JACS, Nature Chemistry, Nature Methods, Nature Commun., PLOS Comput. Bio., Phys. Rev. Letter, Phys. Rev. E., JCTC, JCIM, accomplishing an h-index of 45 with over 1380 citations/ year in 2022.

In 2006, I co-founded Acellera Ltd and in 2012 Acellera Labs SL its R&D division. Acellera's mission is to enable computable drug discovery, developing the algorithms to automate drug discovery via high-throughput computations and machine learning methods. The company pioneered the use of graphical processing units in molecular simulations and drug discovery. Currently Acellera and its affiliate Acellera Labs employ a dozen people and have an annual turnover of approximately 1M Euro working together with several of the top-10 pharmas.

CURRENT POSITIONS

ICREA Research Professor, Head of the Computational Science Laboratory, Universitat Pompeu Fabra, ES · 2014 - now

Created GPUGRID.net, the second largest distributed computing project harnessing several thousands GPUs. Co-project leaders of OpenMM/ACEMD, one of the leading molecular dynamics packages, jointly with University of Stanford and Memorial Sloan Kettering where we are responsible for the development of machine learning potentials between quantum and classical mechanics and end-to-end simulation approaches. and ranked second in the Unity obstacle tower challenge, an AI testbed for navigation, puzzle solving, etc. We currently own the SOTA on this challenge (arXiv:2007.02622).

Associate Professor, Universitat Pompeu Fabra, ES · 2014 - now

Supervising: 2 postdoc, 5 PhD students (incl. 1 Industrial PhD and 1 MSCA-ITN fellow) and 2 MSc theses.

CEO, CSO Acellera Labs SL, ES · 2012 - now

CEO, Acellera Ltd, UK · 2006 - now

PREVIOUS POSITIONS

Visiting professor UCLA, IPAM, USA · Sep - Dec 2019
Machine Learning for Physics and the Physics of Learning.

Visiting professor Stanford Univ., Clark Center BioX, USA · May 2015

I3 Fellow at UPF, ES · 2012 – 2013

Ramón y Cajal tenure-track fellow at UPF, ES · 2008 – 2012

Visiting professor at UPF, ES · 2006 – 2007

Postdoctoral fellow at University College London, UK · 2003– 2006

Visiting researcher at Chiron Vaccines (now GSK) Siena, IT · 2003

Contracted researcher at University of Siena, IT · 2003

Chief Technology Officer role at Atalab, Florence, IT · 2002 – 2003

EU fellowship at the CINECA Supercomputing Center, IT · 1998 – 1999

EDUCATION

PhD in Chemistry, Center for Computational Science, Queen Mary University of London - UK
1999-2002

Best first year PhD in chemistry

Bachelor in Mathematics, University of Bologna - IT
1993-1997

Graduated 110/110 cum laude (top 2%)

SELECTED INVITED PRESENTATIONS (LAST 4 YEARS)

Regularly invited to speak at international workshops, symposia and conferences and at several pharmaceutical companies.

2022 Machine learning chemistry: From proteins to small molecules, Microsoft Research, Cambridge, UK · (UK - United Kingdom)

2022 Physics and ML-based methods in molecular recognition, EMBL-EBI UK

2022 Coarse-grained potentials for protein thermodynamics, Gordon conference in computational chemistry, 2022 · Spain

2022 Coarse-grained potentials for protein thermodynamics" · Methods in Molecular dynamics and machine learning workshop, Barcelona · (Spain)

2022 Machine Learning for Physics, Machine Learning for Physics Reunion Conference I, Lake Arrowhead Conference Center UCLA, USA

2022 Recent Advances in Machine Learning Accelerated Molecular Dynamics, Pisa, Italy

2021 WE-Heraeus-Seminar on Advanced Physical and Computational Techniques to Investigate Protein Dynamics, Virtual

2020 Physical and Computational Techniques to Investigate Protein Dynamics, Virtual,- invited speaker

2020 Simulations and AI from proteins to bots, IIT, (IT) - invited seminar

2020 From symbolic to machine learning potentials in molecular simulations, (DE)- invited seminar

2020 AI4Science, Amsterdam (NL) - invited speaker

2019 Workshop at Neural Information Processing Systems (NeurIPS), (CA) - invited speaker

2019 IBSA Foundation forum "AI & Pharmaceutical landscape", Lugano (HE) - keynote speaker

2019 Molecular and Chemical Kinetics MolKin, Berlin (DE) - invited speaker

2019 BenevolentAI, London (UK) - internal event - invited talk

2019 Twelfth European Workshop in Drug Design (IT) - invited speaker

2019 British Crystallographic Association Spring Meeting (UK) - keynote speaker

SOFTWARE DEVELOPED (OPEN SCIENCE & COMMERCIAL)

2021 **TORCHMD** - A machine learning framework for molecular simulations. Open source. Currently co-developed with a top-pharma.

2017 **PLAYMOLECULE** - A framework of many deep learning applications for drug discovery and molecular simulations, freely available at playmolecule.org but also commercialized by Acellera to top pharmaceutical companies. Used by thousands of scientists.

2016 **HTMD** - A molecular-specific programmable environment to prepare, handle, simulate, visualize and analyze molecular systems. Commercialized by Acellera to top pharmaceutical companies and biotechs. Free for academia.

2009 **ACEMD** - A high performance molecular dynamics code for biomolecular systems designed specifically for Nvidia GPUs. Commercialized by Acellera to top pharmaceutical companies and academia for the past 15 years with hundreds of licenses sold. Also available for free.

2008 **CELLMD** - A high performance molecular software for the IBM/SONY/TOSHIBA Cell processor (first copy bought by SONY Japan).

PUBLICATIONS

All publications and recent papers:
https://scholar.google.com/citations?user=-_kX4kMAAAAJ&hl=en

For the years 2018-2022:

1. P Thölke, G De Fabritiis, TorchMD-NET: Equivariant Transformers for Neural Network based Molecular Potentials, International Conference on Learning Representations (ICLR), 2022
2. Varela-Rial, Alejandro; Maryanow, Iain; Majewski, Maciej; Doerr, Stefan; Schapin, Nikolai; Jimenez-Luna, Jose; De Fabritiis, Gianni 2022, 'PlayMolecule Glimpse: Understanding Protein-Ligand Property Predictions with Interpretable Neural Networks', Journal Of Chemical Information And

Modeling, 62, 2, 225 - 231.
3. Doerr, Stefan; Majewski, Maciej; Perez, Adria; Kramer, Andreas; Clementi, Cecilia; Noe, Frank; Giorgino, Toni; De Fabritiis, Gianni 2021, 'TorchMD: A Deep Learning Framework for Molecular Simulations', Journal Of Chemical Theory And Computation, 17, 4, 2355 - 2363.
4. Libardi, Gabriele; Dittert, Sebastian; De Fabritiis, Gianni 2021, 'Guided Exploration with Proximal Policy Optimization using a Single Demonstration', International Conference On Machine Learning, Vol 139, 139.
5. Olehnovics, Edgar; Yin, Junqi; Perez, Adria; De Fabritiis, Gianni; Bonomo, Robert A.; Bhowmik, Debsindhu; Haider, Shozeb 2021, 'The Role of Hydrophobic Nodes in the Dynamics of Class A beta-Lactamases', Frontiers In Microbiology, 12, 720991.
6. Varela-Rial, Alejandro; Majewski, Maciej; De Fabritiis, Gianni 2021, 'Structure based virtual screening: Fast and slow', Wiley Interdisciplinary Reviews-computational Molecular Science, e1544.
7. Dainese, Enrico; Oddi, Sergio; Simonetti, Monica; Sabatucci, Annalaura; Angelucci, Clotilde B.; Ballone, Alice; Dufrusine, Beatrice; Fezza, Filomena; De Fabritiis, Gianni; Maccarrone, Mauro 2020, 'The endocannabinoid hydrolase FAAH is an allosteric enzyme (vol 10, 2292, 2020)', Scientific Reports, 10, 1, 5903.
8. Herrera-Nieto, Pablo; Perez, Adria; De Fabritiis, Gianni 2020, 'Small Molecule Modulation of Intrinsically Disordered Proteins Using Molecular Dynamics Simulations', Journal Of Chemical Information And Modeling, 60, 10, 5003 - 5010.
9. Herrera-Nieto, Pablo; Perez, Adria; De Fabritiis, Gianni 2020, 'Characterization of partially ordered states in the intrinsically disordered N-terminal domain of p53 using millisecond molecular dynamics simulations', Scientific Reports, 10, 1, 12402.
10. Husic, Brooke E.; Charron, Nicholas E.; Lemm, Dominik; Wang, Jiang; Perez, Adria; Majewski, Maciej; Kramer, Andreas; Chen, Yaoyi; Olsson, Simon; de Fabritiis, Gianni; Noe, Frank; Clementi, Cecilia 2020, 'Coarse graining molecular dynamics with graph neural networks', Journal Of Chemical Physics, 153, 19, 194101.
11. Martinez-Rosell, Gerard; Lovera, Silvia; Sands, Zara A.; De Fabritiis, Gianni 2020, 'PlayMolecule CrypticScout: Predicting Protein Cryptic Sites Using Mixed-Solvent Molecular Simulations', Journal Of Chemical Information And Modeling, 60, 4, 2314 - 2324.
12. Noe, Frank; De Fabritiis, Gianni; Clementi, Cecilia 2020, 'Machine learning for protein folding and dynamics', Current Opinion In Structural Biology, 60, 77 - 84.
13. Varela-Rial, Alejandro; Majewski, Maciej; Cuzzolin, Alberto; Martinez-Rosell, Gerard; De Fabritiis, Gianni 2020, 'SkeleDock: A Web Application for Scaffold Docking in PlayMolecule', Journal Of Chemical Information And Modeling, 60, 6, 2673 - 2677.
14. Perez, Adria; Herrera-Nieto, Pablo; Doerr, Stefan; De Fabritiis, Gianni 2020, 'AdaptiveBandit: A Multi-armed Bandit Framework for Adaptive Sampling in Molecular Simulations', Journal Of Chemical Theory And Computation, 16, 7, 4685 - 4693.
15. 'PlayMolecule BindScope: Large scale CNN-based virtual screening on the web', M Skalic, G Martínez-Rosell, J Jiménez, G De Fabritiis. 2019, Bioinformatics,

35, 7, 1237 - 1238.
16. PathwayMap: Molecular pathway association with self-normalizing neural networks, J Jiménez Luna, D Sabbadin, A Cuzzolin, G Martínez-Rosell, J Gora, ..., 2019, Journal of Chemical Information and Modeling 59, 3, 1172 - 1181.
17. LigVoxel: inpainting binding pockets using 3D-convolutional neural networks, M Skalic, A Varela-Rial, J Jiménez, G Martínez-Rosell, G De Fabritiis, Bioinformatics, Volume 35, Issue 2, 15 January 2019, Pages 243–250.
18. Galvelis R, Doerr S, Damas JM, Harvey MJ & De Fabritiis G 2019, 'A Scalable Molecular Force Field Parameterization Method Based on Density Functional Theory and Quantum-Level Machine Learning', Journal Of Chemical Information And Modeling, 59, 8, 3485 - 3493.
19. Jimenez-Luna J, Perez-Benito L, Martinez-Rosell G, Sciabola S, Torella R, Tresadern G & De Fabritiis G 2019, 'DeltaDelta neural networks for lead optimization of small molecule potency', Chemical Science, 10, 47, 10911 - 10918.
20. Skalic M, Sabbadin D, Sattarov B, Sciabola S & De Fabritiis G 2019, 'From Target to Drug: Generative Modeling for the Multimodal Structure-Based Ligand Design', Molecular Pharmaceutics, 16, 10, 4282 - 4291.
21. Wang J, Olsson S, Wehmeyer C, Perez A, Charron NE, de Fabritiis G, Noe F & Clementi C 2019, 'Machine Learning of Coarse-Grained Molecular Dynamics Force Fields', Acs Central Science, 5, 5, 755 - 767.
22. Ferruz, Noelia; Doerr, Stefan; Vanase-Frawley, Michelle A.; Zou, Yaozhong; Chen, Xiaomin; Marr, Eric S.; Nelson, Robin T.; Kormos, Bethany L.; Wager, Travis T.; Hou, Xinjun; Villalobos, Anabella; Sciabola, Simone; De Fabritiis, Gianni 2019, 'Dopamine D3 receptor antagonist reveals a cryptic pocket in aminergic GPCRs (vol 8, 897, 2018)', Scientific Reports, 9, 6076.
23. Landin, Erik J. B.; Lovera, Silvia; de Fabritiis, Gianni; Kelm, Sebastian; Mercier, Joel; McMillan, David; Sessions, Richard B.; Taylor, Richard J.; Sands, Zara A.; Joedicke, Lisa; Crump, Matthew P. 2019, 'The Aminotriazole Antagonist Cmpd-1 Stabilises a Distinct Inactive State of the Adenosine 2A Receptor', Angewandte Chemie-international Edition, 58, 28, 9399 - 9403.
24. Lovera, Silvia; Cuzzolin, Alberto; Kelm, Sebastian; De Fabritiis, Gianni; Sands, Zara A. 2019, 'Reconstruction of apo A2A receptor activation pathways reveal ligand-competent intermediates and state-dependent cholesterol hotspots', Scientific Reports, 9, 14199.
25. Skalic, Miha; Jimenez, Jose; Sabbadin, Davide; De Fabritiis, Gianni 2019, 'Shape-Based Generative Modeling for de Novo Drug Design', Journal Of Chemical Information And Modeling, 59, 3, 1205 - 1214.
26. De Mol E, Szulc E, Di Sanza C, Martínez-Cristóbal P, Bertoncini CW, Fenwick RB, Frigolé-Vivas Marta, Masín M, Hunter I, Buzón V, Brun-Heath I, García J, De Fabritiis G, Estébanez-Perpiñá E, McEwan IJ, Nebreda A, Salvatella X 2018, 'Regulation of Androgen Receptor Activity by Transient Interactions of Its Transactivation Domain with General Transcription Regulators', Structure, 26(1):145-152.e3.
27. Ferruz N, Doerr S, Vanase-Frawley MA, Zou Y, Chen X, Marr ES, Nelson RT, Kormos BL, Wager TT, Hou X, Villalobos A, Sciabola S & De Fabritiis G 2018, 'Dopamine D3 receptor antagonist reveals a cryptic pocket in aminergic GPCRs', Scientific Reports, 8, 897.
28. Jimenez J, Skalic M, Martinez-Rosell G & De Fabritiis G 2018, 'K-DEEP: Protein-Ligand Absolute Binding Affinity Prediction via 3D-Convolutional

Neural Networks', Journal Of Chemical Information And Modeling, 58, 2, 287 - 296.
29. Martinez-Rosell G, Harvey MJ & De Fabritiis G 2018, 'Molecular-Simulation-Driven Fragment Screening for the Discovery of New CXCL12 Inhibitors', Journal Of Chemical Information And Modeling, 58, 3, 683 - 691.
30. Perez A, Martinez-Rosell G & De Fabritiis G 2018, 'Simulations meet machine learning in structural biology', Current Opinion In Structural Biology, 49, 139 - 144.

SELECTED GRANTS

Last 5 years

2021-2026 USA, NIH grant "OpenMM: Scalable biomolecular modeling, simulation, and machine learning" (GRANT13012084) 410 564 USD (total project budget 2.57M USD).

2018-2020 Spain, Application of the method of machine learning and data-augmentation for protein folding and molecular recognition" (BIO2017-82628-P)-Programa Estatal De Fomento De La Investigación Científica Y Técnica De Excelencia, 260 150 Euro

2018-2021 Spain, "Development of a fast and accurate tool for the parametrization of force fields, for small molecules, based on automatic learning methods" Programa Torres-Quevedo, 97 755 EUR

2018-2021 Spain, Doctorat Industrial "PlayMolecule: Developing a web platform for biomedical applications" (2017-DI-067) AGAUR 33.960EUR(total project 55 560 EUR)

2019-2023 EU, COMPBIOMED2: A Centre of Excellence in Computational Biomedicine, H2020-INFRAEDI-2018-2020, Grant Agreement:823712) 357 000 EUR (total project budget 7,99M EUR)

2021-2025 EU, AIDD Advanced machine learning for Innovative Drug Discovery (H2020-MSCA-ITN-2020;) 125 452 EUR (total project budget 3.93M EUR).

2020-2021 USA, OpenMM: Key Infrastructure for Biomolecular Modeling and Simulation Chan-Zuckerberg Initiative (EOSS2-0000000172) 35 000 USD (total project budget 230 000 USD)

AWARDS AND SOCIETAL IMPACT

2019 Acellera selected as one of the Top30 AI Drug Discovery companies in the world.

2012 Launched Donate@home project to fund a PhD student via bitcoin mining for science. Over 3500 bitcoins collected from thousands of contributors worldwide.

2009 Appearance of PS3GRID.net on major Spanish newspapers (El Mundo), major national news channels (TV3 and Radio), the Italian scientific program Quark on national television and news in major scientific journals counting over hundreds news items in two years.

2008 Feature article in Science on PS3GRID, *Play me a molecule*, Science 12 September 2008, Vol. 321. no. 5895, p. 14251

2002 Brewin award for the best 1st year PhD student. Queen Mary University of London - UK

LANGUAGE SKILLS

ITALIAN (Native) ENGLISH (C2) SPANISH (C2)