Nicodemo Di Pasquale, PhD

Email: nicodemo.dipasquale@unibo.it

ORCID: 0000-0001-5676-8527
Scholar

RESEARCH INTERESTS

- Process Engineering
- Machine Learning
- Molecular Dynamics
- Computational Fluid Dynamics
- Interfacial Phenomena
- Soft Matter (polymers and biomolecules)
- Population Balance Equation
- Condensed Matter

Education

PhD in Chemical Engineering: 2010-2013

Politecnico di Torino (Italy), Department of Applied Science and Technology. Thesis:
Multiscale simulation of polymer nanoparticles precipitation for pharmaceutical applications

Research Activities:
- Modelling of polymer nanoparticles formation in μ-mixers
- Theoretical description of solvent displacement process in a Confined Impinged Jets Mixer
- Validation of the model for the formation of poly-ϵ-caprolactone nanoparticles
- Development and validation of a dual-resolved model Atomistic/Coarse-grained

PIs: Daniele Marchisio, Antonello Barresi, Paola Carbone

M.Eng. Chemical Engineering: 2008-2009 Politecnico di Torino (Italy)
Final Grade 110/110

PI: Daniele Marchisio

B.Eng. Chemical Engineering: 2004-2007 Politecnico di Torino (Italy)
Final Grade 110/110

Employment History

Università di Bologna (Italy): October 2023 - Present
Associate Professor: Department of Industrial Chemistry "Toso Montanari"

Brunel University London (UK): June 2022 - October 2023
Lecturer in Chemical Engineering: Department of Chemical Engineering and Analytical Science

- Module Leader in the courses of "Fluid Mechanics" and "Process System Engineering"

University of Manchester (UK): September 2020-2022 (0.88 FTE)
Research Associate: Department of Chemical Engineering and Analytical Science

- **VIMMP**: Virtual Materials MarketPlace (in collaboration with IBM and Unilever)

PI: Paola Carbone

University of Nottingham (UK): Jun 2021-present (0.22 FTE)
Research Associate: School of Mathematical Sciences
- Population Balance (PB) Models for Porous Media
PI: Matteo Icardi

University of Nottingham (UK): March 2020 - July 2020
Research Fellow: School of Mathematical Sciences
- **SECURe**: Subsurface Evaluation of Carbon Capture and Storage and Unconventional Risk
PI: Matteo Icardi

University of Nottingham (UK): February 2020 - March 2020
Consultancy: School of Mathematical Sciences
- I designed and optimised a new equipment for food processing for Cranswick plc
- Writing of technical reports for the private partner, technology transfer
PI: Matteo Icardi

University of Leicester (UK): January 2017 - December 2019
Research Associate: School of Mathematics and Actuarial Science
- **VFL:** Virtual Formulation Laboratory (in collaboration with Astrazeneca)
PI: Ruslan Davidchack

University of Manchester (UK): January 2014 - December 2016
Research Associate: School of Chemistry
- Development of a New Polarizable Force-field for proteins with **Machine Learning (ML)**
PI: Paul Popelier

Politecnico di Torino (Italy): January 2013 - December 2013
Research Associate: Department of Applied Science and Technology
- Development and validation of a nucleation kinetic law for polymer precipitation
PI: Daniele Marchisio

Teaching

Experience

Brunel University London (UK): 2022/2023
CL2606 - "Fluids Mechanics" 2nd year students in Chemical Engineering
- Lectures
- Assessment
- Marking

CL5655 - "Process System Engineering" 4th year students in Chemical Engineering
- Lectures
- Set up practical activities (lab sessions)
- Assessment
- Marking

University of Manchester (UK): January - March 2022
The Graphene NOWNANO Centre for Doctoral Training (CDT)

Lecturer: Module of *Fundamentals of Molecular Modelling* (PHYS60653) for Postgraduate Students

- Lectures
- Set up practical activities (lab sessions)
    + Training for Molecular Dynamics Simulations in Gromacs
- Assessment
- Marking

University of Manchester (UK): March - April 2021
Department of Chemical Engineering and Analytical Science

Lecturer: Module of *Molecular Modelling and Simulation in Chemical Engineering* "Molecular Dynamics Simulations" section (equivalent to 5 credits out of 15 in total)(CHEN 40232/60232) for Master Students

- Blended Learning teaching: syncronous/asyncronous lectures
- Set up practical activities (lab sessions)
    + Development of a software for Molecular Dynamics simulations in Matlab
- Assessment
- Marking

Politecnico di Torino (Italy): May 2020
Department of Applied Science and Technology

Invited Virtual Lecture: *Mori-Zwanzig formalism for Dimension Reduction* in the module of "Multiscale modelling and coarse-graining for flow and transport PDEs" for PhD students in Chemical Engineering

University of Nottingham (UK): April 2020
School of Mathematics
Assessment preparation: Modelling with Differential Equations for Master students

- Preparation of the questions for the written exam

University of Leicester (UK): 2017-2019

School of Mathematics and Actuarial Science

Assistant Lecturer: Module of *Scientific Computing* for Master Students

- Matlab tutorials and laboratories
- Marking of coursework
- Delivering viva voce exam for stage-one students

Politecnico di Torino (Italy): 2010-2011

Department of Applied Science and Technology

Teaching Assistant: Module of *Chemical Reactors* for Master Students

- Marking of coursework
- Design of both experiments and set-up of the experimental equipment for demonstration:
  + Measurements of the residence time inside a Continuous Stirred-Tank Reactor
  + Derivation of the residence time distribution

Qualifications

Fellow of the HEA Received in December 2021

Fellowships and Awards

- Winner of the *sandpit grant* (24000£) with the project "Calculation of Surface Free Energy of Atomic and Molecular Systems", awarded by CECAM and CCP5, September 2022-September 2023
- "Instant Access" to "Cirrus" an EPSRC Tier-2 National HPC Facilities with the project "Machine learning interface polarization for generalized electrolytes with particle mesh descriptor" equivalent to 15000 CPU-Core-h
- Institute of Advanced Study Residential Fellowship (1500 £), University of Warwick, January 2017
- Honorary Visiting Fellow in the School of Mathematics and Actuarial Science, University of Leicester, December 2019 - December 2021
- Cover Image of the Journal of Computational Chemistry, vol. 35, issue 16, (2014) (`https://onlinelibrary.wiley.com/doi/10.1002/jcc.23635`)

Editorial duties

Reviewer for: Chemical Engineering Science, The Canadian Journal of Chemical Engineering, Molecular Simulation, The Journal of Physical Chemistry, Chimica oggi-Chemistry today, Materials Letters, Entropy

Publication List

∗=corresponding author

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1. **N. Di Pasquale***, A. R. Finney, J. D. Elliott, P. Carbone, M. Salvalaglio, "Constant chemical potential–quantum mechanical–molecular dynamics simulations of the graphene–electrolyte double layer", The Journal of Chemical Physics 158 (13), 134714, 2023

2. **N. Di Pasquale**, T Hudson, M Icardi, L Rovigatti, M Spinaci, "A systematic analysis of the memory term in coarse-grained models: The case of the Markovian approximation", European Journal of Applied Mathematics 34 (2), 326-345, 2023

3. M. Icardi, **N. Di Pasquale**, E. Crevacore, D. L. Marchisio, M. U. Babler, "Population Balance Models for Particulate Flows in Porous Media: breakage and shear-induced events", Transport in Porous Media 146 (1-2), 197-222, 2023

4. **N. Di Pasquale***, D. Davidchack, "Cleaving Method for Molecular Crystals and Its Application to Calculation of the Surface Free Energy of Crystalline β-d-Mannitol at Room Temperature", Journal of Physical Chemistry A, 126:2134, 2022

5. **N. Di Pasquale**, J. D. Elliott, P. Hadjidoukas, P. Carbone *"Dynamically polarisable force-fields for surface simulations via multi-output classification Neural Networks"*, Journal of Chemical Theory and Computation, 17:4477, 2021

6. F. Municchi, **N. Di Pasquale**, M. Dentz, M. Icardi *"Heterogeneous Multi-Rate mass transfer models in OpenFOAM"*, Computer Physics Communications, 261:107763, 2021

7. **N. Di Pasquale***, R. Davidchack *"Shuttleworth equation: A molecular simulations perspective "*, The Journal of Chemical Physics, 153:154705, 2020

8. E. Greiciunas, F. Municchi, **N. Di Pasquale**, M. Icardi , *"Numerical simulation of crust freezing in processed meat: A fully coupled solid-fluid approach"*, Numerical Heat Transfer, Part A: Applications, 78:378, 2020

9. R. Gowers, and P. Carbone, **N. Di Pasquale***, *"A systematic approach to dual scale models"*, Journal of Computational Physics, 413:109465, 2020

10. **N. Di Pasquale***, T. Hudson, M. Icardi, *Systematic derivation of hybrid coarse-grained models*, Physical Review E, 99:013303, 2019

11. R. Yan, S. D. Ma, R. L. Davidchack, **N. Di Pasquale**, T. Jing, H. B. Dong, *Structural and Mechanical Properties of Homogenous solid-liquid interface of Al modelled with COMB3 potential*, Computational Materials Science, 155:136, 2018

12. **N. Di Pasquale**, S. Davie, P. Popelier, *The accuracy of Ab Initio Calculations without Ab Initio Calculations for charged systems: Kriging Predictions of Atomistic Properties for Ions in Water Solutions*, The Journal of Chemical Physics, 148:241724, 2018

13. F. Zielinski, P. I. Maxwell, T. L. Fletcher, S. J. Davie, **N. Di Pasquale**, S. Cardamone, M. J. L. Mills, P. L. A. Popelier *"Geometry Optimization with Machine Trained Topological Atoms"*, Scientific Reports, 7:12817, 2017

14. **N. Di Pasquale***, P. Carbone, *"Local and Global Dynamics of multi-resolved polymer chains: Effects of the interactions atoms-beads on the dynamic of the chains"*, The Journal of Chemical Physics, 146:084905, 2017

15. A. Lavino, **N. Di Pasquale**, P. Carbone, D. Marchisio, *"A novel multiscale model for the simulation of polymer flash nano-precipitation."*, Chemical Engineering Science, 171:485, 2017

16. S. J. Davie, **N. Di Pasquale**, P. L. A. Popelier, *"Kriging Atomic Properties with a Variable Number of Inputs"*, The Journal of Chemical Physics, 145:104104, 2016

17. **N. Di Pasquale**, M. Bane, S. J. Davie, P. L. A. Popelier, *"FEREBUS: Highly Parallelized Engine for Kriging Training"*, Journal of Computational Chemistry, 37:2606, 2016

18. S. J. Davie, **N. Di Pasquale**, P. L. A. Popelier, *"Incorporation of Local Structure into Kriging Models for the Prediction of Atomistic Properties in the Water Decamer"*, Journal of Computational Chemistry, 37:2409, 2016

19. P. Maxwell, **N. Di Pasquale**, S. Cardamone, P. L. A. Popelier, *"The prediction of topologically partitioned intra-atomic and inter-atomic energies by the machine learning method kriging"*, Theoretical Chemistry Accounts, 135:195, 2016

20. **N. Di Pasquale**, S. J. Davie, P. L. A. Popelier, *"Optimization Algorithms in Optimal Predictions of Atomistic Properties by Kriging"*, Journal of Chemical Theory and Computation, 12:1499, 2016

21. **N. Di Pasquale***, D. Marchisio, P. Carbone and A. Barresi, *"Solvent structuring in water-acetone poly-ϵ -Caprolactone mixtures and its effect on the polymer structure and processability"*, The Journal of Physical Chemistry B, 118:13258, 2014

22. **N. Di Pasquale***, R. Gowers and P. Carbone, *"A multiple time step scheme for multiresolved models of Macromolecules"*, Journal of Computational Chemistry, 35:1199, 2014

23. **N. Di Pasquale***, D. Marchisio, P. Carbone and A. Barresi, *"Identification of nucleation rate parameters with MD and validation of the CFD model for polymer particle precipitation"*, Chemical Engineering Research and Design, 91:2275, 2013

24. **N. Di Pasquale***, D. Marchisio and P. Carbone, *"Mixing atoms and coarse-grained beads in modelling polymer melts"*, The Journal of Chemical Physics, 137:164111, 2012

25. **N. Di Pasquale***, D. Marchisio and A. Barresi, *"Model validation for precipitation in solvent-displacement processes"*, Chemical Engineering Science, 84:671, 2012

Conferences and Schools

Conference Organization

- *"6th InterPore UK conference"*, at Brunel University London, 12th-13th September 2022, London, UK
- *"5th CCPBioSim/CCP5 Manchester Multiscale Conference"*, 3rd-5th April 2023, Manchester, UK

Invited contributions

- *"MMM Hub Software Spotlight - LAMMPS"*, hosted by MMM Hub Software, London, UK, 19 January 2023.
- *''Multiscale modelling Applications: Coupling Strategies from Quantum Mechanics to Coarse-Grain models*, the Statistical Mechanics and Thermodynamics Group of the Royal Society of Chemistry, 08 December, 2021
- *''Mori-Zwanzig projection technique in coarse-grained modelling"*, Mixed-gen Season 2 – Session 1: Multiscale simulations of complex materials. Online meeting - hosted by CECAM-HQ, 27 October 2021

Selected contributions

- *"A coupled Constant Potential/Quantum Mechanical/Molecular dynamics simulations for the description of Graphite-electrolytes double layer"*, presented at the Thomas Young Center 6th Energy Workshop, 14-16 December 2022, London, UK
- *"Heat transfer in radially-arranged packings of arbitrary shaped material: a computational study"*, poster presented at the 13th European Congress of Chemical Engineering and 6th European Congress of Applied Biotechnology, 20-23 September 2021
- *"Machine Learning for Polarisable Force-Fields: Neural- Network models for Graphene-Electrolyte interfaces"*, oral contribution presented at Materials and Molecular Modelling Hub++ Conference 2021, 14 - 15 September 2021
- *"Population balance models for particulate flows in porous media: breakage and shear-driven events"*, oral contribution presented at InterPore21, 31 May - 4 June 2021
- *"Description of Surface Properties of Organic Crystals through Molecular Dynamics Simulations "*, oral contribution presented at Midlands Computational Chemistry meeting, 6-7 January 2021
- *"Calculation of Surface Free Energy in Mannitol Crystals through cleaving"*, poster presented at Insights into Processes at Minerals and Materials Surfaces and Interfaces, 17 June 2019, University of Huddersfield, Huddersfield, UK
- *"Calculation of Surface Free Energy in Mannitol Crystals through cleaving"*, poster presented at Future Formulation III, 4th April 2019, University of Leicester, Leicester, UK
- *"Direct calculation of surface free energy of mannitol by molecular dynamics simulations"*, poster presented at New frontiers in particle-based multiscale and coarse-grained modelling, 17 September 2018, Max Planck Institute for Polymer Research, Mainz, Germany
- *"Kriging Models in Predicting Properties of Ions in Solution from First Principle Calculations "*, poster presented at Second CCPBioSim/CCP5 Multiscale Modelling, 13 April 2016, Manchester, UK

- *"Mixing Atoms and Coarse Grained Beads in Modelling Polymer Melts"*, oral contribution presented at Multiscale Modelling of Condensed Phase and Biological Systems, 7 January 2014, Manchester, UK
- *"New formulation of the Nucleation Law for polymer system and coupling with PBE"*, oral contribution presented at 5^{th} International Conference on Population Balance Modelling, Bangalore, India, 11th September, 2013
- *"Simulation of mixing and precipitation of nanoparticles for pharmaceutical applications with CFD and MD"*, oral contribution presented at 14^{th} European Conference on Mixing, Warsaw, Poland, 9th September, 2012
- *"Hybrid Model Atomistic-Coarse-Grained for soft material molecular dynamics simulations"*, poster presented at Coarse-Grained Methods and Self Assembly , 27 July 2011, CECAM-USI, Lugan, Switzerland
- *"Coupling Molecular Dynamics with Computational Fluid Dynamics Via Parameter Passing for the Simulation of Polymer Nanoparticle Precipitation"* oral contribution presented at AIChE 2011 Annual Meeting, Minneapolis, USA, October 16-21, 2011

Conferences Proceedings

- A. D. Lavino, **N. Di Pasquale**, P. Carbone, D. Marchisio. *" Molecules as building blocks for a CFD-PBE model to describe the effect of fluid dynamics on nanoparticle formation"*. In: International Symposium on Industrial Crystallization, ISIC20, Dublin, Ireland, September 3-6, 2017
- A. D. Lavino, **N. Di Pasquale**, P. Carbone, D. L. Marchisio, *" Soft matter self-assembly in acetone-water mixtures: a multiscale modeling approach"* In: SARA 2016, Edinburgh, UK, December 9, 2016. 22
- D. L. Marchisio, A. D. Lavino, **N. Di Pasquale**, P. Carbone, *"Multiscale modelling of macromolecule self-assembly in solution: the case of poly-ϵ-caprolactone in Acetone-Water Mixtures."* In: AIChE 2016 Annual Meeting, San Francisco, USA, November 16-18, 2016
- A. D. Lavino, **N. Di Pasquale**, P. Carbone, A. A. Barresi, D. L. Marchisio, *"Simulation of macromolecule self-assembly in solution: A multiscale approach."* In: AIP Conference Proceedings, 1695:020036, 2015
- **N. Di Pasquale**, P. Carbone, D. Marchisio, *"Multiscale Modelling of Polycaprolactone Self-Assembly in Water-Acetone Mixtures."* In: 2014 AIChE Annual Meeting, Atlanta, USA, November 16-21, 2014
- **N. Di Pasquale**, P. Carbone, D. L. Marchisio, A. A. Barresi *"Simulation of mixing and precipitation of nanoparticles for pharmaceutical applications with CFD and MD."* In: 14^{th} European Conference on Mixing, Warsaw, Poland, 9th September, 2012

Schools

- *Multiscale Modeling of Flowing Soft Matter and Polymer Systems*, CISM course, Udine (IT), July 2016
- *Hierarchical Methods for Dynamics in Complex Molecular Systems*, IAS Winter School, Forschungszentrum Jülich (DE), March 2012
- *Methods in Molecular Simulation Summer School 2011*, organized by CCP5 and sponsored by CECAM, Belfast (UK), July 2011
- *Advanced calculus Summer School*, organized by CASPUR, Rome (IT), August 2010