CHRISTOPHER D. COOPER

Departamento de Ingeniería Mecánica
Universidad Técnica Federico Santa María
Avenida España 1680
Valparaíso, Chile
+56 32 265 4162

PERSONAL INFORMATION

Full name Christopher David Cooper Villagrán

Date, place of birth November 11th, 1984. Viña del Mar, Chile

Nationality Chilean/Spanish

Email address christopher.cooper@usm.cl

christophercooperv@gmail.com

Phone +56 32 265 4450

Website https://bem4solvation.github.io/

EDUCATION

2010-2015 PhD. Mechanical Engineering. Boston University, Boston, MA. *Advisor:* Prof. Lorena Barba.

2010-2012 MS. Mechanical Engineering. Boston University, Boston, MA. *Advisor:* Prof. Lorena Barba.

2003-2009 Professional Mechanical Engineer. Universidad Técnica Federico Santa María, Valparaíso, Chile.

2003-2007 BSc. Mechanical Engineering. Universidad Técnica Federico Santa María, Valparaíso, Chile.

CURRENT EMPLOYMENT

2019- Assistant Professor (Profesor Asistente). Departamento de Ingeniería Mecánica. Universidad Técnica Federico Santa María. Valparaíso, Chile.

2016- Associate Researcher. Centro Científico Tecnológico de Valparaíso (CCTVal). Valparaíso, Chile.

2015-2019 Instructor (Instructor Académico). Departamento de Ingeniería Mecánica. Universidad Técnica Federico Santa María. Valparaíso, Chile.

Courses taught: Introduction to Fluid Mechanics, Advanced Fluid Mechanics, Statistical Thermodynamics, Fundamentals of Computational Fluid Mechanics, Simulation with Fast Algorithms.

PREVIOUS EXPERIENCE

Research

01-03/2017 Visiting Research Assistant. Mathematics Department, University of Michigan, Ann Arbor, MI.

2010-2014 Research assistant. Boston University, Boston, MA.

2008 Visiting Research Assistant. Research exchange program funded by SCAT-ALFA project (`scat-alfa.eu`). University of Bristol, Bristol, UK.

2007 Research assistant. Department of Mechanical Engineering, Universidad Técnica Federico Santa María, Valparaíso, Chile.

Teaching

Fall 2014 Teaching assistant for Practical Numerical Methods in Python (MOOC developed at GWU)

Department of Mechanical and Aerospace Engineering, George Washington University, Washington, DC.

2011 and 2014 Graduate teaching assistant for Mechanics I course.

Mechanical Engineering Department, Boston University, Boston, MA.

August 2011 Designed and taught a one month course on GPU computing at Universidad Técnica Federico Santa María, Valparaíso, Chile.

2010 Graduate teaching assistant for Fluid Mechanics course.

Mechanical Engineering Department, Boston University, Boston, MA.

2006 - 2009 Teaching assistant for General Fluid Mechanics and Fluid Mechanics II courses.

Mechanical Engineering Department, Universidad Técnica Federico Santa María, Valparaíso, Chile.

2004 Teaching assistant for Mathematics I course.

Mathematics Department, Universidad Técnica Federico Santa María, Valparaíso, Chile.

Industry

2009 Project engineer assistant at a R&D&I office

Sociedad de Consultoría e Inversiones Tecnova S.A., Viña del Mar, Chile

FUNDING

As principal investigator

2023-2024 USM-DGIIE Internal project. "Interoperabilidad para flujos de trabajo computacional simples, rápidos y confiables en modelación molecular".

2016-2019 FONDECYT Iniciación. "Full viruses on your local cluster: parallel simulations of virus-cell electrostatic interactions".

2016 USM-DGIIE Internal project. "Modelación y diseño de prototipo para medir tensiones en compósitos poliméricos".

2015 USM-DGIIE Internal project. "Modelación numérica de moléculas ligando en biosensores".

As co-investigator

2021-2023 FONDECYT Regular. "Graphene-based thermal pump to aneble continuous water flow through slit nanochannels".

2017-2018 FONDEF IDeA en dos etapas. "Preparación y caracterización de metamateriales magnéticos para detección remota de tensiones en neumáticos".

2016 USM-DGIP Internal project. "Dinámica del escurrimiento sobre una superficie porosa: aplicación a la predicción de aluviones".

AWARDS AND HONORS

2020 Excellence in Teaching award. Universidad Técnica Federico Santa María.

2013 Travel award for the 2013 International HPC Summer School in New York University from Xsede, Prace and Riken. New York, NY.

2010 Graduate Teaching Fellow. Boston University, Boston, MA.

2010-2013 "Becas Chile" scholarship for doctoral studies. Chile.

2009 "Colegio de Ingenieros de Chile" Prize. Valparaíso, Chile.

2009 "Federico Santa María" Prize for best Mechanical Engineering graduate. Universidad Técnica Federico Santa María, Valparaíso, Chile.

2008 Mobility grant as part of the Scientific Computing Advanced Training (SCAT) project, funded by the ALFA program to the University of Bristol, Bristol, UK.

2004-2009 University's honor list for outstanding students. Universidad Técnica Federico Santa María, Valparaíso, Chile.

2003 Scholarship for high score in University admissions National Test (PAA). Universidad Técnica Federico Santa María, Valparaíso, Chile.

COMPUTER SKILLS

Languages C/C++, Python, Matlab, CUDA

Libraries MPI, OpenMP

Software iWork, MS Office, LaTeX, Git

OS OSX, Windows, Linux

LANGUAGES

English Bilingual proficiency

Spanish Native proficiency

PUBLICATIONS

Journal publications

I. Addison-Smith, H.V. Guzmán, C.D. Cooper. Accurate boundary-integral formulations for the calculation of electrostatic forces with an implicit-solvent model. *J. Chem. Theory and Comput.* **19** (10) 2996-3006 (2023).

M.A. Ruiz-Rodriguez, C.D. Cooper, W. Rocchia, M. Casalegno, Y.L. de los Santos, G. Raos. Modeling of the Electrostatic Interaction and Catalytic Activity of [NiFe] Hydrogenases on a Planar Electrode. *J. Phys. Chem. B* **126** (43) (2022)

C.D. Cooper, I. Addison-Smith, H.V. Guzmán. Quantitative electrostatic force tomography for virus capsids in interaction with an approaching nanoscale probe. *Nanoscale.* **14** (34) (2022).

S.A. Urzúa, P.Y. Sauceda-Oloño, C.D. García, C.D. Cooper. Predicting the Orientation of Adsorbed Proteins Steered with Electric Fields Using a Simple Electrostatic Model. *Journal of Physical Chemistry B.* **126** (289) (2022)

S.D. Search, C. D. Cooper, and E. van't Wout. Towards optimal boundary integral formulations of the Poisson-Boltzmann equation for molecular electrostatics.*Journal of Computational Chemistry.* **43**(10)(2022)

V. Ramm, J. H. Chaudhry, and C. D. Cooper. Efficient mesh refinements for the Poisson-Boltzmann equation with boundary elements. *Journal of Computational Chemistry.* **42**(12)(2021)

M. Martínez, C. D. Cooper, A. B. Poma, and H. V. Guzmán. Free Energies of the Disassembly of Viral Capsids from a Multiscale Molecular Simulation Approach. *Journal of Chemical Information and Modeling.* **60**(2)(2019)

N. C. Clementi, C. D. Cooper, and L. A. Barba. Computational nanoplasmonics in the quasistatic limit for biosensing applications. *Physical Review E.* **100** (6) (2019)

C. D. Cooper. A boundary-integral approach for the Poisson-Boltzmann equation with polarizable force fields. *Journal of Computational Chemistry.* **40**(18)(2019): 1680-1692. arxiv:1810.03698

N. C. Clementi, G. Forsyth, C. D. Cooper, and L. A. Barba. PyGBe-LSPR: Python and GPU Boundary-integral solver for electrostatics. *Journal of Open Source Software.* **2**, 19 (2017): 36. 10.21105/joss.00306

A. Molavi Tabrizi, S. Goossens, A. Mehdizadeh Rahimi, C. D. Cooper, M. G. Knepley, and J. P. Bardhan. Extending the Solvation-Layer Interface Condition Continum Electrostatic Model to a Linearized Poisson–Boltzmann Solvent. *Journal of Chemical Theory and Computation* **13** (6) (2017): 2897-2914

C. D. Cooper, N. C. Clementi, G. Forsyth, and L. A. Barba. PyGBe: Python, GPUs and Boundary elements for biomolecular electrostatics. *Journal of Open Source Software.* **1** (2016):43. 10.21105/joss.00043

C. D. Cooper and L. A. Barba. Poisson-Boltzmann model for protein-surface electrostatic interactions and grid-convergence study using the PyGBe code. *Comput. Phys. Commun.* 202 (2016): 23-32. arxiv:1506.03745

C. D. Cooper, N. C. Clementi and L. A. Barba. Probing protein orientation near charged nanosurfaces for simulation-assisted biosensor design. *J. Chem. Phys.* 143 **12** (2015): 124709. arXiv:1503.08150

C. D. Cooper, J. P. Bardhan, L. A. Barba. A biomolecular electrostatics solver using Python, GPUs and boundary elements that can handle solvent-filled cavities and Stern layers. *Comput. Phys. Commun.* 185 **3** (2014): 720-729. arXiv:1309.4018

Conference presentations

C. D. Cooper, M. O. Fenley, and H. V. Guzmán. Computing electrostatics interactions of biomolecular and bio-materials complexes with a robust and user-friendly PB framework. *Protein Electrostatics Conference.* Genoa, Italy. June 2023.

C. D. Cooper. A boundary integral computational framework for molecular electrostatics modeling. *SIAM Conference on Computational Science and Engineering.* Amsterdam, Netherlands. March, 2023.

S. Urzúa and C. D. Cooper. Evaluación del efecto de campos eléctricos en la interacción proteína -superficie usando un modelo continuo y el método de elementos de frontera. *XIX Jornada de Mecánica Computacional.*. Valparaíso, Chile. October, 2021.

M. Guerrero and C. D: Cooper. Acoplamiento BEM-FEM para la simulación de nanoestructuras disueltas en un medio salino, a partir de la ecuación de Poisson-Boltzmann. *XIX Jornada de Mecánica Computacional.*. Valparaíso, Chile. October, 2021.

C. D. Cooper and P. Fernández. An analysis of the approximations and errors in a boundary integral solution of the Poisson-Boltzmann equation. *SIAM Conference on Computational Science and Engineering.* Spokane, WA. February, 2019.

C. D. Cooper. Polarizable force fields in an implicit solvent model with a boundary integral approach. *SIAM Conference on the Life Sciences.* Minneapolis, MN. August, 2018.

C. D. Cooper. Biomolecular electrostatics calculations using polarizable force fields in a continuum ionic solvent, with algorithmic and hardware acceleration. *13^{th} World Congress on Computational Mechanics.* New York, NY. July, 2018.

C. D. Cooper. Numerical simulations of sensitivity in LSPR biosensors. *X Conferencia Iberoamericana de Sensores Ibersensor 2016.* Viña del Mar, Chile (October, 2016).

S. Flores and C. D. Cooper. Jupyter notebooks como herramienta versátil para docencia en cursos STEM. *XIXX Congreso Chileno de Educación en Ingeniería, SOCHEDI 2016.* Pucón, Chile (October, 2016).

C. D. Cooper. Modelación numérica de nano-biosensores con modelos continuos. *XVI Congreso Chileno de Ingeniería Mecánica, COCIM 2015.* Valparaíso, Chile (November, 2015).

C. D. Cooper and L. A. Barba. Implicit solvent model using Python and GPUs for proteins interacting with charged surfaces. *XXVI IUPAP Conference on Computational Physics, CCP 2014.* Boston, MA (August, 2014).

C. D. Cooper, J. P. Bardhan and L. A. Barba. Efficient boundary element methods for molecular electrostatics using Python and GPUs. *SIAM Conference on Computational Science and Engineering.* Boston, MA (February, 2013).

C. D. Cooper and L. A. Barba. Fast tree methods and GPUs for protein electrostatics. *Symposium of the International Association for Boundary Element Method, IABEM 2013.* Santiago, Chile (January, 2013).

C. D. Cooper and L. A. Barba. Efficient Boundary Element Methods in Python with GPUs. *10^{th} World Congress on Computational Mechanics.* Sao Paulo, Brazil (July, 2012).

F. A. Cruz, C. D. Cooper, R. Yokota, L. A. Barba. Parallel Implementation of the Panel-free Boundary Conditions for the Viscous Vortex Method. *21^{st} International Conference on Parallel Computational Fluid Dynamics.* Moffet Field, CA (2009).

C. D. Cooper, L. A. Barba. Panel-free Boundary Conditions for the Viscous Vortex Method. *19^{th} AIAA Computational Fluid Dynamics Conference.* San Antonio, TX (2009).

Posters and other presentations

C. D. Cooper. Using a simple electrostatic model to study the interaction between proteins and surfaces. *Department of Chemistry, Materials, and Chemical Engineering Seminar.* Politecnico di Milano, Milan, Italy. June, 2023 (Invited talk)

C. D. Cooper. Why should we talk more about boundary integrals to computational chemists?. *UCL-Imperial Numerics Seminar.* UCL, London, UK. February, 2023. (Invited talk)

C. D. Cooper. Poisson-Boltzmann calculations with AMOEBA from a Jupyter notebook. *Tinker Developer Workshop.* NIH, Bethesda, MD. June, 2022. (Invited talk)

C. D. Cooper. Keeping it simple at large scales: a Python-based Poisson-Boltzmann tool to aid in the road to Exascale. *CECAM Workshop: Advances in Electrostatic calculations: the road towards the Exascale.* July, 2021 (Invited talk)

C. D. Cooper. A fast and accurate solution of the Poisson-Boltzmann equation with boundary elements. *Department of Mathematics and Statistics Seminar.* Department of Mathematics and Statistics, University of New Mexico, Albuquerque, NM. October, 2019. (Invited talk)

C. D. Cooper. Modeling molecular solvation with continuum models from a boundary integral perspective. *Molecular Biophysics Seminar.* Oden Institute, University of Texas, Austin. October, 2019. (Invited talk)

C. D. Cooper. Dissolving proteins with continuum models: electrostatics and boundary integral methods. *Colloquim of the Centro Interdisciplinario de Neurociencias de Valparaíso.* University of Valparaíso. July, 2019. (Invited talk)

M. Martínez, H. V. Guzmán, and C. D. Cooper. Implicit solvent calculations at large scale: virus-level Poisson-Boltzmann and multiscale simulations for electrostatics. *Biophysical Society Meeting.* Baltimore, MD. March, 2019. (Poster) DOI: `https://doi.org/10.1016/j.bpj.2018.11.1574`.

C. D. Cooper. Disolviendo moléculas con modelos continuos. *X Escuela de Nanoestructuras*, Departamento de Física, Universidad Técnica Federico Santa María. Valparaíso, Chile. January, 2019. (Invited talk)

C. D. Cooper. GPUs en computación científica: programación y aplicaciones. *Presentation for undergraduate level course on HPC at Pontificia Universidad Católica de Chile.*. November, 2018. (Invited talk)

C. D. Cooper. Biomolecular solvation from the interface: boundary integrals and HPC for bioelectrostatics. *Seminario del Centro Científico Tecnológico de Valparaíso (CCTVal)*, Universidad Técnica Federico Santa María. Valparaíso, Chile. August, 2018. (Invited talk)

C. D. Cooper. Biomolecular solvation from the interface: Poisson-Boltzmann, GPUs and boundary elements. *Department of Biomedical Engineering Seminar, The University of Iowa.* Iowa City, IA. August, 2018. (Invited talk)

C. D. Cooper. A boundary integral approach for protein electrostatics with polarizable force fields. *SIAM Conference on the Life Sciences.* Minneapolis, MN. August, 2018. (Poster).

C. D. Cooper. Biomolecular Simulations in a Continuum Ionic Solvent with Polarizable Force Fields, Using Python and GPUs. *Biophysical Society Meeting 2018.* San Francisco, CA. February, 2018. (Poster) DOI: `https://doi.org/10.1016/j.bpj.2017.11.3644`.

C. D. Cooper. Dissolving proteins with continuum models: a Poisson-Boltzmann solver in Python, with GPUs and boundary elements. *Theoretical and Computational Biophysics Group Seminar.* Beckman Institute, University of Illinois, Urbana-Champaign, IL. March, 2017. (Invited talk)

C. D. Cooper. Simulating protein electrostatics with Python and GPUs: implementation and applications. *First Chilean Symposium on Boundary Element Methods.* Pontificia Universidad Católica de Chile, Santiago, Chile. December, 2016. (Invited talk)

C. D. Cooper. Solvating proteins with continuum models: a Poisson-Boltzmann solver in Python, with GPUs and boundary elements. *Computational Methods in Biology and Biomedicine.* Pontificia Universidad Católica de Chile, Santiago, Chile. September, 2016. (Invited talk)

C. D. Cooper. Electrostática en proteínas: presente y futuras direcciones. Centro Científico Tecnológico de Valparaíso (CCTVal), Universidad Técnica Federico Santa María, Valparaíso, Chile. March, 2016. (Invited talk)

C. D. Cooper. Biomolecular electrostatics with continuum models: a boundary integral implementation and applications to biosensors. Invited talk. *Coloquio de Informática.* Departamento de Informática, Universidad Técnica Federico Santa María, Valparaíso, Chile. March, 2015. (Invited talk)

C. D. Cooper and L. A. Barba. Using GPUs for the boundary element method. *CUDA Research Fast Forward - NVIDIA Booth, Supercomputing 2011.* Seattle, WA. November, 2011.

EVENT ORGANIZATION

Second Chilean Symposium on Boundary Element Methods. Universidad Técnica Federico Santa María, Valparaíso, Chile. December, 2018.

WORKSHOPS

International Summer School on HPC Challenges in Computational Sciences. Organized by Xsede, Prace and Riken. New York, NY (July, 2013).

Pan-American Advanced Studies Institute: Scientific computing in the Americas, the challenges of massively parallel. Organized by L. Barba with NSF funding. Valparaíso, Chile (January, 2011).

RESEARCH INTERESTS

Boundary element methods

Continuum electrostatics for biomolecular simulations

Treecodes and Fast Multipole Methods

GPU computing

Computational Fluid Dynamics