Henrique Musseli Cezar

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A Ph.D. candidate working with computational physics/chemistry and developing scientific software. My main research interest is the efficient sampling of molecular structure and thermodynamic properties, specially using Monte Carlo methods.

Education

2015– **PH.D. CANDIDATE in Physics, Institute of Physics, University of São Paulo**
Implementation and Development of Efficient Algorithm for Intramolecular Deformation with the Monte Carlo Method
CNPq Ph.D. Fellowship - Advisor: Dr. Kaline R. Coutinho

2013–2015 **MASTER'S in Computational Physics, São Carlos Institute of Physics, University of São Paulo**
Implementation of the Parallel Tempering Monte Carlo Method to the Study of Thermodynamic Properties of Nanoclusters
FAPESP Master Fellowship - Advisor: Dr. Juarez L. F. Da Silva

2009–2012 **B.S. in Computational Physics, São Carlos Institute of Physics, University of São Paulo**
Undergraduate Research with Dr. Leonardo P. Maia: Fluid Dynamics in Porous Media with Lattice Boltzmann - CNPq Scientific Initiation Fellowship

Complementary Education

2015 COURSERA ONLINE COURSE: Algorithms: Design and Analysis, Part 1. (Duration: 36h). Stanford University

2006–2008 TECHNICAL COURSE in Informatics, Colégio Divino Salvador

Computational Skills

Proficient with programming languages (from more to less proficient): Fortran (legacy and modern), C, Python, C++ and Bash. I have experience with OpenMP parallelization, code profiling and optimization, and also have knowledge in MPI and Pthreads parallelization.

Research overview

My research is mainly focused on the development of algorithms and computer code to efficiently sample properties of organic molecules and metallic nanoclusters with intricate potential energy surface and/or embedded in solvent. Specifically, I have experience with Monte Carlo methods and extended ensemble methods such as replica exchange. I also have some experience in global optimization and clustering. Recently, my work has been focused on the development of a Bias Monte Carlo method to sample internal degrees of freedom of organic molecules and peptides in solution, which is the main subject of my Ph.D. thesis. To achieve the objectives of my research, my work rely on high performance computing, and for this reason, I also have some interest in this field.

Software development

Apart from several scripts and smaller software, I am one of the main developers of two scientific softwares:

Cezar HM, Canuto S, Coutinho K

Dice

A Monte Carlo code for simulation of liquids and gases, specifically, solute/solvent systems. My main contribution is the coding and development of a Configurational Bias Monte Carlo method to add the sampling of internal degrees of freedom of molecules. The code is written in Fortran and has OpenMP parallelization.

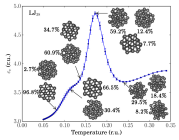
Rondina GG, **Cezar HM**, Da Silva JLF

GOTNano

A code for global optimization and to obtain thermodynamic properties of nanoclusters. My main contribution is the implementation of the Parallel Tempering Monte Carlo algorithm to sample the thermodynamic properties. The code is written in C and has OpenMP parallelization.

Publications

Submitted and Under Review



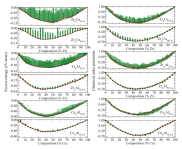
Cezar HM, Rondina GG, Da Silva JLF

Parallel Tempering Monte Carlo Combined with Clustering Euclidean Metrics Analysis to Study the Thermodynamic Stability of Lennard-Jones Nanoclusters

Under review at Journal of Chemical Physics ·

We use a clustering algorithm to analyze trajectories from a Parallel Tempering Monte Carlo simulation of Lennard-Jones nanoclusters, identifying the phase changes and most most frequent structures with great accuracy using a simple approach.

Published



De Souza DG, **Cezar HM**, Rondina GG, De Oliveira MF, Da Silva JLF

A Basin-hopping Monte Carlo Investigation of the Structural and Energetic Properties of 55- and 561-atom Bimetallic Nanoclusters: the Examples of the ZrCu, ZrAl, and CuAl Systems

Journal of Physics: Condensed Matter 28:175302, 2016 · DOI

We report a basin-hopping Monte Carlo investigation of the structural and energetic properties of bimetallic ZrCu, ZrAl, and CuAl nanoclusters with 55 and 561 atoms, showing how the atoms of the different species are distributed in the structure and a trend of more spherical structures at 50-50 compositions.

The LaTeX template for this CV is forked from https://github.com/jchodera/latex-cv