Workshop on Monte Carlo Simulations

It is intended for students and reasearchers in chemistry, physics, chemical engeneering and biological fields.

Goal: Learning the basics of Monte Carlo methods and their applications in phase equilibria and adsorption of fluids in porous materials.

Professor: ***Jeffrey Potoff,*** ***Wayne University, USA.***
Dates: ***May 17th (10:00 to 18:00) and 18th (10:00 to 13:00)***
Place: ***Hotel Ritz, Zócalo, Mexico City.***
Cost: $660.00 MXN for two days coffee and one meal.
The accommodation is not included in the price.
Registration: montecarlogomc@yahoo.com
Registration Deadline: May 14th.
Maximum number of participants: 30.

Theory and practice:

1. The Monte Carlo Method.
2. Force Fields/Models.
3. Ensembles: NVT, NPT, GCMC and Gibbs ensemble.
4. Adsorption.
5. Histogram reweighting.
6. Advanced sampling methods.
7. Use of multi-core CPU and GPU architecture to increase code performance.

The payment has to be done before May 14th to:
Hotelera Centro Histórico SA de CV
Bank: Banamex
Account: 7745806
Sucursal 100

Exercises using GOMC: *GPU Optimized Monte Carlo is a parallel molecular simulation code designed for high-performance simulation of large systems.*

Every participant must download and install the program in advance from http://gomc.eng.wayne.edu

Organizers

Dr. José Alejandre. UAM-Iztapalapa
Dr. Edgar Núñez Rojas. CONACyT – UAM-Iztapalapa

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