

JOURNAL PAPERS

Refereed Journal Papers

1. Orkoulas, G., "Spatial updating Monte Carlo algorithms in particle simulations", *Molecular Simulation*, in press, (2010).
2. Noon, D. P. and G. Orkoulas, "Simulation of phase transitions via spatial updating and tempering", *Molecular Simulation*, in press, (2010).
3. Zhang, X., G. Hu, G. Orkoulas and P. D. Christofides, "Controller and Estimator Design for Regulation of Film Thickness, Surface Roughness and Porosity in a Multiscale Thin Film Growth Process," *Ind. Eng. Chem. Res.*, in press, (2010).
4. Orkoulas, G., "An Overview of Monte Carlo methods for Fluid Simulation," *Computing in Science and Engineering*, **11**(5) 76, (2009); invited review article.
5. Orkoulas, G. and D. P. Noon, "Spatial updating in the great grand canonical ensemble," *J. Chem. Phys.*, **131** 161106 (2009).
6. O'Keeffe, C. J. and G. Orkoulas, "Parallel Canonical Monte Carlo Simulations through Sequential Updating of Particles," *J. Chem. Phys.*, **130** 134109, (2009).
7. Hu, G., J. Huang, G. Orkoulas and P. D. Christofides, "Investigation of Film Surface Roughness and Porosity Dependence on Lattice Size in a Porous Thin Film Deposition Process via Kinetic Monte Carlo Simulations," *Phys. Rev. E*, **80** 041122, (2009).
8. Hu, G., G. Orkoulas and P. D. Christofides, "Stochastic Modeling and Simultaneous Regulation of Surface Roughness and Porosity in Thin Film Deposition," *Ind. Eng. Chem. Res.*, **48** 6690, (2009).
9. Hu, G., G. Orkoulas and P. D. Christofides, "Regulation of Film Thickness, Surface Roughness and Porosity in Thin Film Growth Using Deposition Rate," *Chem. Eng. Sci.*, **64** 3903, (2009).
10. Hu, G., G. Orkoulas and P. D. Christofides, "Modeling and Control of Film Porosity in Thin Film Deposition," *Chem. Eng. Sci.*, **64** 3668, (2009).
11. O'Keeffe, C. J., R. Ren and G. Orkoulas, "Spatial Updating Grand Canonical Monte Carlo Algorithms for Fluid Simulation: Generalization to Continuous Potentials and Parallel Implementation," *J. Chem. Phys.*, **127** 194103, (2007).
12. Orkoulas, G., "Acceleration of Monte Carlo Simulations through Spatial Updating in the Grand Canonical Ensemble," *J. Chem. Phys.*, **127** 084106, (2007).
13. Ren, R. and G. Orkoulas, "Parallel Markov Chain Monte Carlo Simulations," *J. Chem. Phys.*, **126** 211102, (2007).
14. Ren, R., C. J. O'Keeffe and G. Orkoulas, "Sequential Metropolis algorithms for fluid simulations," *Int. J. Thermophys.*, **28** 520, (2007).
15. Ren, R., C. J. O'Keeffe and G. Orkoulas, "Sequential updating algorithms for grand canonical Monte Carlo simulations," *Molecular Physics*, **105** 231, (2007).
16. Ren, R., C. J. O'Keeffe and G. Orkoulas, "Scaling fields and pressure mixing in the Widom-Rowlinson model," *J. Chem. Phys.*, **125** 144505, (2006).
17. Ren, R., C. J. O'Keeffe and G. Orkoulas, "Simulation of symmetric tricritical behavior in electrolytes," *J. Chem. Phys.*, **125** 124504, (2006).

18. Pérez-Pellitero, J., P. Ungerer, G. Orkoulas and A. D. Mackie, "Critical point estimation of the Lennard-Jones pure fluid and binary mixtures," *J. Chem. Phys.*, **125** 054515, (2006).
19. Ren, R. and G. Orkoulas, "Acceleration of Markov chain Monte Carlo simulations through sequential updating," *J. Chem. Phys.*, **124** 064109, (2006).
20. Son, J., G. Orkoulas and A. B. Kolomeisky, "Monte Carlo simulation of rigid biopolymer growth processes," *J. Chem. Phys.*, **123** 124902, (2005).
21. Kim, Y. C., M. E. Fisher and G. Orkoulas, "Asymmetric fluid criticality. I. Scaling with pressure mixing," *Phys. Rev. E*, **67** 061506, (2003).
22. Orkoulas, G., S. K. Kumar and A. Z. Panagiotopoulos, "Monte Carlo study of Coulombic criticality in polyelectrolytes," *Phys. Rev. Lett.*, **90** 048303, (2003).
23. Orkoulas, G., M. E. Fisher and A. Z. Panagiotopoulos, "Precise simulation of criticality in asymmetric fluids," *Phys. Rev. E*, **63** 051507, (2001).
24. Romero-Enrique, J. M., G. Orkoulas, A. Z. Panagiotopoulos and M. E. Fisher, "Coexistence and criticality in size-asymmetric hard-core electrolytes," *Phys. Rev. Lett.*, **85** 4558, (2000).
25. Orkoulas, G., A. Z. Panagiotopoulos and M. E. Fisher, "High resolution study of fluid criticality," *Computer Simulation Studies in Condensed Matter Physics XIII*, (2000).
26. Orkoulas, G., M. E. Fisher and C. Üstün, "The Yang-Yang relation and the specific heats of propane and carbon dioxide," *J. Chem. Phys.*, **113** 7530, (2000).
27. Fisher, M. E. and G. Orkoulas, "The Yang-Yang anomaly in fluid criticality: Experiment and scaling theory," *Phys. Rev. Lett.*, **85** 696, (2000).
28. Orkoulas, G., M. E. Fisher and A. Z. Panagiotopoulos, "Criticality and crossover in accessible regimes," *Phys. Rev. E*, **61** 5930, (2000).
29. Orkoulas, G. and A. Z. Panagiotopoulos, "Phase behavior of the restricted primitive model and square-well fluids from Monte Carlo simulations in the grand canonical ensemble," *J. Chem. Phys.*, **110** 1581, (1999).
30. Orkoulas, G. and A. Z. Panagiotopoulos, "Phase Diagram of the two-dimensional Coulomb Gas: A thermodynamic scaling Monte Carlo study," *J. Chem. Phys.*, **104** 7205, (1996).
31. Orkoulas, G. and A. Z. Panagiotopoulos, "Free energy and phase equilibria for the restricted primitive model of ionic fluids from Monte Carlo simulations," *J. Chem. Phys.*, **101** 1542, (1994).
32. Orkoulas, G. and A. Z. Panagiotopoulos, "Chemical Potential in ionic systems from Monte Carlo simulations with distance-biased test particle insertions," *Fluid Phase Equil.*, **83** 223, (1993).

Refereed Conference Proceedings Papers

1. Hu, G., X. Zhang, G. Orkoulas and P. D. Christofides, "Simultaneous Regulation of Film Thickness, Surface Roughness and Porosity in a Multiscale Thin Film Growth Process," *Proceedings of the 48th IEEE Conference on Decision and Control, Shanghai, China*, 2387, (2009).
2. Hu, G., G. Orkoulas and P. D. Christofides, "Simultaneous Regulation of Surface Roughness and Porosity in Thin Film Growth," *Proceedings of International Symposium on Advanced Control of Chemical Processes, Istanbul, Turkey*, 6 pages, paper 169, (2009).
3. Hu, G., G. Orkoulas and P. D. Christofides, "Model Predictive Control of Film Porosity in Thin Film Deposition," *Proceedings of the American Control Conference, St. Louis, MO*, 4797, (2009).

4. Hu, G., G. Orkoulas and P. D. Christofides, “Stochastic Modeling of Film Porosity in Thin Film Deposition,” *Proceedings of the American Control Conference, St. Louis, MO*, 4771, (2009).
5. Lou, Y., G. Hu, P. D. Christofides and G. Orkoulas, “Parameter identification for nonlinear stochastic PDE model of a sputtering process,” *Proceedings of the 8th IFAC Symposium on Dynamics and Control of Process Systems*, **3** 217, (2007).

Submitted for Publication

1. Zhang, X., G. Hu, G. Orkoulas and P. D. Christofides, “Predictive Control of Surface Mean Slope and Roughness in a Thin Film Deposition Process,” *Chem. Eng. Sci.*, submitted, (2010).
2. Huang, J., G. Hu, G. Orkoulas and P. D. Christofides, “Dynamics and Lattice-Size Dependence of Surface Mean Slope in Thin Film Deposition,” *Ind. Eng. Chem. Res.*, submitted, (2010).
3. Zhang, X., G. Hu, G. Orkoulas and P. D. Christofides, “Estimation-Based Control of Film Surface Roughness, Porosity and Thickness in a Multiscale Thin Film Growth Process,” *Proceedings of the 49th IEEE Conference on Decision and Control*, submitted, Atlanta, Georgia, (2010).
4. Hu, G., J. Huang, G. Orkoulas and P. D. Christofides, “Dependence of Film Surface Roughness on Lattice Size and Temperature in Thin Film Deposition,” *Proceedings of the 49th IEEE Conference on Decision and Control*, submitted, Atlanta, Georgia, (2010).
5. Zhang, X., G. Hu, G. Orkoulas and P. D. Christofides, “Simultaneous Regulation of Thin Film Surface Mean Slope and Roughness For Light Trapping Optimization Using Predictive Control,” *Proceedings of the 49th IEEE Conference on Decision and Control*, submitted, Atlanta, Georgia, (2010).
6. Zhang, X., G. Hu, G. Orkoulas and P. D. Christofides, “Model Predictive Control of Surface Mean Slope in a Thin Film Deposition Process,” *Proceedings of 9th International Symposium on Dynamics and Control of Process Systems*, submitted, 6 pages, Leuven, Belgium, (2010).
7. Huang, J., G. Hu, G. Orkoulas and P. D. Christofides, “Lattice-Size Dependence and Dynamics of Surface Mean Slope in a Thin Film Deposition Process,” *Proceedings of 9th International Symposium on Dynamics and Control of Process Systems*, submitted, 6 pages, Leuven, Belgium, (2010).

In Preparation

1. Cerdeiriña, C. A., G. Orkoulas and M. E. Fisher “The Yang-Yang Anomaly in Fluid Criticality: Exactly Soluble Models,” in preparation.

PRESENTATIONS

Summary of Contributed Presentations

47 contributed and invited presentations at conferences.