Position: **Ricercatore**

Affiliation: **IPCF - Consiglio Nazionale delle Ricerche**

Address: **Physics Dept, University "La Sapienza"P.le A. Moro 2, 00185, Rome, Italy**

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Research Interests My work focuses on complex and biological flows investigated via simulation, with target systems ranging from molecular fluids to macromolecules and suspensions in aqueous and ionic environments. I am specially interested in biofluids such as blood, described from the red blood cells up to large scale physiological level.

I take advantage of simulations techniques, such as Molecular Dynamics, Monte Carlo, Lattice Boltzmann and Density Functional Theory. I actively develop new methods aimed at a unified multiscale modeling, ranging from Gibbs to Boltzmann descriptions applied to microscopic, mesoscopic or macroscopic scenarios.

Ongoing Projects

- **Biofluidics and Hemodynamics**
- **Multi Scale Modelling: From Atoms to Hydrodynamics**
- **Biological water, DNA and proteins**

Related Links

- Harvard Hemodynamics
- DLPROTEIN distribution site and development site

Curriculum Vitae

Professional Address:

IPCF – CNR, Dipartimento di Fisica – Università La Sapienza

P.le A. Moro 2, 00185 Rome, Italy

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+39 06 4991 4239 (office)

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Professional Profile:

Computational physicist of biological and physiological systems

Education

- Master degree in Physics (1993), University of Rome La Sapienza. Title of the thesis: Molecular Dynamics methods for solid mixtures at constant temperature and pressure. Application to the solution of deuterium in palladium. Advisors: Prof. G. Ciccotti and Prof. A. Tenenbaum.

- PhD in Chemistry (1997), University of Rome La Sapienza. Title of the thesis: Structural study of monomeric microperoxidases in water and water/methanol solution by molecular dynamics simulations. Advisor Prof. M. Barteri. Thesis accepted without amendments.

Employment

- Ecole Polytechnique Fédérale de Lausanne, Switzerland (Research Scientist, 2009-2010)

- Harvard University, School of Engineering and Applied Sciences (Research Scientist, 2007-2009)
- National Research Council, Italy (Senior Research Scientist, Permanent Position, 2005-)
- Ylichron Ltd., Italy (2004-2005)
- National Research Council, Italy (Junior Research Scientist, 2003-2004)
- Institute for Condensed Matter (INFM, CNR), Italy (Post-doc, 2002)
- University of Cambridge, department of Chemistry (Post-doc, 1998-2001)
- University of Rome La Sapienza, department of Physics (Post-doc, 1998)
- Ecole Polytechnique Fédérale de Lausanne, IRRMA (Post-doc, 1998)

Work experience

- Multiscale cardiovascular response

1. Plasma and cellular dynamics from micrometric to millimetric scales
2. Microrheology at varying hematocrit level, vessel morphology and pulsatility

- Soft materials at molecular level: proteins, oligopeptides, DNA, lipids, membranes

1. Structure and dynamics at varying conditions (hydration, thermodynamic point, etc)
2. Electronic structure and function of biomolecules
3. Sampling analysis and enhancement
4. DNA translocation for sequencing in solid-state nanopores

- Water, colloids and ionic solvents

1. Phase coexistence and intermittency of water under confinement
2. Non-equilibrium loads and ratchet effect
3. Electro-osmotic and dielectric forces
4. Depletion interactions

Methodological expertise

- Multi-scale modeling and simulations

1. Hybrid methods for suspended bodies of finite size
2. Synthetic models via Lattice Boltzmann and Lattice Fokker-Planck methods
3. Structure, thermodynamics and dynamics of inhomogeneous fluids
4. Statistical foundations for particle-based and field-based numerical methods
5. Electrostatics and polarizable media

- Particle-based simulations via Molecular Dynamics and Monte Carlo

1. Deterministic and stochastic simulation methods
2. Constrained and multiple time-step molecular dynamics
3. Kinetic methods for correlated atomic systems
4. Ensemble transformations via feed-backs
5. Enhanced sampling of rare events
6. Force field modeling and statistical inversion

- General-purpose numerical analysis

1. Complexity, robustness and feasibility
2. Truncation and finite-precision control
3. Optimization and algorithmic design

High Performance Computing

- Design and deployment of large scale software packages (DLPROTEIN, IMAGE, MUPHY)
- Parallel Programming with message passing and shared memory paradigms
- Distributed clusters and highly scalable platforms (Blue Gene)
- HPC on General Purpose Graphical Processing Units (GP-GPU)
- Objected-oriented, procedural, scripting programming and scientific visualization

Consultancy and Collaborations

- Harvard Medical School, Brigham and Women’s Hospital, USA
- University of Cambridge, UK
- Council for New Technologies, Energies and Environment (ENEA), Italy

- ENI R&D, Donegani Institute, Italy
- Institute for Applied Mathematics IAC, CNR, Italy
- University of Trento, Italy
- University of Rome 2, Italy
- University of Rome 1, Italy
- Université Libre de Bruxelles, Belgium

Awards and Fellowships

- Gordon Bell Honorable Mention, Supercomputing Conference, Seattle (2011)
- Finalist at the Gordon Bell Award, Supercomputing Conference, New Orleans (2010)
- Best Invited Talk, International Conference on Computational Science, Beijing (2007)
- Research Fellowship, CINECA Supercomputing center, Casalecchio di Reno (2001)
- Research Fellowship, Leverhulme Trust, UK (1998)
- INFM Prize for Junior Research, Italy (1997)
- Research fellowship of the European Human Capital Mobility Program, EU (1997)
- Silicon Graphics Prize for Junior Research, Italy (1996)
- PhD Fellowship in Chemistry, Italy (1994)

Teaching and Educational Activity

- Academic Years 2004-2006: Course “Computational methods for biological applications”, Graduate Level, Faculty of Engineering, University of Rome La Sapienza, Italy.

- Years 2001-2002: Course “Biosimulation with DLPROTEIN”. University of Rome la Sapienza.

- Years 2000-2001: “HPC simulation methods in biology”. Supercomputing Center Cineca, Italy.

- Academic Years 1996-1998: Course “Computer Programming, Architectures and Algorithmic Design”, Undergraduate Level, Faculty of Environmental Science, University of Tuscia, Italy.

- Joint supervision of the graduate students:

1. Marcello Sega, Department of Physics, University of Trento. 1998-2002
2. Michelle Borkin, School of Engineering and Applied Sciences, Harvard University, 2008-
3. Amanda Peters, School of Engineering and Applied Sciences, Harvard University, 2008-

- 2005-2006: Joint supervision of the master students:

1. Raffaele Sinibaldi, Department of Physics, University of Rome La Sapienza. 2001-2002
2. John Russo, Department of Physics, University of Rome La Sapienza. 2002-2003

Supervision of 6 undergraduate students, University of Cambridge.

Grants

Co-Principal Investigator of the Grant from the Swiss Competence Centre for Materials Science and Technology “Biocompatible films, foams, fabrics and surfaces from poly(isobutylene)-oligopeptide conjugates”, 2010-2012.

Co-Principal Investigator of the Italian National Grant (PRIN) “Physical properties in nanosized bio-matrices based on polymers”, 2007-2008.

Co-Principal Investigator of the Italian National Grant (PRIN) “Structural, dynamical and functional properties of proteins in non-liquid systems containing residual water”, 2005-2006.

Principal Investigator of the industrial grant from ENI R&D “Multi-lamellar structure of binary and ternary polymer blends via computer modelling and small angle neutron scattering” 2002-2003.

Co-Principal Investigator of the Italian National Grant (PRIN) “Dynamical processes in self-organized structure of polysaccharides in aqueous solvents.” 2003-2004.

Organizational activities

CECAM Workshop on “Trends in computational hemodynamics”, 10-12 May 2010. Organizers: S. Melchionna, E. Kaxiras, A. Quarteroni

CECAM Workshop on “Common trends between kinetic theory, dynamic density functional theory and mesoscopic methods based on effective free energy models”, 2-5 October 2008. Organizers: S. Melchionna, U. Marini Bettolo Marconi, I. Pagonabarraga

International Conference “Computational Physics CCP2004”, Genova 1-4 September 2004. Scientific secretaries: S. Melchionna, C. Pierleoni, M. Ferrario

Euroconference “Monte Carlo and Molecular Dynamics of Condensed Matter Systems”, Como, July 1995. Organizers: K. Binder, G. Ciccotti.

Keynotes and invited talks

Invited talk “Cardiovascular blood flows with suspended red blood cells via computer simulation”, Conference Micro and Nano flows, Thessaloniki, 2011.

Invited talk “Thermal response of proteins and hydration water”, CECAM Workshop on Models for bulk, confined water and aqueous solutions upon supercooling, Lausanne, 2011.

Invited talk “Dynamics of charged fluids in nanospaces: the effect of excluded volume interactions”, CECAM Workshop on New Challenges for the simulation of electrokinetic

phenomena, Paris, 2011.

Keynote talk, “Multiscale cardiovascular hemodynamics: heart-size circulation at red blood cell resolution”, Workshop on Multiscale fluid mechanics with the Lattice Boltzmann method, Leiden, 2011.

Invited talk “Multiscale cardiovascular hemodynamics: heart-size circulation at red blood cell resolution”, SuperComputing, New Orleans, 2010.

Invited talk “Cardiovascular blood flows with suspended red blood cells via computer simulation”, Nanomedicine, Beijing, 2010.

Invited talk “Hydrokinetic approach to hemodynamics: a showcase for anisotropic suspended particles”, International workshop: Novel simulation approaches to soft matter systems, Dresden, 2010.

Invited talk “Blood flows via suspended particles and the Lattice Boltzmann method”, World Congress on Computational Mechanics ECCOMAS – CFD Minisymposium, Lisbon, 2010.

Invited talk “Multi-scale modeling of blood flows in large scale coronary systems”, 5th Conference “From Solid State to Biophysics: from Physics to Life Sciences”, Dubrovnik, 2010.

Invited talk “DNA translocation in nanopores: departure from scaling behavior”, XII International Workshop on Complex Systems, Andalo, 2010.

Invited talk “Multi-scale simulations of blood flow in realistic coronary arteries”, 5th MIT Conference on Computational Fluid and Solid Mechanics, Boston, 2009.

Invited talk “Multi-scale methods for mesoscopic flows with application to hemodynamics”, Black Forest Focus on Soft Matter, Freiburg, 2009.

Invited talk “Role of water in stabilizing thermophilic proteins”, CECAM Workshop, Lausanne, 2009.

Invited talk “Multi-scale simulations of DNA and arterial systems”, BECAT-IBM Symposium on High Performance Computational Science and Engineering, University of Connecticut, 2008.

Invited talk “Recent advances in multi-scale modeling of DNA translocation and hemodynamics”, Conference on Discrete Simulation in Fluid Dynamics, Florianopolis, 2008.

Invited talk “Multi-scale simulations with a combined Lattice Boltzmann/Molecular Dynamics approach” World Congress on Computational Mechanics ECCOMAS – WCCM Minisymposium, Venice, 2008.

Invited talk “Multi-scale simulations of complex materials for engineering and biological applications” 6th International Congress on Industrial and Applied Mathematics, Minisimposium, Zurich, 2007.

Invited talk “Multiscale modeling of biopolymer translocation through nanopores”, International Conference on Computational Science, Beijing, 2007.

Invited talk “Multiscale modeling of DNA translocation: a Lattice Boltzmann-Molecular Dynamics study”, 3rd International Conference on Multiscale Materials Modeling, Freiburg, 2006.

Plenary talk “Multiscale modeling of DNA translocation and colloids in presence of hydrodynamics”, Conference on Discrete Simulation in Fluid Dynamics, Geneva, 2006.

Invited talk “Electrorheology in nanopores via Lattice Boltzmann methods”, Europhysics Conference in Computational Physics, Genova, 2004.

Keynote lecture ”Rare events and constrained statistical mechanics”, Congress of the Italian Mathematical Society, Chia Laguna. 2002.

Invited talk “Thermal response and glass-like behavior of a protein” 16th congress on Theoretical Physics and Condensed Matter, Fai della Paganella, 1997.

Invited talk “Structure and dynamics of Microperoxidases in solution”, National School in Biophysics, Bressanone,1995.

Invited talk “Isothermal and isobaric methods for Molecular Dynamics”, Congress of the Italian Chemical Society, Rome,1993.

Publications

Soft Matter, Electrochemistry and Biomolecules

1. C.W. Hsu, M. Fyta, G. Lakatos, S. MELCHIONNA, E. Kaxiras, *Ab initio determination of coarse-grained interactions in double-stranded DNA*

, J. Chem. Phys., in press (2012).

2. U. Marini Bettolo Marconi, S. MELCHIONNA,*Charge transport in nanochannels: a molecular theory,* Langmuir, in press (2012).

3. F. Sterpone, S. MELCHIONNA, *Thermophilic proteins: insight and perspective from in silico experiments* , Chem. Soc. Rev., 41, 1665 (2012).

4. S. MELCHIONNA, G. Pontrelli, M. Bernaschi, M. Bisson, I. Halliday, T.J. Spencer, S. Succi, *The Lattice Boltzmann method as a general framework for blood flow modeling and simulations* , book chapter in Nano and Micro Flow Systems for Bioanalysis, M.W. Collins and C. Koenig eds, Springer (2012).

5. S. MELCHIONNA, U. Marini Bettolo Marconi, *Electro-osmotic flows under nanoconfinement: a self-consistent approach*
, Europhys. Lett., 95, 44002 (2011).

6. U. Marini Bettolo Marconi, S. MELCHIONNA, *Multicomponent diffusion in nanosystems,* J. Chem. Phys., 044104, 135 (2011).

7. M. Fyta, S. MELCHIONNA, S. Succi, *Translocation of biomolecules through solid-state nanopores: theory meets experiments* , Polymer Phys., 49, 985 (2011).

8. S. MELCHIONNA, E. Kaxiras, M. Bernaschi, S. Succi, *Endothelial shear stress from large-scale blood flow simulations* ,
Phil. Trans. A Royal Soc., 369, 2354 (2011).

9. F. Sterpone, S. MELCHIONNA, *Role of packing, hydration and fluctuations on*

thermostability, book chapter in *Thermostable Proteins: Structural stability and design,*
L. Nilsson and S. Sen Eds., Taylor and Francis (2011).

10. A. Gizzi, M. Bernaschi, D. Bini, C. Cherubini, S. Filippi, S. MELCHIONNA, S. Succi, *Three -band decomposition analysis of wall shear stress in pulsatile flows*
, Phys. Rev. E, 83, 032902 (2011).

11. U. Marini Bettolo Marconi, S. MELCHIONNA, *Dynamics of fluid mixtures in nanospaces*, J. Chem. Phys., 134, 064118 (2011).

12. F. Sterpone, C. Bertonati, G. Briganti, S. MELCHIONNA, *Water around thermophilic proteins: the role of charged and apolar atoms*
, J. Phys.: Condens. Matter, 22, 284113 (2010).

13. S. MELCHIONNA, M. Bernaschi, M. Fyta, E. Kaxiras, S. Succi, *Quantized biopolymer translocation through nanopores: departure from simple scaling*
, Phys.Rev.E 79, 030901 (2009).

14. M. Fyta, S. MELCHIONNA, M. Bernaschi, E. Kaxiras, S. Succi, *Numerical simulation of conformational variability in biopolymer translocation through wide nanopores*
, J. Stat. Mech. Theo. Expt., P06009 (2009).

15. F. Sterpone, C. Bertonati, G. Briganti, S. MELCHIONNA, *Key role of proximal water in regulating thermostable proteins*
. J. Phys. Chem. B, 113, 131 (2009).

16. M. Fyta, S. MELCHIONNA, S. Succi, E. Kaxiras, *Hydrodynamic correlations in the translocation of a biopolymer through a nanopore: theory and multiscale simulations*
, Phys. Rev. E 78, 036704 (2008).

17. M. Chinappi, S. MELCHIONNA, C.M. Casciola, S.Succi, *Mass flux through asymmetric nanopores: microscopic versus hydrodynamic motion*
, J.Chem.Phys. 129, 124717 (2008).

18. F. Sterpone, C. Pierleoni, S. MELCHIONNA, G. Briganti, *Pressure induced core packing and interfacial dehydration in nonionic C12E6 micelle in aqueous solution*
, Langmuir 26, 6067 (2008).

19. M. Bernaschi, S. MELCHIONNA, S. Succi, M. Fyta, E. Kaxiras, *Quantized current blockade and hydrodynamic correlations in biopolymer translocation through nanopores: evidence from multiscale simulations*
, Nanoletters 8, 1115 (2008).

20. M. Sega, R. Vallauri, P. Brocca, L. Cantù, S. MELCHIONNA, *Short range structure of a GM3 ganglioside membrane: comparison between experimental WAXS and computer simulation results* , J. Phys. Chem. B, 111, 10965 (2007).

21. M. Fyta, S. MELCHIONNA, S. Succi, E. Kaxiras, *Multiscale modeling of biopolymer translocation through a nanopore* ,
Lecture Notes in Computer Science, 4487, 786 (2007).

22. J. Russo, S. MELCHIONNA, F. De Luca, C. Casieri, *Water confined in nanopores: spontaneous formation of microcavities*
, Phys.Rev. B, 76, 195403 (2007) Cond-mat/0705.2348v1.

23. S. MELCHIONNA, M. Fyta, E. Kaxiras, S. Succi, *Exploring DNA translocation through a nanopore via a multiscale Lattice-Boltzmann Molecular Dynamics methodology*
, Intl. J. Mod. Phys. C, 18, 685 (2007).

24. M. Fyta, S. MELCHIONNA, E. Kaxiras, S. Succi, *Multiscale coupling of molecular dynamics and hydrodynamics: application to DNA translocation through a nanopore*

, MultiScale Modelling and Sim., 5, 1156 (2006).

25. M. Chinappi, E. De Angelis, S. MELCHIONNA, C.M. Casciola, S.Succi, R. Piva, *Molecula r dynamics simulation of ratchet motion in an asymmetric nanochannel* , Phys. Rev. Lett., 97, 144509 (2006).

26. S. MELCHIONNA, R. Sinibaldi, G. Briganti, *Explanation of the stability of thermophilic proteins based on unique micromorphology* , Biophys. J. 90, 4204 (2006).

27. R. Sinibaldi, C. Casieri, S. MELCHIONNA, G. Onori, A.L. Segre, S. Viel, L.Mannina, F.De Luca, *The role of water coordination in binary mixtures. A study of two model amphiphilic molecules in aqueous solutions by Molecular Dynamics and NMR* , J. Phys. Chem. B, 110, 8885 (2006).

28. M. Sega, R. Vallauri, S. MELCHIONNA, *Diffusion of water in confined geometry: The case of a multilamellar bilayer* , Phys. Rev. E, 72, 41201 (2005).

29. M. Sega, P. Brocca, S. MELCHIONNA, R. Vallauri, *Molecular dynamics simulation of a GM3 ganglioside bilayer* , J. Phys. Chem. B, 108, 20322 (2004).

30. S. MELCHIONNA, G. Briganti, P. Londei, P. Cammarano, *Water induced effects on the thermal response of a protein* , Phys.Rev.Lett., 92, 158101 (2004).

31. R. Allen, J.-P. Hansen, S. MELCHIONNA, *A Molecular Dynamics investigation of water permeation through nanopores* , J.Chem.Phys., 119, 3905 (2003). Reprinted in Virtual Journal of Biological Physics Research, August 1, 2003 and Virtual Journal of Nanoscale Science & Technology, August 11, 2003.

32. R. Allen, J.-P. Hansen, S. MELCHIONNA, *Permeation of nanopores by water: the effects of channel polarization* , J.Phys.Cond.Matt. 15, S297 (2003).

33. R. Allen, J.-P. Hansen, S. MELCHIONNA, *Intermittent permeation of cylindrical nanopores by water* , Phys.Rev.Lett. 89, 175502-1 (2002). Reprinted in Virtual Journal of Biological Physics Research, October 15, 2002 and Virtual Journal of Nanoscale Science & Technology, October 21, 2002.

34. D. Goulding, S. MELCHIONNA, *Accurate calculation of three-body depletion interactions*, Phys. Rev. E 64, 11403 (2001).

35. D. Goulding, S. MELCHIONNA, J.-P. Hansen, *Entropic selectivity of microporous materials* , Phys.Chem.Chem.Phys. 3, 1644 (2001).

36. S. Makholizo, S. MELCHIONNA, *Molecular Characterization of a laminin-derived oligopeptide with implications in biomimetic applications* , Biophys.Chem. 89, 129 (2001).

37. G. Briganti, R. Giordano, S. MELCHIONNA, L. Abis, G. Marra, C. Giannotta, A. Gennaro, *Small Angle Neutron Scattering from isotopic mixtures of binary and ternary polymer blends* , J. of Colloids and Surfaces A, 176, 161 (2001).

38. G.-M. Rignanese, F. De Angelis, S. MELCHIONNA, A. De Vita, *Glutathione S-Transferase: a First-Principles Study of the Active Site* , J.Am.Chem.Soc. 122, 11963 (2000).

39. D. Goulding, S. MELCHIONNA, J.-P. Hansen, *Size selectivity of narrow pores*, Phys. Rev. Lett. 85, 1132 (2000).

40. S. MELCHIONNA, J.-P. Hansen, *Triplet depletion forces from density functional optimization* , Phys.Chem.Chem.Phys. 2, 3465 (2000).

41. M. Falconi, S. MELCHIONNA, A. Desideri, *Molecular dynamics simulations of Cu, Zn superoxide dismutase: Effect of temperature on dimer asymmetry, Biophys* . Chem. 81, 197 (1999).

42. S. MELCHIONNA, A. Desideri, *Origin of the low-frequency modes of globular proteins*, Phys.Rev.E 60, 4664 (1999).

43. L. Stella, S. MELCHIONNA, *Equilibration and sampling in molecular dynamics simulations of biomolecules* , J. Chem. Phys. 109, 10115 (1998).

44. S. MELCHIONNA, M. Falconi, A. Desideri, *Effect of temperature and hydration on protein fluctuations: molecular dynamics simulation of Cu,Zn superoxide dismutase at six different temperatures. Comparison with neutron scattering data* , J. Chem. Phys. 108, 6033 (1998).

45. S. MELCHIONNA, M. Falconi, A. Desideri, *Molecular dynamics simulation of Cu,Zn superoxide dismutase as a function of temperature* , in Biological Macromolecular Dynamics, edited by Cusack, S., Buttner, H., Ferrand, M., Langan, P., Timmins, P. (Adenine Press, 1997).

46. S. MELCHIONNA, M. Barteri, G. Ciccotti, *Molecular dynamics study of microperoxidases in aqueous and non-aqueous solutions* , J.Phys.Chem. 100, 19241 (1996).

47. S. MELCHIONNA, M. Barteri, G. Ciccotti, *Molecular dynamics study of monomeric heme undecapeptide of Cytochrome c* , J. Comp.

Aided Mat. Des. 2, 9 (1995).

Computational methodology: Multi-Scale and Kinetic approaches

1. H. Basagaoglu, S. MELCHIONNA, S. Succi, V. Yakot, *Fluctuation-dissipation relation for a FLB-BGK model* , Europhys. Lett. 99, 64001 (2012).

2. S. MELCHIONNA, U. Marini Bettolo Marconi, *Stabilized Lattice Boltzmann-Enskog method for compressible flows and its application to one and two-component fluids in nanochannels* , Phys. Rev. E, 85 ,036707 (2012).

3. G. Pontrelli, I. Halliday, S. MELCHIONNA, T.J. Spencer, S. Succi, *The Lattice Boltzmann method and Multiscale hemodynamics: recent advances and perspectives,* book chapter in *Nano and Micro flow systems for bioanalysis* , M.W. Collins and C.S. Konig eds, Springer Verlag (2012).

4. I. Mazzitelli, M. Venturoli, S. MELCHIONNA, S. Succi, *Towards a mesoscopic model of water-like fluids with hydrodynamic interactions* , J. Chem. Phys., 135, 124902 (2011).

5. S. MELCHIONNA, *A model for red blood cells in simulations of large-scale blood flows*, Macromol. Theory & Simul., 20, 548 (2011).

6. S. MELCHIONNA, *Incorporation of smooth spherical particles in the Lattice Boltzmann method* , J. Comput. Phys., 230, 3966 (2011).

7. U. Marini Bettolo Marconi, S. MELCHIONNA, *Dynamic density functional theory and Kinetic theory of simple fluids* , J. Phys.: Condens. Matt., 22, 364110 (2010).

8. S. MELCHIONNA, M. Bernaschi, S. Succi, E. Kaxiras, F.J. Rybicki, D. Mitsouras, A.U. Coskun, C.L. Feldman, *Hydrokinetic approach to large-scale cardiovascular blood flow*, Comput. Phys. Comm., 181, 462 (2010).

9. U. Marini Bettolo Marconi, S. MELCHIONNA, *Kinetic theory of correlated fluids: from dynamic density functional to Lattice Boltzmann methods* , J. Chem. Phys., 131, 014105 (2009).

10. F.J. Rybicki, S. MELCHIONNA, D. Mitsouras, A.U. Coskun, A.G. Whitmore, M. Steigner, L. Nallamshetty, F. Welt, M. Bernaschi, M., Borkin, J. Sircar, E. Kaxiras, S. Succi, P.H. Stone, C.L. Feldman, *Prediction of coronary artery plaque progression and potential rupture from 320-detector row prospectively ECG-gated single heart beat CT angiography: Lattice Boltzmann evaluation of endothelial shear stress* . Intl. J. of Cardiovasc. Imaging, DOI 10.1007/s10554-008-9418-x (2009).

11. M. Fyta, S. MELCHIONNA, E. Kaxiras, S. Succi, *Multiscale simulation of nanobiological flows* , Computing in Science and Engineering, 10, 10 (2008).

12. S. MELCHIONNA, F.J. Rybicki, D. Mitsouras, A.U. Coskun, S. Succi, M. Bernaschi, E. Kaxiras, P.H. Stone, C.L. Feldman, *Non-invasive Prediction of Localization and Progression of Coronary Disease in Man Using Shear Stress Profiles Derived from 320-Row Detector Computed Tomography: Implications for Widespread Screening* , Circ., S845, 118 (2008).

13. S. MELCHIONNA, U. Marini Bettolo Marconi, *Lattice Boltzmann method for inhomogeneous fluids* , Europhys. Lett., 81 34001 (2008).

14. U. Marini Bettolo Marconi, P. Tarazona, F. Cecconi, S. MELCHIONNA, *Beyond dynamic density functional theory: the role of inertia* . J. Phys.: Condens. Matter 20, 494233 (2008).

15. U. Marini Bettolo Marconi, S. MELCHIONNA, *Phase-space approach to dynamical density functional theory* , J. Chem. Phys., 126, 184109 (2007).

16. S. MELCHIONNA, *Design of quasi-symplectic propagators for Langevin dynamics*, J. Chem. Phys. 127, 044108 (2007).

17. M. Fyta, S. MELCHIONNA, E. Kaxiras, S. Succi, *Multiscale coupling of molecular dynamics and hydrodynamics: application to DNA translocation through a nanopore* , MultiScale Modelling and Sim., 5, 1156 (2006).

18. S. MELCHIONNA, *Numerical integration of projective Hamiltonian dynamics*, Mol. Phys., 104, 3045 (2006).

19. D. Moroni, B. Rotenberg, J.-P. Hansen, S. MELCHIONNA, S. Succi, *Solving the Fokker-Planck kinetic equation on a lattice* , Phys. Rev. E, 73, 066707 (2006).

20. D. Moroni, J.-P. Hansen, S. MELCHIONNA, S. Succi, *On the use of the lattice Fokker-Planck schemes for hydrodynamics* , Europhys. Phys. Lett., 75, 399 (2006).

21. S. MELCHIONNA, S. Succi, J.-P. Hansen, *Simulation of single-file ion transport with the lattice Fokker-Planck equation* , Phys. Rev. E 73, 107701 (2006).

22. S. Succi, S. MELCHIONNA, J.-P. Hansen, *Lattice Fokker-Planck equation*, Intl. J. Mod. Phys. C, 17, 459 (2006).

23. S. MELCHIONNA, S. Succi, *Lattice Boltzmann-Poisson method for electrorheological nanoflows in ion channels* , Comp.Phys.Comm., 169 203 (2005).

24. S. MELCHIONNA, *Altered inertial response of generic degrees of freedom*, J. Chem. Phys., 121, 4534 (2004).

25. S. MELCHIONNA, *Molecular Dynamics simulation of biosystems: perspectives and open problems* , Mem. S.A.It., 4, 75 (2004).

26. S. MELCHIONNA, S. Succi, *Electro-rheology in nanopores via Lattice Boltzmann*, J.Chem.Phys., 120, 4492 (2003).

27. R. Allen, J.-P. Hansen, S. MELCHIONNA, *Electrostatic potential inside ionic solutions confined by dielectrics: a variational approach* , Phys. Chem. Chem. Phys. 3, 4177 (2001).

28. G. Ciccotti, G.J. Martyna, S. MELCHIONNA, M.E. Tuckerman, *Constrained isothermal-isobaric molecular dynamics with full atomic virial,* J.Phys.Chem.B 105, 6710 (2001).

29. J.-P. Ryckaert, G. Arialdi, S. MELCHIONNA, *Molecular dynamics of polymers with explicit but frozen hydrogens* , Mol.Phys. 99, 155 (2001).

30. S. MELCHIONNA, *Enhanced sampling of rare events*, Phys. Rev. E 62, 8762 (2000).

31. S. MELCHIONNA, *Constrained systems and statistical distribution*, Phys. Rev. E 61, 6165 (2000). Phys.Rev.E 62, 5864 (2000).

32. S. MELCHIONNA, G. Ciccotti, *Atomic stress isobaric scaling for systems subjected to holonomic constraints* , J.Chem.Phys. 106, 195 (1997).

33. S. MELCHIONNA, G. Ciccotti, B.L. Holian, *Comment on constant pressure molecular dynamics algorithms* , J.Chem.Phys. 105, 346 (1996).

34. S. MELCHIONNA, G. Ciccotti, B.L. Holian, *Hoover NpT dynamics for systems varying in shape and size* , Mol.Phys. 78, 533 (1993).

High-□□ Performance□ Computing

1. M. Bernaschi, M. Bisson, M. Fatica, S. MELCHIONNA, S. Succi, *Petaflop hydrokinetics simulations of complex flows on massive GPU clusters*
, Comm. Comput. Phys., in press (2012).

2. M. Bisson, M. Bernaschi, S. MELCHIONNA, S. Succi, E. Kaxiras, *Multiscale*

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