Han Wang

CAEP Software Center for High Performance Numerical Simulation
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Educational Background & Employment

2014 –	**Research Scientist**	CAEP Software Center for High Performance Numerical Simulation, Beijing, P.R. China
2011 – 2014	**Postdoctoral Researcher**	Department of Mathematics & Computer Science, Freie Universität Berlin, Germany
2006 – 2011	**Ph.D. in Computational Math.**	School of Mathematical Sciences, Peking University, Beijing, P.R. China *Supervisor:* Prof. Pingwen Zhang
2007 – 2008	**Visiting Study**	Max-Planck Institute for Polymer Research, Mainz, Germany
2002 – 2006	**B.S. in Computational Math.**	School of Mathematical Sciences, Peking University, Beijing, P.R. China

Current Research Interests

Adaptive resolution simulation.

Nonequilibrium molecular dynamics simulation and response theory.

Fast and accurate methods for molecular simulation.

Error estimate of the force computation in molecular dynamics simulations.

Inhomogeneous dispersion correction.

Parameter optimization.

List of Publications

1. Han Wang and Huazhong Tang*,
An efficient adaptive mesh redistribution method for a non-linear Dirac equation,
Journal of Computational Physics, **222**, 1, 176–193 (2007).

2. Han Wang, Kun Li and Pingwen Zhang*,
Crucial properties of the moment closure model FENE-QE,
Journal of Non-Newtonian Fluid Mechanics, **150**, 2–3, 80–92 (2008).

3. Han Wang, Christoph Junghans* and Kurt Kremer,
Comparative atomistic and coarse-grained study of water: What do we lose by coarse-graining?
The European Physical Journal E: Soft Matter and Biological Physics, **28**, 2, 221–229 (2009).

4. Han Wang*, Florian Dommert and Christian Holm,
Optimizing working parameters of the smooth particle mesh Ewald algorithm in terms of accuracy and efficiency,
The Journal of Chemical Physics, **133**, 034117 (2010).

5. Han Wang, Luigi Delle Site and Pingwen Zhang*,
On the existence of a third-order phase transition beyond the Andrews critical point: A molecular dynamics study,
The Journal of Chemical Physics, **135**, 224506 (2011).

6. Han Wang*, Christof Schütte and Pingwen Zhang,
Error estimate of short-range force calculation in inhomogeneous molecular systems,
Physical Review E, **86**(2), 026704 (2012).

7. Han Wang*, Pingwen Zhang and Christof Schütte,
On the Numerical Accuracy of Ewald, Smooth Particle Mesh Ewald, and Staggered Mesh Ewald Methods for Correlated Molecular Systems,
Journal of Chemical Theory and Computation, **8**(9), 3243–3256 (2012).

8. Han Wang, Christof Schütte and Luigi Delle Site*,
Adaptive Resolution Simulation (AdResS): A smooth thermodynamic and structural transition from atomistic to coarse grained resolution and vice versa in a Grand Canonical fashion,
Journal of Chemical Theory and Computation, **8**(8), 2878–2887 (2012).

9. Han Wang*, Dan Hu, Pingwen Zhang,
Measuring the spontaneous curvature of bilayer membranes by molecular dynamics simulations,
Communications in Computational Physics, **13**(4), 1093–1106 (2013).

10. Han Wang, Carsten Hartmann, Christof Schütte and Luigi Delle Site*,
Grand-canonical-like molecular-dynamics simulations by using an adaptive-resolution technique,
Physical Review X, **3**(1), 011018 (2013).

11. Han Wang, Carsten Hartmann, Christof Schütte*,
Linear response theory and optimal control for a molecular system under non-equilibrium conditions,
Molecular Physics, **111**(22-23), 3555-3564 (2013).

12. Jinglong Zhu, Pingwen Zhang, Han Wang*, and Luigi Delle Site,
Is there a third order phase transition for supercritical fluids?
The Journal of Chemical Physics, **140**, 014502 (2014).

13. Han Wang*, Christof Schütte, Giovanni Ciccotti and Luigi Delle Site,
Exploring the conformational dynamics of a large molecule in solution using an external electric field: A nonequilibrium molecular dynamics simulation,
Journal of Chemical Theory and Computation, **10**(4), 1376–1386 (2014).

14. Animesh Agarwal, Han Wang*, Christof Schütte and Luigi Delle Site*,
Chemical potential of liquids and mixtures via Adaptive Resolution Simulation,
The Journal of Chemical Physics, **141**, 034102 (2014).

15. Han Wang*,
Error estimates for calculating the non-bonded interactions in molecular dynamics simulations (in Chinese),
Scientia Sinica Mathematica, **44**, 823-836 (2014).

16. Wei Zhang, Han Wang, Carsten Hartmann*, Markus Weber and Christof Schütte,
Applications of the cross-entropy method to importance sampling and optimal control of diffusions,
SIAM Journal on Scientific Computing, **36**(6), A2654–A2672 (2014).

17. Han Wang* and Christof Schütte*,
Building Markov State Models for Periodically Driven Non-Equilibrium Systems,
Journal of Chemical Theory and Computing, **11**(4), 1819–1831 (2015).

18. Han Wang* and Animesh Agarwal,
Adaptive resolution simulation in equilibrium and beyond,
The European Physical Journal Special Topics, **224**, 2269–2287, (2015).

19. Animesh Agarwal, Jinglong Zhu, Carsten Hartmann, Han Wang and Luigi Delle Site*,
Molecular dynamics in a grand ensemble: Bergmann-Lebowitz model and adaptive resolution simulation,
New Journal of Physics, **17**(8), 083042 (2015).

20. Shuyu Chen†, Han Wang†, Tiezheng Qian and Ping Sheng*,
Determining hydrodynamic boundary conditions from equilibrium fluctuations,
Physical Review E, **92**, 043007, (2015).

21. Han Wang*, Haruki Nakamura, Ikuo Fukuda*,
A Critical Appraisal of the Zero-Multipole Method: Structural, Thermodynamic, Dielectric, and Dynamical Properties of a Water System,
The Journal of Chemical Physical, **144**, 114503 (2016).

22. Xingyu Gao, Jun Fang, Han Wang*,
Sampling the isothermal-isobaric ensemble by Langevin dynamics,
The Journal of Chemical Physical, **144**, 124113 (2016).

23. Jun Fang, Xingyu Gao, Haifeng Song, Han Wang*,
On the existence of the optimal order for wavefunction extrapolation in Born-Oppenheimer molecular dynamics,
The Journal of Chemical Physical, **144**, 244103 (2016).

24. Han Wang*, Xingyu Gao and Jun Fang
Multiple Staggered Mesh Ewald: Boosting the Accuracy of the Smooth Particle Mesh Ewald Method,
Journal of Chemical Theory and Computation, **12**(11), 5596-5608 (2016).

25. Xingyu Gao, Zeyao Mo, Jun Fang, Haifeng Song, Han Wang*,
Parallel 3-dim fast Fourier transforms with load balancing of the plane waves,
Computer Physics Communications, **211**, 54-60 (2017).

26. GuoMin Han, Han Wang, De-Ye Lin, XueYan Zhu, ShenYang Hu*, HaiFeng Song*,
Phase-field modeling of void anisotropic growth behavior in irradiated zirconium,
Computational Materials Science, **133**, 22-34 (2017).

27. Gao Xingyu, Jun Fang, Han Wang*,
Kaiser-Bessel basis for particle-mesh interpolation,
Physical Review E, **95**, 063303 (2017).

28. Han Wang*, Jun Fang, Gao Xingyu,
The optimal particle-mesh interpolation basis,
The Journal of Chemical Physics, **147**, 124107 (2017).

* To whom correspondence should be addressed.

† Equal contribution.

Conference and Seminar Presentations

- Optimizing Working Parameters of the Smooth Particle Mesh Ewald Algorithm
  - Invited talk. *2009 Frontiers of Computational and Applied Mathematics*, Tsinghua University, Beijing, P.R. China, Aug. 2009.
- Measuring Spontaneous Curvature by Molecular Dynamics Simulations

  - Invited talk. *East Asian Postgraduate Workshop on Soft Matter*, Hong Kong University of Science and Technology, Hong Kong, Apr. 2010.
  - Invited talk. *2010 Frontiers of Computational and Applied Mathematics*, Suzhou University, Suzhou, P.R. China, Jul. 2010.
  - Invited seminar talk. Institute of Natural Sciences, Shanghai Jiao Tong University, P.R. China, Aug. 2010.

- Some theoretical considerations of the Adaptive Resolution Simulation (AdResS)
  - *Physical Principles of Multiscale Modeling, Analysis and Simulation in Soft Condensed Matter*, UC Santa Barbara, CA, U.S., Apr. 2012.

- The numerical accuracy of force computation in inhomogeneous and correlated molecular systems
  - Invited seminar talk. Institute of Natural Sciences, Shanghai Jiao Tong University, P.R. China, Jun. 2012.

- Adaptive Resolution Simulation (AdResS): A smooth thermodynamic and structural transition from atomistic to coarse-grained resolution and vice versa in a grand canonical fashion
  - Invited talk. *Modeling the Dynamics of Complex Molecular Systems*, Lorentz Center, Leiden University, Leiden, the Netherlands, Aug. 2012.

- Grand-Canonical-Like Molecular Dynamics by Using an Adaptive-Resolution Technique.
  - *German Physical Society (DPG) Spring Meeting*, University of Regensburg, Germany, Apr. 2013

- The numerical accuracy of force computation in inhomogeneous and correlated molecular systems.
  - Invited seminar talk. *Applied Mathematics Seminar*, School of Mathematics and Center for Numerical Algorithms and Intelligent Software (NAIS), University of Edinburgh, U.K., Apr. 2013

- Grand-canonical-like molecular-dynamics simulations by using an adaptive-resolution technique
  - Invited talk. *American Chemical Society (ACS) 246th National Meeting*, Indianapolis, U.S., Sep. 2013. (Not be able to travel due to the visa issue.)

- On the numerical accuracy of Ewald, smooth particle mesh Ewald, and staggered mesh Ewald methods for inhomogeneous and correlated molecular systems.
  - Invited talk. *American Chemical Society (ACS) 246th National Meeting*, Indianapolis, U.S., Sep. 2013. (Not be able to travel due to the visa issue.)

- Linear response theory and optimal control for a molecular system under non-equilibrium conditions
  - Invited talk. *International Conference on Scientific Computation and Differential Equations (SciCADE) 2013*, Valladolid, Spain, Sep. 2013.

- Dynamical non-equilibrium molecular dynamics simulation and the response theory
  - Invited talk. *Interdisciplinary Workshop on Recent Progress in Set-Oriented Numerics and Networks Research*, Davos, Switzerland, Mar. 2014.

- A Critical Appraisal of the Adaptive Resolution Simulation in Sampling the Grand-Canonical Ensemble
  - Invited talk. *CECAM workshop: Scale-Bridging Techniques in Molecular Simulation: A Critical Appraisal*, Berlin, Germnay, Sep. 2014.

- Building Markov State Models for Periodically Driven Non-Equilibrium Systems.

  - Invited talk. *The 2014 Workshop for Young Chinese Computational Mathematicians*, Wuhan, China, Dec. 2014.
  - Invited seminar talk. Lawrence Berkeley National Laboratory, Berkeley, U.S., Apr. 2015.
  - Invited seminar talk. Peking University, Beijing, China, May 2015.

- On the numerical accuracy of Ewald, smooth particle mesh Ewald, and staggered mesh Ewald methods for inhomogeneous and correlated molecular systems.
  - Invited seminar talk. City University, Hong Kong, Jul. 2015.
  - Invited talk. The International Congress on Industrial and Applied Mathematics (ICIAM), Beijing, Aug. 2015.

- Large-scale first-principles molecular dynamic simulations for threshold displacement energy calculations of metals
  - Invited talk. NSCC-GZ/Hartree workshop on multiscale simulation of advance materials, NSCC, Guangzhou, Oct. 2015.
  - Invited talk. Workshop on Frontiers in Computational and Applied Mathematics, Tsinghua Univ., Beijing, Nov. 2015.

- Multiple staggered mesh: boosting the accuracy of particle mesh Ewald method.
  - Invited talk. 2016 Conference on numerical methods and applications, Dalian, Jun. 2016.
  - Invited talk. NSFC-RGC Forum for young scholars, Shenzhen, Jul. 2016.
  - Invited talk. Workshop on Computational Problems in Materials Science, Beijing, Oct. 2016.
  - Invited talk. 2017 International Workshop on Soft Matter and Biophysics Theories, Beijing, Jan. 2017.

- On the existence of the optimal order for wavefunction extrapolation in Born-Oppenheimer molecular dynamics
  - The 4th International Conference on Molecular Simulation, Shanghai, Oct. 2016.
  - Invited talk 10th International conference on Computational Physics, Maco, Jan. 2017.

- Deep neural network for interatomic potentials
  - Invited seminar talk. The Institute of Computational Mathematics and Scientific/Engineering Computing of Chinese Academy of Sciences, Jun. 2017.

- On the numerical accuracy of the particle-mesh Ewald method
  - Invited seminar talk. The Institute of Computational Mathematics and Scientific/Engineering Computing of Chinese Academy of Sciences, Jun. 2017.
  - Invited seminar talk. School of Mathematics, Sichuan University, Sep. 2017.

- The equilibrium melting path of the hexagonal ice.
  - Invited talk. The National Conference of Computational Mathematics, Xi'an, Jul. 2017.

- Deep Potential Molecular dynamics: a scalable model with the accuracy of quantum mechanics
  - Invited seminar talk. School of Mathematics, Sichuan University, Sep. 2017.
  - Invited talk. CSIAM 2017, Qingdao, Oct. 2017.
  - Invited seminar talk. The Institute of Computational Mathematics and Scientific/Engineering Computing of Chinese Academy of Sciences, Nov. 2017.

Teaching Experiences

Teaching Assistant, Introduction to Computation, spring 2009, Peking University.

Teaching Assistant, Linear Algebra, spring 2010, Peking University.

Awards and Fellowships

Hua Wei Fellowship, Peking University, 2006–2007.

Youth Paper Award, second class, China Society for Computational Mathematics, 2009.

New Scientist Award for Ph.D. Students, Ministry of Education of the P.R. China, 2010.

Excellent Doctoral Dissertation Award of Beijing, (2012).