Alexander V. Shapeev

Position: *Associate Professor*
Affiliation: *Skolkovo Institute of Science and Technology*
Skolkovo Innovation Center, Nobel str. 3
Moscow 143026, Russia
Website: www.shapeev.com

Research

Skolkovo Institute of Science and Technology (Skoltech)
Associate Professor **since 2019**
Assistant Professor **since 2014**

Institute of Pure and Applied Mathematics, UCLA, USA
Departmental Scholar **2016**

University of Minnesota, School of Mathematics
Postdoctoral researcher **2011–2014**

Swiss Federal Institute of Technology (EPFL)
Postdoctoral researcher **2009–2011**

Lavrentyev Institute of Hydrodynamics (SB RAS, Russia)
Research Engineer **2009**

National University of Singapore, Dept. of Math.
Research Assistant **2008**
PhD student **2004–2008**

Lavrentyev Institute of Hydrodynamics (SB RAS, Russia)
Junior Researcher **1999–2004**

Grants and Contracts

- PI in a Skolkovo Foundation grant (NGP) on elastic strain engineering **2016–2019**
- PI in the RScF grant on machine-learning interatomic potentials **2018–2020**
- PI in an industrial contract on materials design with a major Russian company **since 2019**
- co-PI in an industrial contract with a major mining company **since 2017**

Teaching

Skolkovo Institute of Science and Technology
Professor **since 2015**
- Numerical PDEs, MSc level (Spring 2015)
  - lectures (about 10 students), problem solving sessions, application project; co-taught with Ivan Oseledets

- Multiscale Methods, MSc level (Fall 2015)
  - lectures (2 students), problem solving sessions, application project
- Numerical PDEs, MSc level (Spring 2016)
  - lectures (3 students), problem solving sessions, application project
- Computational Science and Engineering II, MSc level (Spring 2017)
  - lectures (about 10 students), problem solving sessions, application project.
    (Based on Numerical PDEs course.)
- Computational Science and Engineering I and II, MSc level (Spring 2018)
  - lectures (about 10 students), problem solving sessions, application project.
    (Merged with Athanasios Polimeridis's course that was read in Academic Year 2016–17.)

University of Minnesota, School of Mathematics
Instructor **since 2012**

- Introduction to Numerical Methods I
  - lectures (33 students), computer project, office hours, grading
- Differential Equations (ordinary)
  - lectures and problem solving sessions (25–30 students), office hours, grading

Swiss Federal Institute of Technology (EPFL)
Teaching Assistant **2009–2011**

- Linear Algebra, Analysis I and II
  - problem solving sessions (30 students), office hours, grading

National University of Singapore, Dept. of Math.
Teaching Assistant **2004–2008**

- Mathematics I and II (calculus and differential equations)
  - problem solving sessions (30 students), office hours, grading
- Calculus (single-variable)
  - lab sessions (30 students), grading

Novosibirsk State University, Specialized Educational Scientific Center
Teacher (high school) **2003–2004**

- Computer Science
  - lectures on algorithm design (10 students)

Novosibirsk State University
Teacher (high school) **2002–2004**

- Computer Science
  - discussion sessions on programming in C (15 students)

Academic Supervision

Skolkovo Institute of Science and Technology
2 postdocs, 6 PhD students, 6 MSc students, 2 research interns **since 2014**

University of Minnesota
One PhD thesis, co-supervised with Prof. M. Luskin **since 2012**

Two senior projects (undergraduate) **2012**

Swiss Federal Institute of Technology (EPFL)

One MSc thesis (co-supervised with Prof. A. Abdulle) **2011**

Two MSc semester projects (co-supervised with Prof. A. Abdulle) **2009, 2010**

Education

National University of Singapore

PhD in Mathematics (GPA: 5.0 out of 5.0) **2009**

Novosibirsk State University

MSc in Mechanics (GPA: 5.0 out of 5.0) **2003**

BSc in Mechanics (GPA: 5.0 out of 5.0) **2001**

Honors and Achievements

- SIAM Outstanding Paper Prize **2013**
- Letters of Commendation for Graduate Tutor, Dept. of Math., National University of Singapore **2008, 2009**
- Best Graduate Researcher Award, National University of Singapore **2007**
- Third Prize, EASIAM Student Paper Competition **2007**
- ACM International Collegiate Programming Contest World Finals **2000, 2002**
- Scholarship of the President of Russian Federation, Novosibirsk State University **1999**

Professional Development

University of Minnesota

Teaching in Higher Education **2012**

University of Minnesota

Preparation for College Teaching **2012**

National University of Singapore

Several half-day courses **2005–2007**

Areas of Expertise

- computational materials science
- machine learning
- numerical analysis
- scientific computing
- continuum mechanics
- numerical multiscale methods

Alexander V. Shapeev

List of Publications

Submitted (4)

1. T. Kostiuchenko, F. Körmann, J. Neugebauer, A. Shapeev. *Impact of local lattice relaxations on phase stability and chemical ordering in bcc NbMoTaW high-entropy alloys explored by ab initio based machine-learning potentials*, arXiv:1810.10820, http://arxiv.org/abs/1810.10820.
2. C. Nyshadham, M. Rupp, B. Bekker, A. V. Shapeev, T. Mueller, C. W. Rosenbrock, G. Csányi, D. W. Wingate, G. L. W. Hart. *General machine-learning surrogate models for materials prediction*, arXiv:1809.09203, http://arxiv.org/abs/1809.09203.
3. B. Grabowski, Y. Ikeda, F. Körmann, C. Freysoldt, A. I. Duff, A. Shapeev, J. Neugebauer. *Ab initio vibrational free energies including anharmonicity for multicomponent alloys.*
4. E.A. Meshkov, I. I. Novoselov, A. V. Shapeev, A. V. Yanilkin. *Sublattice formation in CoCrFeNi high-entropy alloy.*

Accepted (3)

5. Z. Shi*, E. Tsymbalov*, M. Dao, S. Suresh, A. Shapeev, J. Li. *Deep Elastic Strain Engineering of Bandgap through Machine Learning* accepted to PNAS.
   * both authors contributed equally
6. E. V. Podryabinkin, E. V. Tikhonov, A. V. Shapeev, A. R. Oganov. *Accelerating crystal structure prediction by machine-learning interatomic potentials with active learning*, accepted to PRB, arXiv:1802.07605, http://arxiv.org/abs/1802.07605.
7. I. I. Novoselov, A. V. Yanilkin, A. V. Shapeev, E. V. Podryabinkin. *Moment tensor Potentials as a Promising Tool to Study Diffusion Processes*, accepted to Computational Materials Science, arXiv:1812.02946, http://arxiv.org/abs/1812.02946.

Published (25)

8. E. Tsymbalov, M. Panov, A. Shapeev. *Dropout-Based Active Learning for Regression*, in International Conference on Analysis of Images, Social Networks and Texts, Springer (2019), 247–258.
9. K. Gubaev, E.V. Podryabinkin, G.L.W. Hart, A.V. Shapeev. *Accelerating high-throughput searches for new alloys with active learning of interatomic potentials*, Computational Materials Science, 156 (2019), pp. 148–156.
10. I.S. Novikov, Y.V. Suleimanov, A.V. Shapeev. *Automated Calculation of Thermal Rate Coefficients using Ring Polymer Molecular Dynamics and Machine-Learning Interatomic Potentials with Active Learning*, Phys. Chem. Chem. Phys., 20 (2018), pp. 29503–29512.

11. K. Gubaev, E. V. Podryabinkin, A. V. Shapeev. *Machine learning of molecular properties: locality and active learning*, The Journal of Chemical Physics, 148 (2018), 241727.
12. M. Luskin and A.V. Shapeev, *Approximation of Crystalline Defects at Finite Temperature*, Multiscale Modeling & Simulation 15 (2017), pp. 1830–1864.
13. E. V. Podryabinkin and A. V Shapeev, *Active learning of linearly parametrized interatomic potentials*, Computational Materials Science, 140 (2017), pp. 171–180.
14. Alexander Shapeev, *Accurate representation of formation energies of crystalline alloys with many components*, Computational Materials Science, 139 (2017), pp. 26–30.
15. A. Abdulle and A. S. O. Jecker, *An optimization based coupling method for multiscale problems*, Multiscale Model. Simul., 14 (2016), pp. 1377–1416.
16. V. Ehrlacher, C. Ortner, and A. Shapeev, *Analysis of boundary conditions for crystal defect atomistic simulations*, Archive for Rational Mechanics and Analysis, 222 (2016), pp. 1217–1268.
17. X. H. Li, C. Ortner, A. V. Shapeev, and B. Van Koten, *Analysis of blended atomistic/continuum hybrid methods*, Numerische Mathematik, 134 (2016), pp. 275–326.
18. A. Shapeev, *Moment tensor potentials: a class of systematically improvable interatomic potentials*, Multiscale Model. Simul., 14 (2016), pp. 1153–1173.
19. D. Olson, P. Bochev, M. Luskin, and A. V. Shapeev, *Analysis of an optimization-based atomistic-to-continuum coupling method for point defects*, ESAIM: Mathematical Modelling and Numerical Analysis, 50 (2016), pp. 1–41. arXiv:1411.4027.
20. D. Olson, P. Bochev, M. Luskin, and A. V. Shapeev, *An optimization-based atomistic-to-continuum coupling method*, SIAM J. Numer. Anal., 52 (2014), pp. 2183–2204. arXiv:1304.4976.
21. C. Ortner, A. Shapeev, and L. Zhang, *(In-)stability and stabilisation of QNL-type atomistic-to-continuum coupling methods*, Multiscale Model. Simul., 12 (2013), pp. 1258–1293. arXiv:1308.3894.
22. X. H. Li, M. Luskin, C. Ortner, and A. V. Shapeev, *Theory-based benchmarking of the blended force-based quasicontinuum method*, Computer Methods in Applied Mechanics and Engineering, 268 (2014), pp. 763–781. arXiv:1304.1368.
23. A. Abdulle, P. Lin, and A. Shapeev, *A priori and a posteriori $W^{1,\infty}$ error analysis of a QC method for complex lattices*, SIAM J. Numer. Anal., 51 (2013), pp. 2357–2379. arXiv:1210.2076.
24. C. Ortner and A. V. Shapeev, *Analysis of an energy-based atomistic/continuum approximation of a vacancy in the 2D triangular lattice*, Math. Comp., 82 (2013), pp. 2191–2236. arXiv:1210.2076.
25. A. V. Shapeev, *Consistent energy-based atomistic/continuum coupling for two-body potentials in three dimensions*, SIAM J. Sci. Comput., 34 (2012), pp. B335–B360. arXiv:1108.2991.
26. A. Abdulle, P. Lin, and A. V. Shapeev, *Numerical methods for multilattices*, Multiscale Model. Simul., 10 (2012), pp. 696–726. arXiv:1107.3462.
27. M. Dobson, C. Ortner, and A. V. Shapeev, *The spectrum of the force-based quasicontinuum operator for a homogeneous periodic chain*, Multiscale Model. Simul., 10 (2012), pp. 744–765. arXiv:1004.3435.
28. A. V. Shapeev, *Consistent energy-based atomistic/continuum coupling for two-body potentials in one and two dimensions*, Multiscale Model. Simul., 9 (2011), pp. 905–932.

arXiv:1010.0512.
Winner of 2013 SIAM Outstanding Paper Prize

29. A. V. Shapeev and P. Lin, *An asymptotic fitting finite element method with exponential mesh refinement for accurate computation of corner eddies in viscous flows*, SIAM J. Sci. Comput., 31 (2009), pp. 1874–1900.
30. A. V. Shapeev, *Investigation of mixed spectral and finite difference approximation on the basis of problem of viscous flow in a diffuser*, Siberian Journal of Numerical Mathematics, 8 (2005), pp. 149–162. in Russian.
31. A. V. Shapeev, *Unsteady self-similar flow of a viscous incompressible fluid in a plane divergent channel*, Fluid Dynamics, 39 (2004), pp. 36–41.
32. A. V. Shapeev and V. P. Shapeev, *High-order accurate difference schemes for elliptic equations in a domain with a curvilinear boundary*, Computational Mathematics and Mathematical Physics, 40 (2000), pp. 213–221.

Book Chapter (1)

33. A. V. Shapeev, *Applications of Machine Learning for Representing Interatomic Interactions*, Chapter in Computational Materials Discovery (Artem R Oganov, Gabriele Saleh, Alexander G Kvashnin, eds.), The Royal Society of Chemistry (2019).

Preprints and Proceedings (13)

34. D. Olson, P. Bochev, M. Luskin, and A. V. Shapeev, *Development of an optimization-based atomistic-to-continuum coupling method*, 2013. arXiv:1309.5988.
35. C. Ortner and A. V. Shapeev, *Interpolants of lattice functions for the analysis of atomistic/continuum multiscale methods*, 2012. arXiv:1204.3705.
36. A. Abdulle, P. Lin, and A. V. Shapeev, *Homogenization-based analysis of quasi-continuum method for complex crystals*, 2010. arXiv:1006.0378.
37. P. Lin and A. V. Shapeev, *Energy-based ghost force removing techniques for the quasicontinuum method*, 2009. arXiv:0909.5437.
38. A. V. Shapeev, *Viscous incompressible axisymmetric flows in cones*, Preprint 2-09, Lavrentyev Institute of Hydrodynamics SB RAS, 2009. In Russian.
39. G. Carre, S. D. Pino, K. P. Gostaf, E. Labourasse, and A. Shapeev, *Polynomial least-squares reconstruction for semi-lagrangian cell-centered hydrodynamic schemes*, in ESAIM Proceedings, CEMRACS 2008 - Modelling and Numerical Simulation of Complex Fluids, vol. 28, 2009, pp. 100–116.
40. A. V. Shapeev, *A numerical-asymptotic method for computation of infinite number of eddies of viscous flows in domains with corners*, in Computational Fluid Dynamics, 2008.
41. G. Czichowski, A. V. Shapeev, and V. P. Shapeev, *Pattern formation – group theoretical and numerical points of view*, Preprint 15/2002, Ernst-Moritz-Arndt-Universitat Greifswald, Institut fur Mathematik und Informatik, 2002.
42. A. V. Shapeev, *Unconditionally stable explicit high-order scheme for the nonlinear schrodinger equation*, in Proceedings of the Youth Scientific Conference dedicated to the

10th anniversary of Institute of Computational Technologies SB RAS, vol. 2, Novosibirsk, Russia, 2001, pp. 175–179. in Russian.

43. A. V. Shapeev, *Numerical simulation of 3d motions of locally heated liquid films*, in Proceedings of the Third Russian National Conference on Heat Transfer, Moscow, Russia, October 2002, pp. 103–105. in Russian.
44. A. V. Shapeev, *Proof of convergence of numerical methods of solving weakly nonlinear problems*, in Problems of Continuous Media Mechanics: Proceedings of the 33rd Regional Youth Conference, Ekaterinburg, Russia, 2002, pp. 189–193. in Russian.
45. A. V. Shapeev and V. P. Shapeev, *Solution of elliptical problems with singularities using high-order schemes*, in Problems of Continuous Media Mechanics: Proceedings of the 32nd Regional Youth Conference, Ekaterinburg, Russia, 2001, pp. 62–66. in Russian.
46. A. V. Shapeev and V. P. Shapeev, *High order approximation schemes*, in Proceedings of the 3rd European Conference on Numerical Mathematics and Advanced Applications, World Scientific, 2000, pp. 715–724.