

Shibabrat Naik

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Current position

- 11/2021 –: **Research fellow**, Mathematics Institute, University of Warwick.

Expertise

Combining **dynamical systems theory** and **data-driven methods** for applications in Engineering Science and Mechanics.

Education

08/2010–12/2016	Ph.D., Engineering Mechanics, Virginia Tech, USA. Title: Geometric Approaches in Phase Space Transport and Partial Control of Escaping Dynamics Advisor: Prof. Shane D. Ross
01/2015–12/2016	Graduate Certificate, Computational Engineering Science and Mechanics, Virginia Tech, USA.
06/2006–05/2010	B.E., Civil Engineering, Jadavpur University, India.

Professional appointments

- 06/2018 – 09/2021: **Postdoctoral Research Associate**, Applied Mathematics, University of Bristol.
- 09/2017 – 06/2018: **Research Associate**, Engineering Mechanics, Virginia Tech.
- 04–08/2017: **Postdoctoral Researcher**, Mechanical Engineering and Applied Mechanics, University of Pennsylvania.
- 01–03/2017: **Postdoctoral Researcher**, Mechanical Engineering, University of Delaware and **Visiting Scholar**, Mechanical Engineering and Mechanics, Drexel University.
- 08–10/2016: **Tutoring Lab Staff**, Virginia Tech Math Emporium, Department of Mathematics, Virginia Tech.
- 01/2012–07/2016: **Graduate Research Assistant** in Dynamical systems theory and applications, Ross Dynamics Lab, Engineering Mechanics, Virginia Tech. .
- 06–12/2013: **Research Intern**, Mechatronics, Mitsubishi Electric Research Laboratory, Boston, Massachusetts.
- 08/2010–12/2011: **Graduate Teaching Assistant** for Statics, Mechanics of deformable bodies and Dynamics, Department of Engineering Science and Mechanics, Virginia Tech

Awards and recognitions

- **Royal Society JSPS Standard Postdoctoral Fellowship 2021** in Prof. Tamiki Komatsuzaki's group at Hokkaido University. Declined due to personal reason and conflict with the research fellow position at Mathematics Institute, Warwick, due to start in Sept'21.
- **Front cover image** in *International Journal of Bifurcation and Chaos*, [April 2020 issue](#).
- **Outstanding Student Paper** award by Nonlinear Geophysics focus group for poster on "Lobe dynamics and homoclinic tangles in atmospheric flows", American Geophysical Union, Fall meeting, San Francisco, CA, 2012.
- **Pratt Presidential Fellowship**, Virginia Tech, 2010-2011.
- **First prize** for the Industrial Design Problem in student design competition, MEGALITH, organized by Indian Institute of Technology, Kharagpur, India, 2010.
- **Best student proposal** award for the project "Correlation of Air and Noise Quality with Urban Traffic Characteristics for Kolkata Metropolis" for the Project Proposal Competition for "Services to Community and Economy" under Technical Education Quality Improvement Program, Jadavpur University, India, 2009.

Publications

Journal articles

Most significant papers published within the past 5 years are shown in bold

14. P. Pandey, S. Naik, and S. Keshavamurthy. Influence of low frequency modes on dynamical concertedness in double proton transfer dynamics. *Communications in Nonlinear Science and Numerical Simulation*, 109:106326, 2022. [Arxiv DOI](#)
13. V. Krajiňák, S. Naik, and S. Wiggins. Predicting trajectory behaviour via machine-learned invariant manifolds. *Chemical Physics Letters*, page 139290, 2021. [Arxiv DOI](#)
12. **S. Naik, V. Krajiňák, and S. Wiggins. Support vector machines for learning reactive islands. *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 31(10):103101, October 2021. [Arxiv DOI](#)**
11. W. Lyu, S. Naik, and S. Wiggins. Hamiltonian pitchfork bifurcation in transition across index-1 saddles. *Communications in Nonlinear Science and Numerical Simulation*, 103:105949, 2021. [DOI](#)
10. P. Pandey, S. Naik, and S. Keshavamurthy. Classical and Quantum Dynamical Manifestations of Index-2 Saddles: Concerted Versus Sequential Reaction Mechanisms. *Regular and Chaotic Dynamics*, 26(2):165–182, March 2021. [DOI](#)
9. W. Lyu, S. Naik, and S. Wiggins. The Role of Depth and Flatness of a Potential Energy Surface in Chemical Reaction Dynamics. *Regular and Chaotic Dynamics*, 25(5):453–475, September 2020. [DOI](#)
8. **S. Naik and S. Wiggins. Detecting reactive islands in a system-bath model of isomerization. *Physical Chemistry Chemical Physics*, 22(32):17890–17912, 2020. [DOI](#)**

7. W. Lyu, [S. Naik](#), and S. Wiggins. UPOsHam: A Python package for computing unstable periodic orbits in two-degree-of-freedom Hamiltonian systems. *Journal of Open Source Software*, 5(45):1684, January 2020. [DOI](#)
6. V. J. García-Garrido, [S. Naik](#), and S. Wiggins. Tilting and Squeezing: Phase Space Geometry of Hamiltonian Saddle-Node Bifurcation and its Influence on Chemical Reaction Dynamics. *International Journal of Bifurcation and Chaos*, 30(04):2030008, March 2020 [DOI](#)
5. [S. Naik](#) and S. Wiggins. **Finding normally hyperbolic invariant manifolds in two and three degrees of freedom with Hénon-Heiles-type potential.** *Physical Review E*, 100(2):022204, August 2019. [DOI](#)
4. [S. Naik](#), V. J. García-Garrido, and S. Wiggins. Finding NHIM: Identifying high dimensional phase space structures in reaction dynamics using Lagrangian descriptors. *Communications in Nonlinear Science and Numerical Simulation*, 79:104907, December 2019. [DOI](#)
3. S. D. Ross, A. E. BozorgMagham, [S. Naik](#), and L. N. Virgin. **Experimental validation of phase space conduits of transition between potential wells.** *Physical Review E*, 98(5):052214, 2018. [DOI](#)
2. [S. Naik](#), F. Lekien, and S. D. Ross. Computational method for phase space transport with applications to lobe dynamics and rate of escape. *Regular and Chaotic Dynamics*, 22(3):272–297, 2017. [DOI](#)
1. [S. Naik](#) and S. D. Ross. Geometry of escaping dynamics in nonlinear ship motion. *Communications in Nonlinear Science and Numerical Simulation*, 47:48–70, 2017. [DOI](#)

Conference proceedings

3. M. L. Bujorianu, R. S. MacKay, T. Grafke, [S. Naik](#), and E. Boulougouris. A new stochastic framework for ship capsizing. In *Proceedings of STABES*, 2021. arXiv: 2105.05965
2. [S. Naik](#) and S. D. Ross. Partial control and avoidance of escape from a potential well. XXIV ICTAM, 21-26 August 2016, Montréal, Canada.
1. S. D. Ross, A. E. BozorgMagham, [S. Naik](#), and L. N. Virgin. Escape from potential wells in multi-dimensional experimental systems. XXIV ICTAM, 21-26 August 2016, Montréal, Canada.

Open-source books and technical reports

7. W. Lyu, [S. Naik](#), and S. Wiggins. Quantum dynamics of a one degree-of-freedom hamiltonian saddle-node bifurcation, 2021. [Arxiv](#)
6. M. Agaoglou, B. Aguilar-Sanjuan, V. J. García-Garrido, R. García-Meseguer, F. González-Montoya, M. Katsanikas, V. Krajňák, [S. Naik](#), and S. Wiggins. *Lagrangian Descriptors: Discovery and Quantification of Phase Space Structure and Transport*. Zenodo v1.0.0, Jul 2020. https://champsproject.github.io/lagrangian_descriptors
5. W. Lyu, [S. Naik](#), and S. Wiggins. Elementary exposition of realizing phase space structures relevant to chemical reaction dynamics. *arXiv:2004.05709*, April 2020
4. M. Agaoglou, B. Aguilar-Sanjuan, V. J. García-Garrido, R. García-Meseguer, F. González-Montoya, M. Katsanikas, V. Krajňák, [S. Naik](#), and S. Wiggins. *Chemical Reactions: A Journey into Phase Space*. Zenodo v0.1.0, Dec 2019. <https://www.chemicalreactions.io>

3. T. Mandal, S. Ghosh, and S. Naik. Study on the strength of fly ash based geopolymer concrete, 2010
2. S. Naik and W. Malik. Experimental modal testing for estimating the dynamic properties of a cantilever beam, 2010
1. S. Naik and H. P. Majumdar. Group Theoretic approach to the analysis of boundary layer flow over shrinking sheet with suction, 2010.

Contributed and invited talks

8. Ship capsize and phase space transport: Application of geometric and probabilistic approaches of phase space transport; S. Naik, S. D. Ross; MIR@W Ship capsize, 2021.
7. Tilting and Squeezing: Implications of Hamiltonian saddle-node bifurcation for reaction dynamics; S. Naik, W. Lyu, V. J. García-Garrido, S. Wiggins; BMC-BAMC Glasgow, 2021.
6. Finding NHIM: Identifying High Dimensional Phase Space Structures using Lagrangian Descriptors; S. Naik, S. Wiggins; SIAM-DS 2019, Salt Lake, Utah, USA.
5. Escape from potential wells in multi-degree of freedom systems: phase space geometry and partial control; S. Naik, S. D. Ross; SIAM-DS 2015, Salt Lake, Utah, USA.
4. Partial control approach for avoiding capsize; S. Naik, S. D. Ross; SIAM Mid-Atlantic Student Conference, Washington D.C., USA.
3. Probabilistic approaches of phase space transport and mixing; S. Naik, S. D. Ross, P. Grover; Invited talk for SIAM Student Chapter at Virginia Tech, Blacksburg, USA.
2. Thermal coherent sets and heat transfer in chaotic laminar flows; S. Naik, P. Grover; APS Division of Fluid Dynamics 2013, Pittsburgh, PA, USA.
1. Lobe dynamics and homoclinic tangles in atmospheric flows; S. Naik, S. D. Ross; Poster at AGU fall meeting 2012, San Francisco, CA, USA.

Research funding

- **London Mathematical Society** summer research bursary 2019 (Grant ref: 18-19-58, Mr Wenyang Lyu), 2020 (Grant ref: 19-20-28, Mr Piero Sarti), 2021 (Grant ref: URB-2021-82, Mr Alexander Hind). Joint recipient with Prof. Stephen Wiggins and respective students. Amount: £4880.00 equally supported by LMS and the School of Mathematics.

Synergistic Activities

Professional service

- Serving as co-organizer for the Institute of Applied Mathematics *Fluids and Materials seminar* since 2020.
- Volunteer member of Equality, Diversity, and Inclusion Committee in the School of Mathematics, University of Bristol.
- Served as session chair for [Topics in Bifurcation Theory](#) at SIAM-DS 2015. Co-organizer of minisymposium on [High Dimensional Phase Space Structures in Chemical Reaction Dynamics](#) at SIAM-DS 2019, [Integrating dynamical systems with data-driven methods](#) at virtual BMC-BAMC Glasgow 2021.

- Reviewed for Journal of Open Source Software, Communications in Computational Physics, PLOS ONE, Discrete and Continuous Dynamical Systems - Series B.
- Member of Society of Industrial and Applied Mathematics, American Physical Society.

Supervision experience

Funding provided by London Mathematical Society, School of Mathematics Summer Research bursary at Bristol, Warwick, and EPSRC funded project, [CHAMPS](#) and co-supervisor with Prof. Stephen Wiggins and Prof. Robert S. MacKay.

- 2022: Alex McSweeney-Davis (University of Warwick)
- 2021: Will Simpkins, Alexander Hind (University of Bristol)
- 2020: Bing En Gan, Annie Hu, Piero Sarti, Sam Spedding (University of Bristol)
- 2019-2021: Wenyang Lyu (University of Bristol)

Outreach

- Collaborative art on mathematics behind my research for the international Pint of Science festival 2019, [Creative Reactions](#).

Training and skills

- 2016: Certified Tutor, Level I, CRLA's International Tutor Training Program, Dept. of Mathematics, Virginia Tech Math Emporium, USA.
- Attended training workshops for staff development on research methods, project planning, peer-review, and related academic skills.
- Workshop on Machine learning and dynamical systems at Imperial College, London and University of Washington, Seattle. Democracy hackthon at PyData London 2019.
- Computational science: Jupyter, C/C++, Python, MATLAB, \LaTeX , MPI, OpenMP, Fortran, Java, Javascript, Julia, Xmgrace, COMSOL, Paraview, Tecplot, GNU-Scientific Library, C++ Standard Template Library, Numpy, Scipy, Matplotlib, Pandas, Scikit-learn.
- MOOC courses and certifications: Machine Learning, Linear and Integer programming, Computing for Data analysis, Python: Data Analysis, C++ Essential Training, Learning C++, Computational Engineering Science and Mechanics. Extensive coursework in machine learning and data science using online courses on LinkedIn and Coursera.

Research interests

- Dynamical systems theory
 - Geometric and statistical methods of chaotic dynamics.
 - Discovery of structures (invariant sets and manifolds) in phase space transport.
 - Partial control of escape and transition dynamics.
 - Phase space structures based control.
- Data-driven methods
 - Transport barriers in atmosphere and ocean.
 - Machine learning phase space structures.

- Reduced order modelling.
- Defect and anomaly detection in structural dynamics.
- Applications
 - Engineering science and mechanics: ship dynamics and capsizing, transport and optimization in fluid mechanics.
 - Chemical physics: isomerization and solution-phase reaction dynamics, machine learning of phase space structures.
 - Plasma physics: isodrastic magnetic fields for plasma confinement.
 - Robotics: multi-agent systems, distributed control and coordination.

References

- Robert S. MacKay, Professor, Mathematics Institute, University of Warwick, UK. Contact: r.s.mackay@warwick.ac.uk
- Stephen Wiggins, Professor of Applied Mathematics, School of Mathematics, University of Bristol, UK. Contact: s.wiggins@bristol.ac.uk
- Shane D. Ross, Professor of dynamical systems and fluid mechanics, Department of Aerospace and Ocean Engineering, Virginia Tech, USA. Contact: sdross@vt.edu
- Nicole Abaid, Associate Professor, Department of Mathematics, Virginia Tech, USA. Contact: nabaid@vt.edu
- Piyush Grover, Assistant Professor, Department of Mechanical & Materials Engineering, University of Nebraska – Lincoln, USA. Contact: piyush.grover@unl.edu