

Molei Tao

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RESEARCH KEYWORDS

understanding deep learning, dynamics-inspired learning algorithms, AI/ML for sciences and scientific computing (e.g., learning dynamics from data); numerical analysis, multiscale methods; nonlinear dynamical systems; geometric integrators, variational methods, Hamiltonian and Lagrangian mechanics; applied probability, rare events, sampling, optimal transport, and generative modeling; control and optimization

PROFESSIONAL EXPERIENCE

- Associate Professor, School of Mathematics, Georgia Tech 2020-
- Assistant Professor, School of Mathematics, Georgia Tech 2014-2020
- Courant Instructor, New York University 2012-2014
- Postdoc in Computing & Mathematical Sciences, Caltech 2011-2012

EDUCATION

- Ph.D. in Control & Dynamical Systems (from Dept. Computing + Mathematical Sciences) June 2011
Graduate Minor in Physics June 2011
California Institute of Technology, USA
Advisors: Prof. Houman Owhadi and Prof. Jerrold E. Marsden (deceased)
- B.S. in Mathematics and Physics, with Honor July 2006
Tsinghua University, China

LIST OF PUBLICATIONS

PUBLISHED OR ACCEPTED: (*: corresponding author; †: student or postdoc mentee)

- X. Li, F. Lu, **M. Tao**, F. Ye. NySALT: Nyström-type inference-based schemes adaptive to large time-stepping. *J. Comput. Phys.* (conditionally accepted 2022)
- O. So†, G. Li, E.A. Theodorou, and **M. Tao***. Data-driven discovery of non-Newtonian astronomy via learning non-Euclidean Hamiltonian. *NeurIPS 2022* (workshop)
- A. Wibisono, **M. Tao**, and G. Piliouras. Alternating Mirror Descent for Constrained Min-Max Games. *NeurIPS 2022*
- R. Chen†, G. Li, and **M. Tao***. Low Spin-Axis Variations of Circumbinary Planets. *Mon. Notices Royal Astron. Soc.* (2022)
- R. Li†, H. Zha, and **M. Tao***. Hessian-Free High-Resolution Nesterov Acceleration for Sampling. *ICML 2022*
- Y. Chao† and **M. Tao***. Parametric resonance for enhancing the rate of metastable transition. *SIAM J. Applied Math.* (2022)
- Y. Wang†, M. Chen, T. Zhao, and **M. Tao***. Large Learning Rate Tames Homogeneity: Convergence and Balancing Effect. *ICLR 2022*
- R. Li†, H. Zha, and **M. Tao***. Mean-Square Analysis with An Application to Optimal Dimension Dependence of Langevin Monte Carlo. *ICLR 2022*

- R. Li[†], **M. Tao**, S.S. Vempala, and A. Wibisono*. The Mirror Langevin Algorithm Converges with Vanishing Bias. ALT 2022
- T. Lee*, **M. Tao**, and M. Leok. *Variational Symplectic Accelerated Optimization on Lie Groups*. CDC 2021
- R. Chen[†] and **M. Tao***. *Data-driven Prediction of General Hamiltonian Dynamics via Learning Exactly-Symplectic Maps*. ICML 2021
- **M. Tao*** and S. Jin. *Accurate and efficient simulations of Hamiltonian mechanical systems with discontinuous potentials*. J. Comput. Phys. (2021) accepted
- R. Li[†], X. Wang[†], H. Zha, and **M. Tao***. *Improving sampling accuracy of SG-MCMC methods via non-uniform subsampling of gradients*. Discrete Contin. Dyn. Syst. (2021) accepted
- R. Chen[†], G. Li*, and **M. Tao**. *GRIT: a package for structure-preserving simulations of gravitationally interacting rigid-bodies*. Astrophys. J. (2021) accepted
- S. Al-Abri, T. Lin, **M. Tao**, and F. Zhang. *A Derivative-Free Optimization Method with Application to Functions with Exploding and Vanishing Gradients*. IEEE Control Systems Letters. (2021) 5(2): 587–592
- L. Kong[†] and **M. Tao***. *Stochasticity of Deterministic Gradient Descent: Large Learning Rate for Multiscale Objective Function*. NeurIPS 2020
- K. Huang[®], Y. Wang^{†®}, **M. Tao**, and T. Zhao*. *Why Do Deep Residual Networks Generalize Better than Deep Feedforward Networks? — A Neural Tangent Kernel Perspective*. NeurIPS 2020
([®]: joint first authors)
- **M. Tao*** and Tomoki Ohsawa. *Variational Optimization on Lie Groups, with Examples of Leading (Generalized) Eigenvalue Problems*. International Conference on Artificial Intelligence and Statistics (AISTATS) 2020 (Best Paper Award)
- A. Garzon*, W. Rodriguez, F. Cristancho, and **M. Tao**. *AhKin: a modular and efficient code for the Doppler Shift Attenuation Method*. Comput. Phys. Comm. (2020) 246: 106854
- M. Oudich, Y. Deng, **M. Tao**, and Y. Jing*. *Space-time phononic crystals with anomalous topological edge states*. Phys. Rev. Res. (2019) 1: 033069
- D. Dylewsky*, **M. Tao**, and J. Nathan Kutz. *Dynamic mode decomposition for multiscale nonlinear physics*. Phys. Rev. E (2019) 99: 063311
- **M. Tao***. *Simply improved averaging of coupled oscillators and weakly nonlinear waves*. Commun. Nonlinear Sci. Numer. Simul. (2019) 71: 1–21
- P. Xie[†] and **M. Tao***. *Parametric resonant control of macroscopic behaviors of multiple oscillators*. American Control Conference 2019
- S. Surappa, **M. Tao**, and F.L. Degertekin*. *Analysis and design of capacitive parametric ultrasonic transducers for efficient ultrasonic power transfer based on a 1D lumped model*. IEEE Trans. Ultrason. Ferroelectr. Freq. (2018) 65(11): 2103–2112
- A. Souza[†] and **M. Tao**. *Metastable transitions in inertial Langevin systems: what can be different from the overdamped case?* Eur. J. Appl. Math. (2019) 5: 830–852
- **M. Tao***. *Hyperbolic periodic orbits in nongradient systems and small-noise-induced metastable transitions*. Physica D (2018) 363: 1–17.
- **M. Tao***. *Explicit symplectic approximation of nonseparable Hamiltonians: algorithm and long time performance*. Phys. Rev. E (2016) 94: 043303.
- G. Li, M.J. Holman, and **M. Tao***. *Uncovering circumbinary planetary architectural properties from selection biases*. Astrophys. J. (2016) 831(1), 96–111.
- **M. Tao***. *Explicit high-order symplectic integrators for charged particles in general electromagnetic fields*. J. Comput. Phys. (2016) 327:245–251.

- **M. Tao*** and H. Owhadi. *Temporal homogenization of linear ODEs, with applications to parametric super-resonance and energy harvest*. Arch. Rat. Mech. Anal. (2016) Vol. 220, 261–296.
- **M. Tao*** and H. Owhadi. *Variational and linearly-implicit integrators, with applications*. IMA J. Numer. Anal. (2016) 36(1), 80–107.
- S. Han*, **M. Tao**, U. Topcu, H. Owhadi, and R.M. Murray. *Convex optimal uncertainty quantification*. SIAM J. Optim. (2015) Vol. 25, 1368–1387.
- Y. Jing*, **M. Tao**, and J. Cannata. *An improved wave-vector-frequency-domain method for nonlinear wave modeling*. IEEE Trans. Ultrason. Ferroelectr. Freq. (2014) Vol. 61, 515–524.
- S. Ober-Blöbaum*, **M. Tao**, M. Cheng, H. Owhadi, and J.E. Marsden. *Variational integrators for electric circuits*. J. Comput. Phys. (2013) Vol. 242, 498–530.
- W.S. Koon*, H. Owhadi, **M. Tao**, and T. Yanao. *Control of a Model of DNA Division via Parametric Resonance*. Chaos (2013) Vol. 23, 013117.
- S. Han, U. Topcu, **M. Tao**, H. Owhadi, and R.M. Murray. *Convex optimal uncertainty quantification: algorithms and a case study in energy storage placement*. American Control Conference 2013. (Best Student Paper Award Finalist).
- N. Friedman, A.T. Jennings, G. Tsekenis, J-Y. Kim, **M. Tao**, J.T. Uhl, J.R. Greer, and K.A. Dahmen*. *Statistics of Dislocation Slip Avalanches in Nanosized Single Crystals Show Tuned Critical Behavior Predicted by a Simple Mean Field Model*. Phys. Rev. Lett. (2012) Vol. 109, 095507.
- **M. Tao***, H. Owhadi, and J.E. Marsden. *From efficient symplectic exponentiation of matrices to symplectic integration of high-dimensional Hamiltonian systems with slowly varying quadratic stiff potentials*. Appl. Math. Res. Expr.(2011) Num. 2, 242–280. (Most-Cited Articles #8 as of September 1, 2016)
- **M. Tao***, H. Owhadi, and J.E. Marsden. *Space-time FLAVORS: finite difference, multisymplectic, and pseudospectral integrators for multiscale PDEs*. Dyna. Part. Diff. Eq. (2011) Vol. 8, 21–46.
- Y. Jing, **M. Tao**, and G. Clement*. *Evaluation of a wave vector frequency domain method for nonlinear wave propagation*. J. Acous. Soc. Amer. (2011) Vol. 129, 32–46.
- **M. Tao**, H. Owhadi*, and J.E. Marsden. *Nonintrusive and structure preserving multiscale integration of stiff ODEs, SDEs and Hamiltonian systems with hidden slow dynamics via flow averaging*. SIAM Multi. Model. Simul. (2010) Vol. 8, 1269–1324.
- Q. Hou[®], **M. Tao[®]**, and Y. Li. *A fast and reliable two-sequence local alignment algorithm*. China National Computer Conference 2005. ([®]: joint first authors; in Chinese)

PREPRINTS:

- L. Kong[†], Y. Wang[†], and **M. Tao**. Momentum Stiefel Optimizer, with Applications to Suitably-Orthogonal Attention, and Optimal Transport.
- Q. Zhang, **M. Tao**, and Y. Chen. gDDIM: generalized denoising diffusion implicit models.
- S. Surappa, C. Wei, **M. Tao**, and F.L. Degertekin. Electromechanical frequency comb generation in fluid media with a parametrically driven capacitive microresonator.

OTHER MANUSCRIPTS:

- **M. Tao** (2011) *Multiscale geometric integration of deterministic and stochastic systems*. (Ph.D. Dissertation)
- **M. Tao**, H. Owhadi, and J.E. Marsden (2010) *Temperature and friction accelerated sampling of Boltzmann-Gibbs distribution*. arXiv:1007.0995
- **M. Tao**, H. Owhadi, and J.E. Marsden (2010) *Structure preserving stochastic impulse methods for stiff Langevin systems with a uniform global error of order 1 or 1/2 on position*. arXiv:1006.4657 (serves as supplementary material for [Tao et al., AMRX 2011]).

- **M. Tao** (2007) *Thermodynamic and structural consensus principle predicts mature miRNA location and structure, categorizes conserved interspecies miRNA subgroups, and hints new possible mechanisms of miRNA maturization.* (English version of Bachelor Thesis) arXiv:0710.4181

AWARDS, GRANTS AND RECOGNITIONS

- GT-Emory Joint AI.Humanity Award (2023, \$100,000, GT PI)
- **Cullen-Peck Scholar Award** (recognition of research accomplishments led by GT College of Sciences faculty at the associate professor or advanced assistant professor level) (2022, \$10,000)
- Georgia Tech Grant ‘Pushing Frontiers of Astrophysics with Application-Driven Advancement of Scientific Machine Learning’ (2021, \$44,853, co-PI, PI: Laura Cadonati)
- IEEE EFTF-IFCS 2021 **Best Student Paper Finalist** (for ‘Phononic Frequency Comb Generation in a Micromechanical Resonator Operating in Air and Liquid Environments’ by S. Surappa, M. Tao & F.L. Degertekin)
- Georgia Tech Grant ‘Nucleating Artificial Intelligence and Machine Learning Collaborations in the College of Sciences’ (2021, \$18,000, co-PI, PI: Roman Grigoriev)
- **AISTATS 2020 Best Paper Award** (for ‘Variational Optimization on Lie Groups, with Examples of Leading (Generalized) Eigenvalue Problems’ by M. Tao & T. Ohsawa)
- NSF Grant ECCS 1936776 (2019-2022, \$349,923, co-PI, PI: F Levent Degertekin)
- **NSF CAREER Award** DMS 1847802 (2019-2023, \$400,330, single PI)
- NSF Grant ECCS 1829821 (2018-2019, \$79,971, co-PI, PI: F Levent Degertekin)
- ‘Thank a Teacher’ Certificates for excellence in teaching, Georgia Tech, 2016, 2019(*2), 2022
- NSF Grant DMS 1521667 (2015-2019, \$209,912, single PI)
- AMS – Simons Travel Grant Award, 2015 (\$4,000, single PI, partially returned upon receipt of NSF)
- 2013 American Control Conference (ACC) **Best Student Paper Award Finalist** (for joint work with Shuo Han, Ufuk Topcu, Houman Owhadi, and Richard Murray)
- **W.P. Carey Ph.D. Prize in Applied Mathematics**, 2011
- Caltech Institute Fellowship, 2006
- Tsinghua Outstanding Undergraduate Thesis, 2006
- Tsinghua Scholarships, 2004, 2005
- Gold medals in various Olympiads in Informatics (*8) and Mathematics (*2), 1995-2002 (China or Jiangsu province)

STUDENTS AND POSTDOCTORAL SCHOLARS

Current:

- Yuqing Wang (Math PhD student at Georgia Tech)
- Lingkai Kong (Math PhD student at Georgia Tech)
- Kevin Rojas (Machine Learning PhD student at Georgia Tech)
- Keunwoo Lim (undergrad at Seoul National University, math)
- Aadarsh Vavilikolanu (undergrad at Georgia Tech, computer science)
- Joan Gimeno (postdoc collaborator at Georgia Tech, math, main mentor: Rafael de la Llave)

Alumni:

- Oswin Chun Man So (GT Computer Science undergrad (co-mentored, with Evangelos Theodorou); 1st position after: PhD student at MIT)

- Minshuo Chen (GT ISyE PhD student of significant collaboration (advisor: Tuo Zhao); 1st position after: postdoc at Princeton University)
- Lin Li (visiting undergrad from Peking University (PKU); 1st position after: Peking University, School of Math Probability+Stats undergrad)
- Sriharsha Kocherla (K12 student at South Forsyth High School)
- Kowshik Arko Dey (undergrad at ZJU-UIUC, computer engineering; 1st position after: ZJU-UIUC)
- Renyi Chen (PhD student at Georgia Tech, math; 1st position after: Google)
- Ruilin Li (previous GT PhD student of significant collaboration, CSE; 1st position after: Hudson River Trading)
- Sushruta Shashidhara (previous GT PhD student of significant collaboration, ME; 1st position after: Stanford University)
- Ying Chao (visiting PhD student from Huazhong Univ. Science and Tech.; 1st position after: Assistant Prof. at Xi'an Jiao Tong Univ. China, Dept. Probability and Statistics)
- Faris El-Katri (undergrad at University of Southern California, math; 1st position after: unknown)
- Giriraj Ramgulam (undergrad at Georgia Tech, math; 1st position after: Georgia Tech Quantitative & Computational Finance Graduate Program)
- Zhehan Cao (GT ECE master student; 1st position after: learnable.ai (startup))
- Yangfei Liao (exchange undergrad from Xi'an Jiaotong Univ., GT Math; 1st position after: undergrad at Xi'an Jiaotong Univ.)
- Andre Souza (postdoc at Georgia Tech, math; 1st position after: scientist at MIT)
- Xin Wang (PhD student at Georgia Tech, math, co-advised; (advisor: Yingjie Liu); 1st position after: Google Research)
- Pengcheng Xie (exchange undergrad from Xi'an Jiaotong Univ., GT Math; 1st position after: PhD student at Chinese Academy of Sciences)
- Terrence Alsup (math undergrad at Georgia Tech; 1st position after: PhD student at Courant Institute)
- Homayoun Yousefi Bakhtiar (undergrad at Georgia Tech, aerospace engineering; 1st position after: graduate student at Georgia Tech)
- Marc Fabritius (exchange master student at Georgia Tech; 1st position after: graduate student at University of Stuttgart)

REU students:

- Gabriell Hall (Spelman College; 2018 summer)
- Huy-Hoang Nguyen (Minerva Schools at KGI; 2018 summer)

Additional students of significant collaboration:

- Qinsheng Zhang (current GT Aerospace PhD student (advisor: Yongxin Chen))
- Guan-Horng Liu (current GT Machine Learning PhD student (advisor: Yongxin Chen))
- Tianrong Chen (current GT ECE PhD student (advisor: Evangelos Theodorou))

Ph.D. Thesis Committee:

- John Dever (Georgia Tech, Mathematics)
- Benjamin Ide (Georgia Tech, Mathematics)
- Bhanu Kumar (Georgia Tech, Mathematics)
- Sushruta Surappa (Georgia Tech, Mechanical Engineering)
- Said Al-Abri (Georgia Tech, Electrical and Computer Engineering)
- Adrián Bustamante (Georgia Tech, Mathematics)

- Shu Liu (Georgia Tech, Math/CSE)
- Yian Yao (Georgia Tech, Mathematics)
- Ruilin Li (Georgia Tech, Math/CSE)
- Patrick Reinbold (Georgia Tech, Physics)
- Shaojun Ma (Georgia Tech, CSE/Math)
- Haiyu Zou (Georgia Tech, Math)
- Hao Wu (Georgia Tech, Math)
- Guan-Horng Liu (Georgia Tech, Machine Learning/Aerospace)
- Tianrong Chen (Georgia Tech, Electrical and Computer Engineering)
- Tian-Yi Zhou (Georgia Tech, Machine Learning/Industrial and Systems Engineering)
- Xinshi Chen (Georgia Tech, Machine Learning/Mathematics)

TEACHING

(see long version)

INVITED TALKS

(see long version)

SCIENTIFIC COMMUNITY SERVICES

Editorial:

- Physica D (invited guest editor)

Referee for journals (multiple times for many of them):

- Chaos
- Discrete Continuous Dynamical Systems
- IMA J. Numerical Analysis
- Journal of Computational Physics
- NATURE Communications
- Numerische Mathematik
- Physica D
- SIAM J. Control and Optimization
- SIAM J. Numerical Analysis
- SIAM J. Scientific Computing
- SIAM J. Applied Dynamical Systems
- SIAM Multiscale Modeling and Simulation
- The Astrophysical Journal
- 10+ more (see long version)

Referee for conferences (multiple times for many of them):

- NeurIPS
- ICML
- ICLR
- IMA Math. Robotics

Panelist for NSF panels