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 2	011
	Graduate Minor in Physics	June 2	011
	California Institute of Technology, USA		
	Advisors: Prof. Houman Owhadi and Prof. Jerrold E. Marsden (deceased)		
•	B.S. in Mathematics and Physics, with Honor	July 2	006
	Tsinghua University, China		

LIST OF PUBLICATIONS

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

- B. Yuan, J. Fan, Y. Wang[†], M. Tao, and Y. Chen^{*}. Markov chain Monte Carlo for Gaussian: A linear control perspective. IEEE Control Systems Letters 2023
- L. Kong[†], Y. Wang[†], and M. Tao. Momentum Stiefel Optimizer, with Applications to Suitably-Orthogonal Attention, and Optimal Transport. ICLR 2023
- Q. Zhang, M. Tao, and Y. Chen. gDDIM: generalized denoising diffusion implicit models. ICLR 2023
- S. Surappa, C. Wei, **M. Tao**, and F.L. Degertekin. Electromechanical frequency comb generation in fluid media with a parametrically driven capacitive microresonator. Physical Review Applied 2023
- X. Li, F. Lu, M. Tao, F. Ye. NySALT: Nyström-type inference-based schemes adaptive to large time-stepping. J. Comput. Phys. 2023
- 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:

• Y. Li, M. Tao, and S. Wang. Landscape classification through coupling method.

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)
- Xinshi Chen (Georgia Tech, Machine Learning/Mathematics)
- 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)
- Yuichiro Aoyama (Georgia Tech, Machine Learning/Aerospace)

TEACHING

(see long version)

INVITED TALKS

(see long version)

SCIENTIFIC COMMUNITY SERVICES

- Editorial: • ICLR 2024 (Area Chair)

 - 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
- Journal of Machine Learning Research
- 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
- 30+ more (see long version)

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

- NeurIPS
- ICML
- ICLR
- IMA Math. Robotics

Panelist for NSF panels