

## Molei Tao

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### RESEARCH KEYWORDS

understanding deep learning, dynamics-inspired learning algorithms, AI for sciences and computations (e.g., learning dynamics from data); numerical analysis, multiscale methods; nonlinear dynamical systems; geometric integrators, variational methods, Hamiltonian and Lagrangian mechanics; applied probability, sampling and rare events; 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

**JOURNAL PAPER:** (\*: corresponding author; †: student or postdoc mentee)

- R. Chen<sup>†</sup>, 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
- 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
- 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<sup>†</sup> 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**<sup>\*</sup>. *Hyperbolic periodic orbits in nongradient systems and small-noise-induced metastable transitions*. Physica D (2018) 363: 1–17.
- **M. Tao**<sup>\*</sup>. *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**<sup>\*</sup>. *Uncovering circumbinary planetary architectural properties from selection biases*. Astrophys. J. (2016) 831(1), 96–111.
- **M. Tao**<sup>\*</sup>. *Explicit high-order symplectic integrators for charged particles in general electromagnetic fields*. J. Comput. Phys. (2016) 327:245–251.
- **M. Tao**<sup>\*</sup> 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**<sup>\*</sup> and H. Owhadi. *Variational and linearly-implicit integrators, with applications*. IMA J. Numer. Anal. (2016) 36(1), 80–107.
- S. Han<sup>\*</sup>, **M. Tao**, U. Topcu, H. Owhadi, and R.M. Murray. *Convex optimal uncertainty quantification*. SIAM J. Optim. (2015) Vol. 25, 1368–1387.
- Y. Jing<sup>\*</sup>, **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<sup>\*</sup>, **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<sup>\*</sup>, H. Owhadi, **M. Tao**, and T. Yanao. *Control of a Model of DNA Division via Parametric Resonance*. Chaos (2013) Vol. 23, 013117.
- N. Friedman, A.T. Jennings, G. Tsekenis, J-Y. Kim, **M. Tao**, J.T. Uhl, J.R. Greer, and K.A. Dahmen<sup>\*</sup>. *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**<sup>\*</sup>, 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**<sup>\*</sup>, 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<sup>\*</sup>. *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<sup>\*</sup>, 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.

#### PEER-REVIEWED CONFERENCE PROCEEDINGS (FULL-SIZED PAPER):

- R. Chen<sup>†</sup> and **M. Tao**<sup>\*</sup>. *Data-driven Prediction of General Hamiltonian Dynamics via Learning Exactly-Symplectic Maps*. ICML 2021
- L. Kong<sup>†</sup> and **M. Tao**<sup>\*</sup>. *Stochasticity of Deterministic Gradient Descent: Large Learning Rate for Multiscale Objective Function*. NeurIPS 2020
- K. Huang<sup>®</sup>, Y. Wang<sup>†®</sup>, **M. Tao**, and T. Zhao<sup>\*</sup>. *Why Do Deep Residual Networks Generalize Better than Deep Feedforward Networks? — A Neural Tangent Kernel Perspective*. NeurIPS 2020  
(<sup>®</sup>: 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)
- P. Xie<sup>†</sup> and **M. Tao\***. *Parametric resonant control of macroscopic behaviors of multiple oscillators*. American Control Conference 2019
- 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).
- S. Ober-Blobbaum, **M. Tao**, M. Cheng, H. Owhadi, and J.E. Marsden. *Variational integrators for electric circuits*. Proceedings of Applied Mathematics and Mechanics 2011. (2-page version of the journal version)
- Q. Hou<sup>®</sup>, **M. Tao<sup>®</sup>**, and Y. Li. *A fast and reliable two-sequence local alignment algorithm*. China National Computer Conference 2005. (<sup>®</sup>: joint first authors; in Chinese)

#### PREPRINTS:

- R. Li<sup>†</sup>, H. Zha, and **M. Tao\***. Mean-Square Analysis with An Application to Optimal Dimension Dependence of Langevin Monte Carlo.
- R. Chen<sup>†</sup>, G. Li, and **M. Tao\***. Obliquity Variations of Circumbinary Planets.
- T. Lee\*, **M. Tao**, and M. Leok. Variational Symplectic Accelerated Optimization on Lie Groups.
- **M. Tao\*** and S. Jin. Accurate and efficient simulations of Hamiltonian mechanical systems with discontinuous potentials.
- R. Li<sup>†</sup>, H. Zha, and **M. Tao\***. Hessian-Free High-Resolution Nesterov Acceleration for Sampling.
- R. Li<sup>†</sup>, X. Wang<sup>†</sup>, H. Zha, and **M. Tao\***. Improving sampling accuracy of SG-MCMC methods via non-uniform subsampling of gradients.

#### 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 maturation*. (English version of Bachelor Thesis) arXiv:0710.4181

#### AWARDS, GRANTS AND RECOGNITIONS

- 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)
- 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)
- 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 and Mathematics, 1995-2002 (Jiangsu province/China)

### STUDENTS AND POSTDOCTORAL SCHOLARS

Current:

- Yuqing Wang (PhD student at Georgia Tech, math)
- Lingkai Kong (PhD student at Georgia Tech, math)
- Keunwoo Lim (undergrad at Seoul National University, math)

Alumni:

- 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)
- Giriraj Ramgulam (undergrad at Georgia Tech, math; 1st position after: Georgia Tech)
- 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: Xi’an Jiaotong Univ.)
- Andre Souza (postdoc at Georgia Tech, math; 1st position after: MIT)
- Xin Wang (PhD student at Georgia Tech, math, co-advised; (advisor: Yingjie Liu); 1st position after: Google AI)
- Pengcheng Xie (exchange undergrad from Xi’an Jiaotong Univ., GT Math; 1st position after: Chinese Academy of Sciences)
- Terrence Alsup (math undergrad at Georgia Tech; 1st position after: Courant Institute)
- Homayoun Yousefi Bakhtiar (undergrad at Georgia Tech, aerospace engineering; 1st position after: Georgia Tech)
- Marc Fabritius (exchange master student at Georgia Tech; 1st position after: 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:

- Minshuo Chen (current GT ISyE PhD student)

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)
- Guan-Hong Liu (Georgia Tech, Machine Learning)

### **TEACHING**

(see long version)

### **INVITED TALKS**

(see long version)

### **SCIENTIFIC COMMUNITY SERVICES**

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 Multiscale Modeling and Simulation
- 10+ more (see long version)

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

- NeurIPS
- ICLR
- IMA Math. Robotics

Panelist for NSF panels