Tom S. Bertalan

Research Software Engineer · Bioreactor Controls · Neural networks for Nonlinear Dynamics

Boston, MA

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Machine learning and dynamical systems researcher specialized in neural system identification and unsupervised representations. Proficient in handling high-dimensional time-series data for both offline parameter optimization and online execution.

PROFESSIONAL EXPERIENCE AND RESEARCH AREAS

University of Massachusetts *Lowell, MA*

Research Software Engineer *1/2024-Present*

- ***Model Predictive Control of CHO Bioreactor***
  - Design and administer virtualization, certificates, remote access, and OPC-UA communication for bioreactor distributed controls.
  - Lead the rewrite of Java-based event-driven pump control logic, including regular review of junior engineers' work.
  - Collect targeted experimental data from a 3-liter bioreactor, characterizing dynamics and responses to control inputs.
  - Supervise the implementation of more rigorous simulation methods for a SBML-encoded bioreactor digital twin.
  - Develop an optimal online model-predictive controller in Aspen DMC to maximize economic factors.

Johns Hopkins University *Baltimore, MD*

Postdoctoral Fellow *2/2020-1/2024*

- ***Neural Differential Equations and Time-Series***
  - Advanced SotA for neural DEs for time series, including CNNs for PDEs; conceived a novel loss function for Hamiltonian systems.
  - Cut RNN inference burn-in from 25 to 5 samples using manifold learning.
  - Derived custom gradients for nets with constraints; promoted theory on error scaling laws; applications in biomanufacturing.
  - Parallelized neural PDE solution sensitivity analysis using SLURM on GPU cluster.
- ***Modeling and Experimental Design for CHO Metabolism***
  - Led a team of biophysics and ML experts in creating a suite of Python/MATLAB simulation and data processing tools.
  - Created a GUI for Bayesian experimental design; mentored team members on its use and maintenance.
- ***Robotic Perception and Control***
  - Developed a variational autoencoder for end-to-end robotic localization.
  - Trained a U-net on both open and custom datasets for real-time (>10hz) on-board semantic segmentation of drivable space.
  - Inferred depth and semantic segmentation in simulation, using pre-trained transformer networks.
  - Profiled depth/segmentation pipeline to ensure pure-GPU inference for real-time inference.
- ***Machine Learning Service Deployment and Administration***
  - Provisioned a local LLAMA2 inference server over VPN for diverse zero-shot microservices, including document renaming, topic extraction, and categorization.
  - Automated conversion of seminar announcements to ICS files via OpenAI API, including curation of a 19.7k-word fine-tuning dataset.
  - Administered lab GPU server for maximum uptime and ease of access for multiple concurrent users.
  - Wrote specifications and solicited bids for an upcoming multi-GPU training server destined for datacenter colocation.

The Massachusetts Institute of Technology *Cambridge, MA*

Postdoctoral Associate *3/2018-2/2020*

- ***Autonomous Vehicle Design and Pathfinding***
  - Developed a model AV with firmware-level speed sensing and control commanded by checksummed bus communications.
  - Designed a jerk-minimizing path planner capable of planing up to two lane switches ahead at 47 mph.
  - Leveraged Ipopt and CppAD to push a model-predictive path follower to a latency of 67 ms in simulation.
  - Taught summer courses on OpenCV, ROS, and CNNs for lane detection, path following, and traffic sign recognition.
  - Wrote wrapper APIs for using video games as robotic simulations.
  - Detected dashcam obstacles via windowed SVM.
- ***Nonlinear dynamics in neuroscience***
  - Wrote object-oriented library for fine- and coarse-grained simulation of neuronal dynamics.
  - Analyzed bifurcation and resonance behavior of a mammalian circadian rhythm model.
  - Played a key role in acquiring a $1.8M grant for an industry-academic partnership.

Princeton University *Princeton, NJ*

NSF Research Assistant *9/2012-3/2018*

Built a rover for particle-filter SLAM with LIDAR using Gazebo and ROS. Created a custom library for visualizing OpenCV pipelines and pruning of computational graphs at execution time. Simulated thousands of neurons in vectorized Numpy and MATLAB, and social agents in OpenMP-accelerated C++.

The University of Alabama *Tuscaloosa, AL*

Student Research Assistant *9/2009-5/2012*

Created a 10-node Beowulf cluster in PHP, explored CUDA for PDE acceleration, and developed a LAMP-based social network. Simulated hierarchy formation in social animals as input to wet-lab experiments. Authored a multigrid subsurface-flow solver with CUDA acceleration.

SKILLS

Libraries, frameworks, & tools

- Python/C++/Java
- NumPy+SciPy+Matplotlib
- Pytorch/TensorFlow/Keras
- Linux, shell scripting, and git
- VSCode/Eclipse+PyDev
- Aspen DMC3 Controls
- OPC-UA, MODBUS/serial, and ROS

Areas of Expertise and Training

- Nonlinear dynamics of time series data
- Deep learning and ML
- Dimension reduction and representation learning
- Probabilistic modeling and theory
- Computer vision
- Research presentation and dissemination
- Trainee and peer mentoring

Other Skills and Interests

- Home automation with Arduino, Raspberry Pi, and 3D printing
- Solo and orchestral violin performance
- Windsurfing and small-boat sailing

EDUCATION & TRAINING

Institutions

- **Johns Hopkins University** *2020 - 2024*
  Postdoctoral Fellow *Che. & Bio. Eng.*
- **The Massachusetts Institute of Technology** *2018 - 2020*
  Postdoctoral Associate *Mech. Engr.*
- **Princeton University** *2012 - 2018*
  NSF Research Fellow *PhD & MA, Che. & Bio. Eng.*
- **The University of Alabama** *2008 - 2012*
  Student Research Assistant *BS Che. & Bio. Eng.; Minor in Math*

Awards

- Princeton Program in Plasma Science and Technology research and academic fellowship
- National Science Foundation research fellowship
- William R. Schowalter fund for scholarly conferences
- National merit finalist scholarship
- University honors program and president's list
- $\Phi\mathrm{H}\Sigma$, $\Omega\mathrm{X}\mathrm{E}$, and $\mathrm{T}\mathrm{B}\Pi$ honor societies

Teaching

- Volunteered in a recurring summer course for high-school seniors and freshmen on employing ROS, OpenCV, and CNNs for lane detection and traffic sign recognition.
- Supervised operations and measurment activities in junior Chemical & Biological Engineering practicum.
- Lectured, held office hours, and graded assignments in senior differential equations course.

SELECTED PUBLICATIONS

Transformations establishing equivalence across neural networks: when have two networks learned the same task? *2024*
Tom Bertalan, F. Dietrich, I. Kevrekidis *Chaos*

Implementation and (Inverse Modified) Error Analysis for implicitly-templated ODE nets *2024*
A. Zhu, B. Zhu, Tom Bertalan, Y. Tang, I. Kevrekidis *SIAMDS*

Data-driven and Physics Informed Modelling of Chinese Hamster Ovary (CHO) Cell Bioreactors *2024*
T. Cui, Tom Bertalan, N. Ndahiro, P. Khare, M. Betenbaugh, C. Maranas, I. Kevrekidis *Comp. & Chem. Engr.*

Certified Invertibility in Neural Networks via Mixed-Integer Programming *2023*
T. Cui, Tom Bertalan, G. Pappas, M. Morari, I. Kevrekidis, M. Fazlyab *L4DC 2023 — PMLR*

Learning emergent PDEs in a learned emergent space *2022*
F. Kemeth, Tom Bertalan, T. Thiem, S. Moon, C. Laing, I. Kevrekidis *Nature Comm.*

Initializing LSTM internal states via manifold learning *2021*
F. Kemeth, Tom Bertalan, N. Evangelou, T. Cui, S. Malani, I. Kevrekidis *Chaos*

Local conformal autoencoder for standardized data coordinates *2020*
E. Peterfreund, O. Lindenbaum, F. Dietrich, Tom Bertalan, M. Gavish, I. Kevrekidis, R. Coifman *PNAS*

On Learning Hamiltonian Systems from Data *2019*
Tom Bertalan, F. Dietrich, Igor Mezic, and I. Kevrekidis *Chaos*

PUBLICATIONS

Integration of Bayesian Optimization and Solution Thermodynamics to Optimize Media Design for Mammalian Biomanufacturing — *In Press*
Nelson Ndahiro, Edward Ma, Tom Bertalan, Marc Donohue, Yannis Kevrekidis, and Michael Betenbaugh — *iScience*

Machine Learning Approaches to Problem Well-Posedness — *In Preparation*
Tom Bertalan, G. Kevrekidis, E. Rebrova, S. Mishra, I. Kevrekidis

Data-driven and Physics Informed Modelling of Chinese Hamster Ovary (CHO) Cell Bioreactors — *2024*
T. Cui, Tom Bertalan, N. Ndahiro, P. Khare, M. Betenbaugh, C. Maranas, I. Kevrekidis — *Comp. & Chem. Engr.*

Implementation and (Inverse Modified) Error Analysis for implicitly-templated ODE nets — *2024*
A. Zhu, B. Zhu, Tom Bertalan, Y. Tang, I. Kevrekidis — *SIAMDS*

Transformations establishing equivalence across neural networks: when have two networks learned the same task? — *2024*
Tom Bertalan, F. Dietrich, I. Kevrekidis — *Chaos*

Certified Invertibility in Neural Networks via Mixed-Integer Programming — *2023*
T. Cui, Tom Bertalan, G. Pappas, M. Morari, I. Kevrekidis, M. Fazlyab — *L4DC 2023 — PMLR*

Some of the variables, some of the parameters, some of the times, with some things known: Identification with partial information — *2023*
Saurabh Malani, Tom Bertalan, T. Cui, M. Betenbaugh, J. Avalos, I. Kevrekidis — *Comp. & Chem. Engr.*

Learning effective stochastic differential equations from microscopic simulations: linking stochastic numerics to deep learning — *2023*
F. Dietrich, A. Makeev, G. Kevrekidis, N. Evangelou, Tom Bertalan, S. Reich, I. Kevrekidis — *Chaos*

Learning emergent PDEs in a learned emergent space — *2022*
F. Kemeth, Tom Bertalan, T. Thiem, S. Moon, C. Laing, I. Kevrekidis — *Nature Comm.*

Personalized Algorithm Generation: A Case Study in Meta-Learning ODE Integrators — *2022*
Y. Guo, F. Dietrich, Tom Bertalan, D. Doncevic, M. Dahmen, I. Kevrekidis, Q. Li — *SIAM J. Sci. Comp.*

Initializing LSTM internal states via manifold learning — *2021*
F. Kemeth, Tom Bertalan, N. Evangelou, T. Cui, S. Malani, I. Kevrekidis — *Chaos*

Development of closures for coarse-scale modeling of multiphase and free surface flows using machine learning — *2021*
C. Linares, Tom Bertalan, E. Koronaki, Jicai Lu, G. Tryggvason, I. Kevrekidis — *APS Bulletin*

Global and local reduced models for interacting, heterogeneous agents — *2021*
T. Thiem, F. Kemeth, Tom Bertalan, Carlo Liang, I. Kevrekidis — *Chaos*

Local conformal autoencoder for standardized data coordinates — *2020*
E. Peterfreund, O. Lindenbaum, F. Dietrich, Tom Bertalan, M. Gavish, I. Kevrekidis, R. Coifman — *PNAS*

Emergent spaces for coupled oscillators — *2020*
T. Thiem, M. Kooshkbaghi, Tom Bertalan, Carol Laing, I. Kevrekidis — *Front. in Comp. Neuro.*

On Learning Hamiltonian Systems from Data — *2019*
Tom Bertalan, F. Dietrich, Igor Mezic, and I. Kevrekidis — *Chaos*

An Emergent Space for Distributed Data with Hidden Internal Order through Manifold Learning — *2017*
F. Kemeth, Sindre Haugland, F. Dietrich, Tom Bertalan, Kevin Höhlein, Q. Li, Erik Bollt, Ronen Talmon, Katharina Krischer, and I. Kevrekidis — *IEEE Access*

Coarse-grained descriptions of dynamics for networks with both intrinsic and structural heterogeneities — *2017*
Tom Bertalan, W. Wu, C. Laing, C. William Gear, and I. Kevrekidis. — *Front. in Comp. Neuro.*

Dimension reduction in heterogeneous neural networks: Generalized Polynomial Chaos (gPC) and ANalysis-Of-VAriance (ANOVA) — *2016*
M. Choi, Tom Bertalan, C. Laing, and I. Kevrekidis. — *Euro. Phys. J., Special Topics*

OpenMG: a new multigrid implementation in Python — *2014*
Tom Bertalan, A. Islam, R. Sidje, and E. Carlson — *Num. Lin. Alg. with App.*

PRESENTATIONS

Symbolic regression and modular neural differential equations for bioprocess engineering and robotics — *2024*
Tom Bertalan, Jaeweon Lee, Zhao Wang, Seongkyu Yoon, I. Kevrekidis — *MLDS 4 (poster)*

Certified Invertibility in Neural Networks via Mixed-Integer Programming — *2023*
T. Cui, Tom Bertalan, G. Pappas, M. Morari, I. Kevrekidis, M. Fazlyab — *Learning for Dyn. Sys.*

Coarse-grained and emergent distributed-parameter systems from data — *2021*
Hassan Arbabi, F. Kemeth, Tom Bertalan, I. Kevrekidis — *American Control Conf.*

Data-driven model reduction and discovery — *2020*
T. Thiem, Tom Bertalan, F. Kemeth, Yorgos Psarellis, I. Kevrekidis — *AIChE*

Dynamical-systems-guided learning of PDEs from data — *2020*
Hassan Arbabi, Tom Bertalan, A. Roberts, I. Kevrekidis — *AIChE*

On the data-driven discovery and calibration of closures — *2020*
S. Lee, Yorgos Psarellis, C. Siettos, Tom Bertalan, D. Amchin, T. Bhattacharjee, S. Datta, I. Kevrekidis — *AIChE*

Connections between residual networks and explicit numerical integrators, and applications to identification of noninvertible dynamical systems — *2020*
T. Cui, Tom Bertalan, Yorgos Psarellis, I. Kevrekidis — *AIChE*

Neural network approach to reduced order modeling of multiphase flows — *2020*
C. Linares, Tom Bertalan, S. Lee, J. Lu, G. Tryggvason, I. Kevrekidis — *APS Div. of Fluid Dyn.*

PDE+PINN: Learning and Solving a PDE at the Same Time — *2020*
Tom Bertalan, F. Kemeth, T. Cui, I. Kevrekidis — *AIChE*

Learning Partial Differential Equations from Discrete Space Time Data: Convolutional and Recurrent Networks, and Their Relations to Traditional Numerical Methods — *2019*
Tom Bertalan, F. Dietrich, T. Thiem, R. Farber, I. Kevrekidis, A. Roberts — *AIChE*

Recurrent Neural Networks, Numerical Integrators and Nonlinear System Identification — *2018*
Tom Bertalan, R. Farber, T. Thiem, F. Dietrich, I. Kevrekidis — *AIChE*

Coarse-Scale PDEs from Microscopic Observations Via Machine Learning — *2019*
S. Lee, M. Kooshkbaghi, C. Siettos, Tom Bertalan, and I. Kevrekidis — *AIChE*

When Have Two Networks Learned the Same Task? Data-Driven Transformations between System Representations — *2019*
Tom Bertalan, F. Dietrich, T. Thiem, I. Kevrekidis — *AIChE*

Coarse modeling of circadian rhythms in heterogeneous neural networks — *3017; 2016*
Tom Bertalan, C. William Gear, Yannis G. Kevrekidis, M. Henson, E. Herzog, and C. Laing — *Dyn. Days 2017; AIChE*

Coarse-graining of heterogeneous neural dynamics — *2015*
Tom Bertalan, M. Choi, C. Laing, I. Kevrekidis — *AIChE*

Heterogeneity and reduction for complex network dynamics — *2014*
I. Kevrekidis, A. Holiday, Tom Bertalan, and C. Laing — *AIChE*

Coarse-graining Network Dynamics — *2013*
A. Holiday and Tom Bertalan — *Network Front.*

nSpyres: an open-source, Python-based framework for simulation of flow through porous media — *2012*
E. Carlson, A. Islam, F. Dumkwu, and Tom Bertalan — *Interpore 2012*

OpenMG: a new multigrid implementation in Python — *2012*
Tom Bertalan, A. Islam, R. Sidje, and E. Carlson — *Proc. 11th Python in Sci. Conf.*

ESIM: a framework for simulation of dominance hierarchy formation in small animal groups — *2012*
Tom Bertalan and R. Earley — *UA Hon. Undergr. Res. Conf.*

An open-source computing cluster for virtual experiments with variable parameters — *2011*
Tom Bertalan and E. Carlson — *UA Hon. Undergr. Res. Conf.*