# Tom S. Bertalan

Research Software Engineer  $\,\cdot\,\,$  Bioreactor Controls  $\,\cdot\,\,$  Neural networks for Nonlinear Dynamics West 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.

# 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, ROS, and sockets

#### **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

# PROFESSIONAL EXPERIENCE AND RESEARCH AREAS

## **University of Massachusetts**

Lowell, MA 1/2024-Present

RESEARCH SOFTWARE ENGINEER

• Model Predictive Control of CHO Bioreactor

- 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 combined quality attributes.
- Lead weekly group meetings, targeting both academic publication and technology transfer to industry partners

#### **Johns Hopkins University**

Baltimore, MD

POSTDOCTORAL FELLOW

3/2020-1/2024

#### · Time Series and PDE Analysis with Neural ODEs

- 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.

#### · Biophysical Experiment and Simulation Enhancement

- 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 Systems Development and Upgrades

- Developed a variational autoencoder for end-to-end robotic localization.
- Used Blender to create synthetic datasets for alternate-view synthesis.
- Upgraded rover with IMU and RealSense, resulting in enhanced odometry for RTAB-MAP SLAM.
- Trained a U-net on both open and custom datasets for real-time (>10hz) on-board semantic segmentation of drivable space.
- Calibrated camera intrinsics for projective geometry of segmented point clouds.
- Profiled depth/segmentation pipeline to ensure pure-GPU inference for real-time inference.

#### · Special Projects and Innovations

- 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.
- Stood up local Llama2 inference server for various internal automation tasks via REST API over VPN.
- 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 3/2018-3/2020

#### · 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.
- 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 9/2012-3/2018 NSF RESEARCH ASSISTANT

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

The University of Alabama Tuscaloosa, AL 9/2009-5/2012 STUDENT RESEARCH ASSISTANT

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.

# 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
- $\Phi H \Sigma$ ,  $\Omega X E$ , and  $T B \Pi$  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

A longer list of publications and presentations is available upon request.

#### Transformations establishing equivalence across neural networks: when have two networks learned the same task?

Thomas Bertalan, Felix Dietrich, Ioannis Kevrekidis

Implementation and (Inverse Modified) Error Analysis for implicitly-templated ODE nets

Aiqing Zhu, Beibei Zhu, Tom Bertalan, Yifa Tang, Ioannis Kevrekidis

Data-driven and Physics Informed Modelling of Chinese Hamster Ovary (CHO) Cell Bioreactors

Tianqi Cui, Tom Bertalan, Nelson Ndahiro, Pratik Khare, Michael Betenbaugh, Costas Maranas, Ioannis Kevrekidis

**Certified Invertibility in Neural Networks via Mixed-Integer Programming** 

Tianqi Cui, <u>Tom Bertalan</u>, George J. Pappas, Manfred Morari, Ioannis Kevrekidis, Mahyar Fazlyab

Learning emergent PDEs in a learned emergent space

Felix Kemeth, Tom Bertalan, Thomas Thiem, Seungjoon Moon, Carlo Laing, Ioannis Kevrekidis

Initializing LSTM internal states via manifold learning

Felix Kemeth, Tom Bertalan, Nikolaos Evangelou, Tianqi Cui, Saurabh Malfani, Ioannis Kevrekidis

Local conformal autoencoder for standardized data coordinates

Erez Peterfreund, Ofir Lindenbaum, Felix Dietrich, Tom Bertalan, Matan Gavish, Ioannis Kevrekidis, Ronald Coifman

On Learning Hamiltonian Systems from Data

Tom Bertalan, Felix Dietrich, Igor Mezic, and Ioannis Kevrekidis

2024; in press

Chaos

2024; in press SIAMDS

Comp. & Chem. Engr.

2023

2024

L4DC 2023 - PMLR

2022

Nature Comm.

2021

Chaos

2020

**PNAS** 

2019 Chaos

### **PUBLICATIONS**

Machine Learning Approaches to Problem Well-Posedness

Tom Bertalan, George Kevrekidis, Elizaveta Rebrova, Siddhartha Mishra, Yannis Kevrekidis

In Preparation

Data-driven and Physics Informed Modelling of Chinese Hamster Ovary (CHO) Cell Bioreactors

Tianqi Cui, <u>Tom Bertalan</u>, Nelson Ndahiro, Pratik Khare, Michael Betenbaugh, Costas Maranas, Ioannis Kevrekidis

2024 Comp. & Chem. Engr.

Implementation and (Inverse Modified) Error Analysis for implicitly-templated ODE nets

Aiqing Zhu, Beibei Zhu, Tom Bertalan, Yifa Tang, Ioannis Kevrekidis

2024; in press

Transformations establishing equivalence across neural networks:

when have two networks learned the same task? Thomas Bertalan, Felix Dietrich, Ioannis Kevrekidis

Identification with partial information

**2024; in press** Chaos

Certified Invertibility in Neural Networks via Mixed-Integer Programming

Tiangi Cui, Tom Bertalan, George J. Pappas, Manfred Morari, Ioannis Kevrekidis, Mahyar Fazlyab

**2023** L4DC 2023 — PMLR

Some of the variables, some of the parameters, some of the times, with some things known:

2023

Saurabh Malani, Tom Bertalan, Tianqi Cui, Michael Betenbaugh, Jose L. Avalos, Ioannis Kevrekidis

Comp. & Chem. Engr.

Learning effective stochastic differential equations from microscopic simulations: linking stochastic numerics to deep learning

Felix Dietrich, Alexei Makeev, George Kevrekidis, Nikolaos Evangelou, <u>Tom Bertalan</u>, Sebastian Reich, Ioannis Kevrekidis

**2023** Chaos

Learning emergent PDEs in a learned emergent space

Felix Kemeth, Tom Bertalan, Thomas Thiem, Seungjoon Moon, Carlo Laing, Ioannis Kevrekidis

**2022** Nature Comm.

Personalized Algorithm Generation: A Case Study in Meta-Learning ODE Integrators

Y. Guo, Felix Dietrich, <u>Tom Bertalan</u>, D. T. Doncevic, M. Dahmen, Ioannis Kevrekidis, Qianxiao Li

2022 SIAM J. Sci. Comp.

Initializing LSTM internal states via manifold learning

Felix Kemeth, Tom Bertalan, Nikolaos Evangelou, Tianqi Cui, Saurabh Malfani, Ioannis Kevrekidis

**2021** Chaos

Development of closures for coarse-scale modeling of multiphase and free surface flows using machine learning

Cristina Linares, Tom Bertalan, Eleni Koronaki, Jicai Lu, Gretar Tryggvason, Ioannis Kevrekidis

**2021** APS Bulletin

Global and local reduced models for interacting, heterogeneous agents

Thomas Thiem, Felix Kemeth, <u>Tom Bertalan</u>, Carlo Liang, Ioannis Kevrekidis

**2021** Chaos

Local conformal autoencoder for standardized data coordinates

Erez Peterfreund, Ofir Lindenbaum, Felix Dietrich, <u>Tom Bertalan</u>, Matan Gavish, Ioannis Kevrekidis, Ronald Coifman

**2020** PNAS

2020

**Emergent spaces for coupled oscillators** 

Thomas Thiem, Mahdi Kooshkbaghi, <u>Tom Bertalan</u>, Carol Laing, Ioannis Kevrekidis

Front. in Comp. Neuro.

On Learning Hamiltonian Systems from Data

Tom Bertalan, Felix Dietrich, Igor Mezic, and Ioannis Kevrekidis

**2019** Chaos

An Emergent Space for Distributed Data with Hidden Internal Order through Manifold Learning

Felix Kemeth, Sindre Haugland, Felix Dietrich, <u>Tom Bertalan</u>, Kevin Höhlein, Qianxiao Li,

Erik Bollt, Ronen Talmon, Katharina Krischer, and Ioannis Kevrekidis

**2017** *IEEE Access* 

Coarse-grained descriptions of dynamics for networks with both intrinsic and structural heterogeneities

Tom Bertalan, Yan Wu, Carlo Laing, C. William Gear, and Ioannis Kevrekidis.

**2017** Front. in Comp. Neuro.

Dimension reduction in heterogeneous neural networks: Generalized Polynomial Chaos (gPC)

and ANalysis-Of-VAriance (ANOVA)

**2016** Euro. Phys. J., Special Topics

Minseok Choi, Tom Bertalan, Carlo Laing, and Ioannis Kevrekidis.

2014

**OpenMG: a new multigrid implementation in Python**<u>Tom Bertalan</u>, Akand Islam, Roger Sidje, and Eric Carlson

Num. Lin. Alg. with App.

# PRESENTATIONS \_\_\_\_\_

Symbolic regression and modular neural differential equations for bioprocess engineering and robotics	<b>2024</b> MLDS 4 (poster)
Tom Bertalan, Jaeweon Lee, Zhao Wang, Seongkyu Yoon, Ioannis Kevrekidis	
Certified Invertibility in Neural Networks via Mixed-Integer Programming Tianqi Cui, <u>Tom Bertalan</u> , George J. Pappas, Manfred Morari, Ioannis Kevrekidis, Mahyar Fazlyab	<b>2023</b> Learning for Dyn. Sys.
Coarse-grained and emergent distributed-parameter systems from data  Hassan Arbabi, Felix Kemeth, Tom Bertalan, Ioannis Kevrekidis	<b>2021</b> American Control Conf.
Data-driven model reduction and discovery  The man Things Tage Destalon Talis Manneth Vergoe Describing Jagonia Manneth Vergoe Describing	<b>2020</b> AIChE
Thomas Thiem, Tom Bertalan, Felix Kemeth, Yorgos Psarellis, Ioannis Kevrekidis	
<b>Dynamical-systems-guided learning of PDEs from data</b> Hassan Arbabi, <u>Tom Bertalan</u> , Anthony Roberts, Ioannis Kevrekidis	<b>2020</b> AIChE
On the data-driven discovery and calibration of closures  Seungjoon Lee, Yorgos Psarellis, Constantinos Siettos, <u>Tom Bertalan</u> , Daniel Amchin, Tapomoy Bhattacharjee, Sujit Datta, Ioannis Kevrekidis	<b>2020</b> AIChE
Connections between residual networks and explicit numerical integrators, and applications to identification of noninvertible dynamical systems  Tianqi Cui, Tom Bertalan, Yorgos Psarellis, Ioannis Kevrekidis	<b>2020</b> AIChE
Neural network approach to reduced order modeling of multiphase flows	2020
Cristina Linares, <u>Tom Bertalan</u> , Seungjoon Lee, Jicai Lu, Gretar Tryggvason, Ioannis Kevrekidis	APS Div. of Fluid Dyn.
PDE+PINN: Learning and Solving a PDE at the Same Time  Tom Bertalan, Felix Kemeth, Tianqi Cui, Ioannis Kevrekidis	<b>2020</b> AIChE
Learning Partial Differential Equations from Discrete Space Time Data: Convolutional and Recurrent Networks, and Their Relations to Traditional Numerical Methods <u>Tom Bertalan</u> , Felix Dietrich, Thomas Thiem, Rob Farber, Ioannis Kevrekidis, Anthony Roberts	<b>2019</b> AIChE
Recurrent Neural Networks, Numerical Integrators and Nonlinear System Identification Tom Bertalan, Rob Farber, Thomas Thiem, Felix Dietrich, Ioannis Kevrekidis	<b>2018</b> AIChE
<b>Coarse-Scale PDEs from Microscopic Observations Via Machine Learning</b> Seungjoon Lee, Mahdi Kooshkbaghi, Constantinos Siettos, <u>Tom Bertalan</u> , and Ioannis Kevrekidis	<b>2019</b> AIChE
When Have Two Networks Learned the Same Task? Data-Driven Transformations between System Representations	2019
Tom Bertalan, Felix Dietrich, Thomas Thiem, Ioannis Kevrekidis	AIChE
Coarse modeling of circadian rhythms in heterogeneous neural networks  Tom Bertalan, C. William Gear, Yannis G. Kevrekidis, Michael Henson, Erik Herzog, and Carlo Laing	<b>3017; 2016</b> Dyn. Days 2017; AlChE
Coarse-graining of heterogeneous neural dynamics	2015
Tom Bertalan, Minseok Choi, Carlo Laing, Ioannis Kevrekidis	AIChE
<b>Heterogeneity and reduction for complex network dynamics</b> Ioannis Kevrekidis, Alexander Holiday, <u>Tom Bertalan</u> , and Carlo Laing	<b>2014</b> AIChE
Polynomial representations of populations with multiple heterogeneities	2014
Tom Bertalan, Yan Wu, Brianna Hnath, and Yannis Kevrekidis	Princeton Grad. Student Symp.
Coarse-graining Network Dynamics Alexander Holiday and Tom Bertalan	<b>2013</b> Network Front.
nSpyres: an open-source, Python-based framework for simulation of flow through porous me-	2012
<b>dia</b> Eric Carlson, Akand Islam, Francis Dumkwu, and Tom Bertalan	Interpore 2012
OpenMG: a new multigrid implementation in Python	2012
Tom Bertalan, Akand Islam, Roger Sidje, and Eric Carlson	Proc. 11 <sup>th</sup> Python in Sci. Conf.
ESIM: a framework for simulation of dominance hierarchy formation in small animal groups <u>Tom Bertalan</u> and Ryan Earley	<b>2012</b> UA Hon. Undergr. Res. Conf.
An open-source computing cluster for virtual experiments with variable parameters <u>Tom Bertalan</u> and Eric Carlson	<b>2011</b> UA Hon. Undergr. Res. Conf.