Introduction to ACC Workshop on Differentiable Programming for Modeling and Control of Dynamical Systems

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Strategic Advisor

PNNL-SA-181885

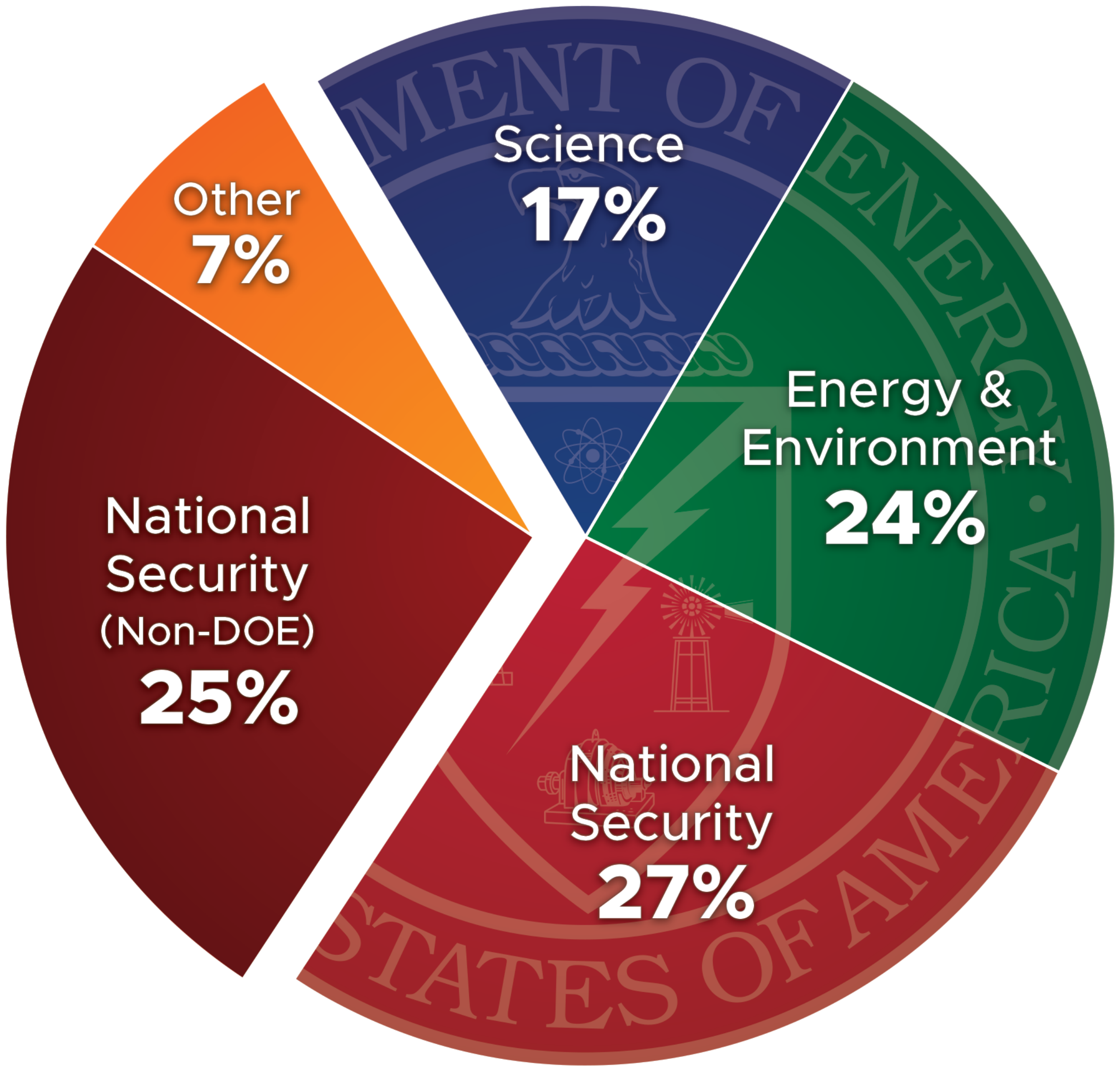
PNNL is one of DOE's **most diversified** national laboratories

$1.34B Spending

5,700 Staff

1,905 Peer-reviewed Publications

272 Invention Disclosures



FY 2022 Spending

Pacific Northwest
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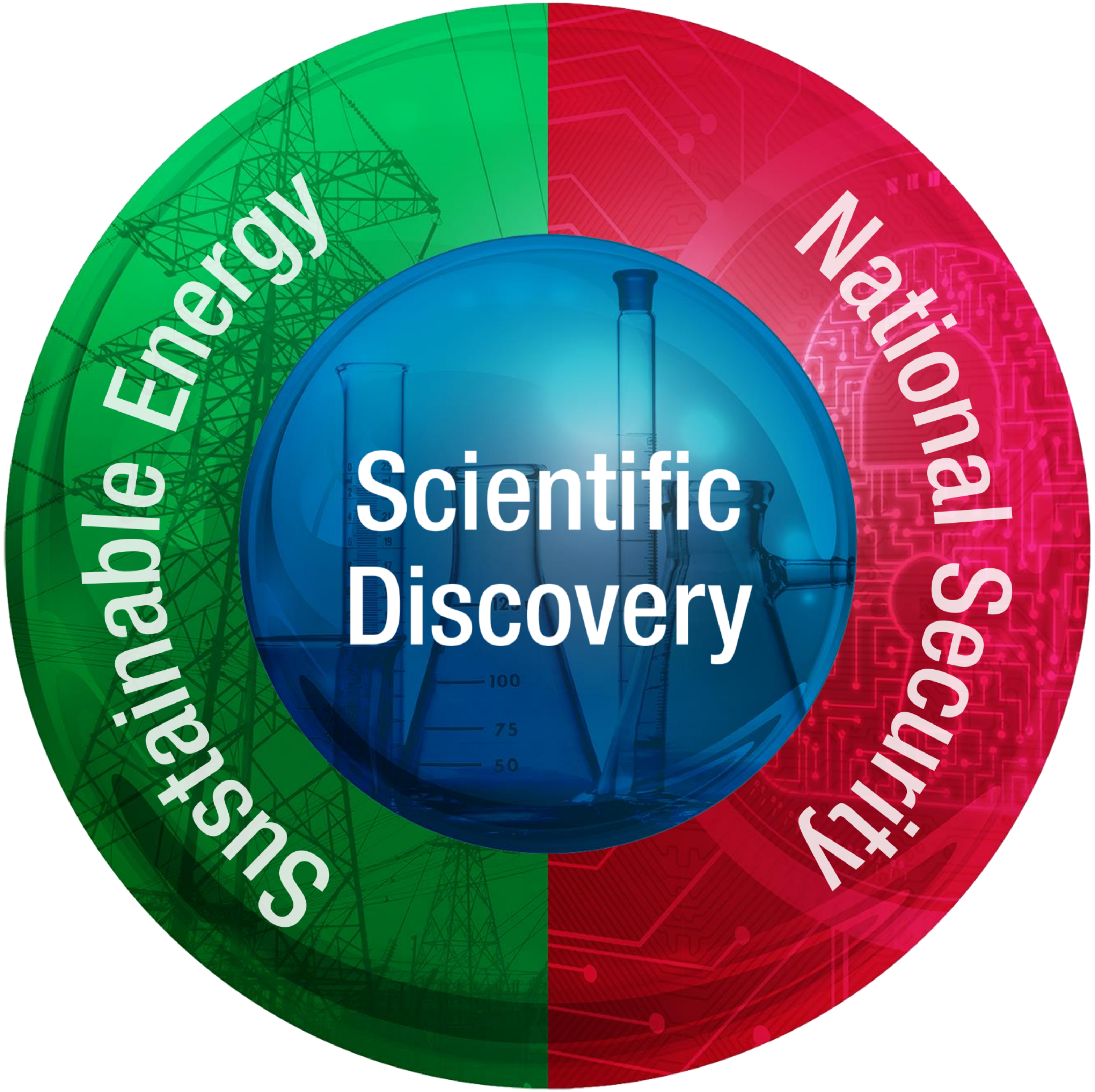
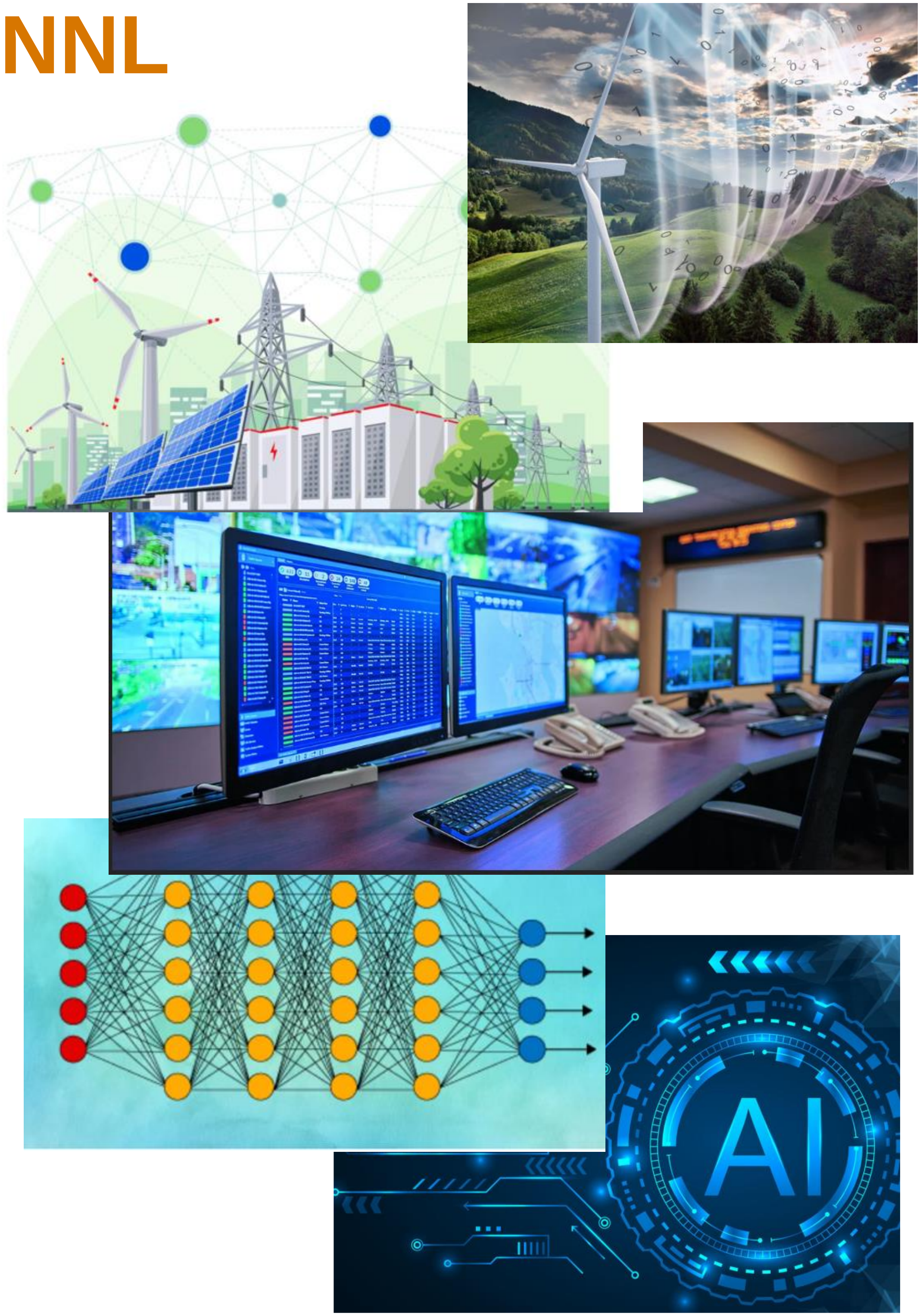
PNNL is **advancing scientific frontiers** and **providing solutions** to critical national needs



Sponsored AI Research at PNNL

- Working with DOE SC to develop new AI methods and computation paradigms for scientific discovery
- Working with ARPA-E, AITO, and DOE applied energy offices in engaging AI capabilities to support their mission objectives in:
    - **Energy Efficiency (including buildings)**
    - **Renewables (including wind)**
    - **Power grid**
    - **Manufacturing**
    - **Transportation**
- Developing and Managing Data Repositories



Overarching Research Challenges

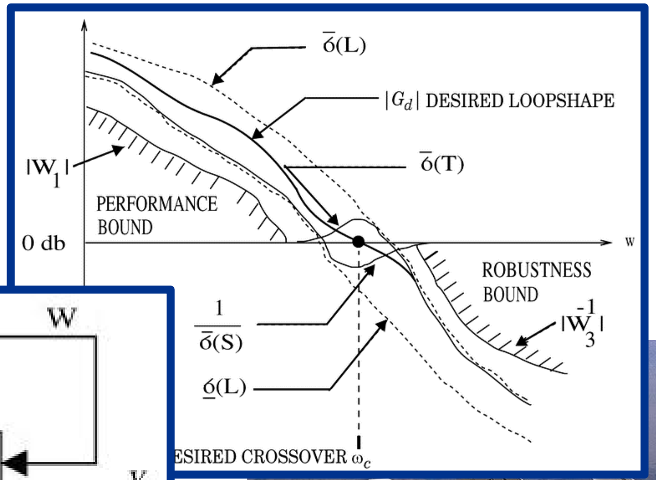
- Learning from limited and uncertain multi-modal data
  - Generation of high-quality and high-coverage data is costly and often unfeasible.
- Integrating data with physics models
  - Convergence of physical, computational and data sciences requires foundational advances in AI/ML and computing.
- Advancing computing systems to support heterogeneous workloads
  - Novel computing frameworks and heterogenous system-on-a-chip designs for converged applications require co-design.
- **Developing AI based operational tools**
  - **Utilize AI in combination with control approaches to develop systems that adapt in real-time to system abnormalities, recover from severe disruptions, and are responsive to human**

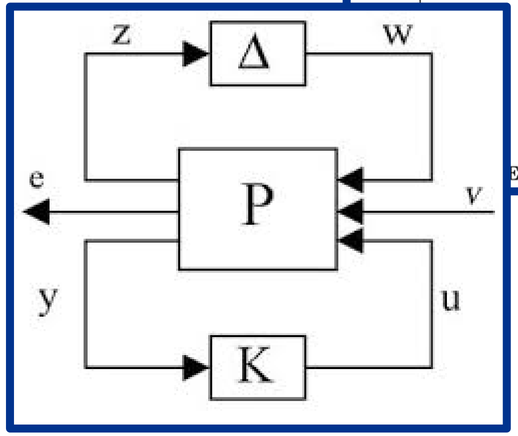
Classic Control Toolbox

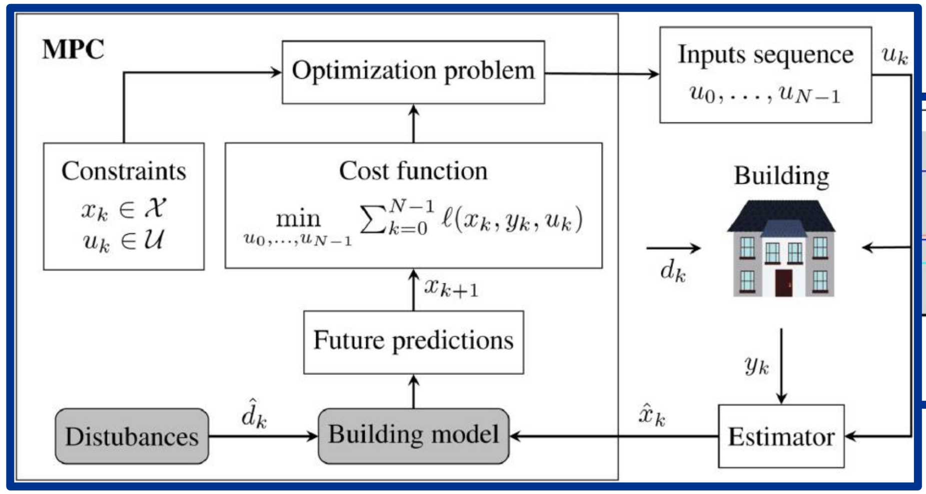
- **Uncertainty Management - Robust Control**
  - Advantage: Optimal performance for systems with parametric and dynamic uncertainty
  - Challenge: Conservative Solution, Sometimes hard to implement

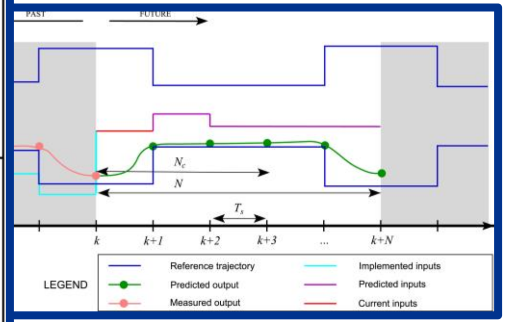
- **Constraint Management - Model Predictive Control**
  - Advantage: Optimal performance; automatic constraint prioritization
  - Challenge: Sensitive to modeling error, Convergence in real-time; Distributed solution hard

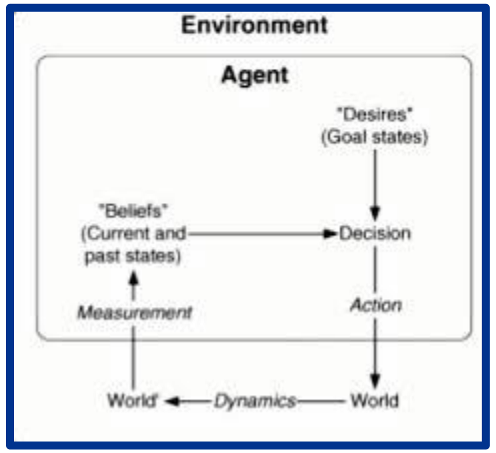
- **Complexity/Scale Management - Agent Based Control**
  - Advantage: Low computation and communication requirements, easy to implement
  - Challenge: Hard to guarantee performance

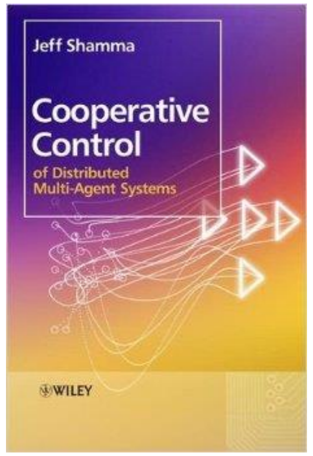




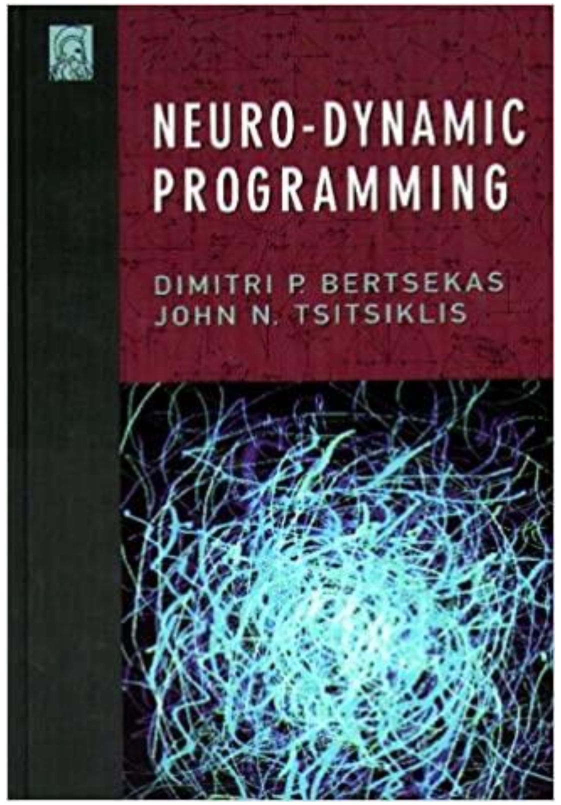


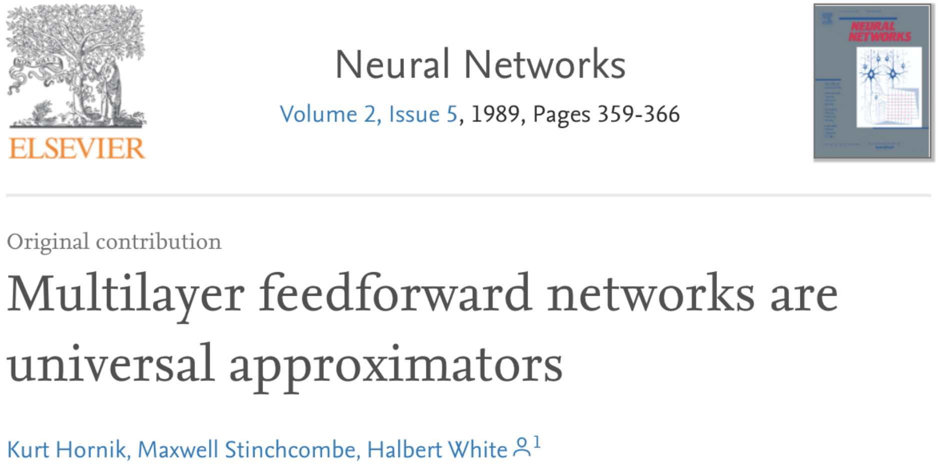






Neural Networks in Control




ELSEVIER

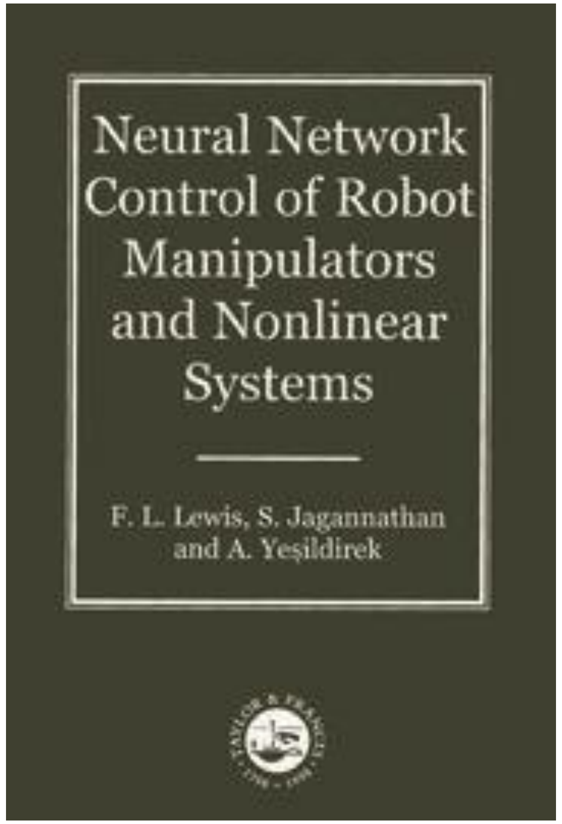
Neural Networks

Volume 2, Issue 5, 1989, Pages 359-366

Original contribution

Multilayer feedforward networks are universal approximators

Kurt Hornik, Maxwell Stinchcombe, Halbert White[1]



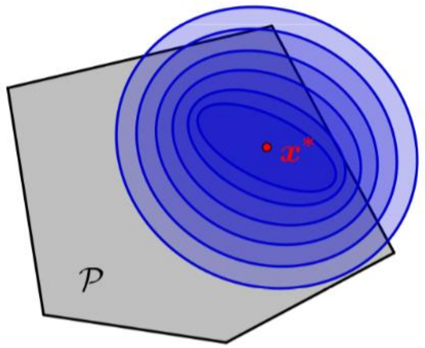
1996 – rigorous explanations of reinforcement learning through the lens of dynamic programming and practical use of function approximation

1999 – rigorous development of training dynamics and practical use of function approximation with performance guarantees during learning

Landscape of Optimization Methods

Online optimization

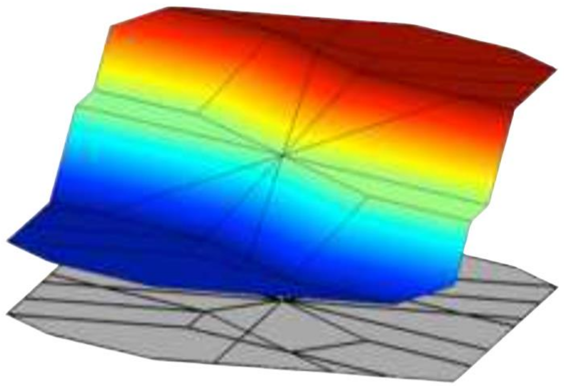
$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{subject to} \quad & b(x) \geq 0 \\ & c(x) = 0. \end{aligned}$$



- “online” solution for given parameter values
- computationally demanding in real-time

Parametric programming

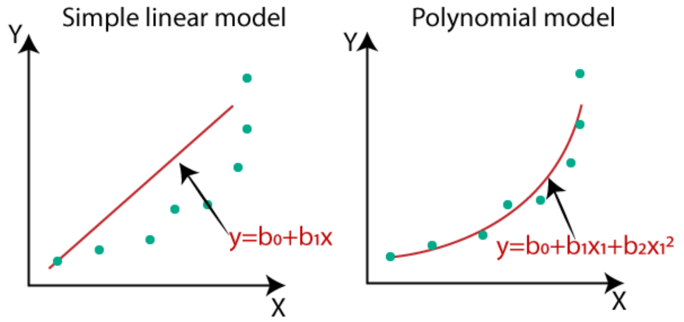
$$J^*(\theta) = \min_{x \in \mathbb{R}^n} f(x, \theta)$$
$$\text{subject to } g(x, \theta) \leq 0.$$
$$\theta \in \Theta \subset \mathbb{R}^m$$



- “offline” optimization obtains a solution map
- classical methods lead to exponential complexity!

Supervised Learning

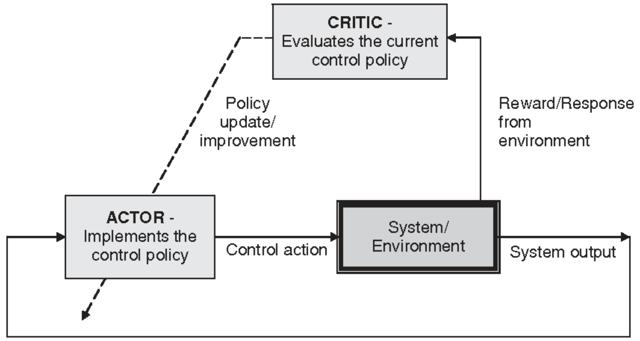
$$\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} L(y^i, f(x^i, \theta))$$



- “offline” optimization obtains a model (map)
- scalable but requires expert optimizer to imitate

Reinforcement Learning

$$\min_{\Theta} \sum_{i=1}^{m} \mathbf{r}(\mathbf{x}, \Theta)$$
$$\text{s.t. } \mathbf{Bellman}(\mathbf{x}, \Theta) = \mathbf{0},$$
$$\mathbf{environment}(\mathbf{x}, \Theta) = \mathbf{0}$$
$$\mathbf{x} \in \Xi$$



- “offline” optimization obtains a policy map
- classically can’t handle constraints

Classic Control Toolbox

Neural Networks in Control

Landscape of Optimization Tools

Classic Control Toolbox

Online optimization

PYOMO

JUMP

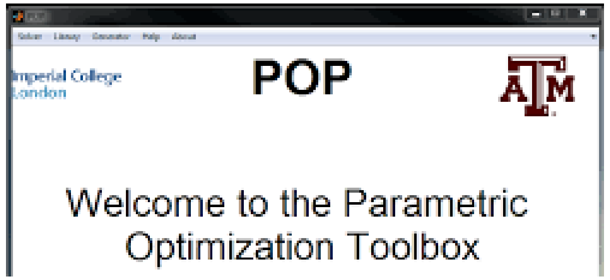
GEKKO DYNAMIC OPTIMIZATION

CVXPY

CasADi

GUROBI OPTIMIZATION

Parametric programming



Multi-parametric Toolbox (MPT)

MATLAB®

Neural Networks in Control

Supervised Learning

Reinforcement Learning

PyTorch

TensorFlow

flux

Gym

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Landscape of Optimization Tools

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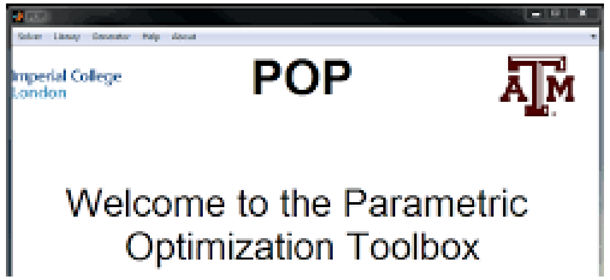


Multi-parametric Toolbox (MPT)

MATLAB®

Supervised Learning

Reinforcement Learning

PyTorch

TensorFlow

flux

Gym

What comes next? … Differentiable programming (DP): a unifying approach for data-driven optimization with solutions based on automatic differentiation (AD)

Differentiable Programming Enables a Wide Array of Applications

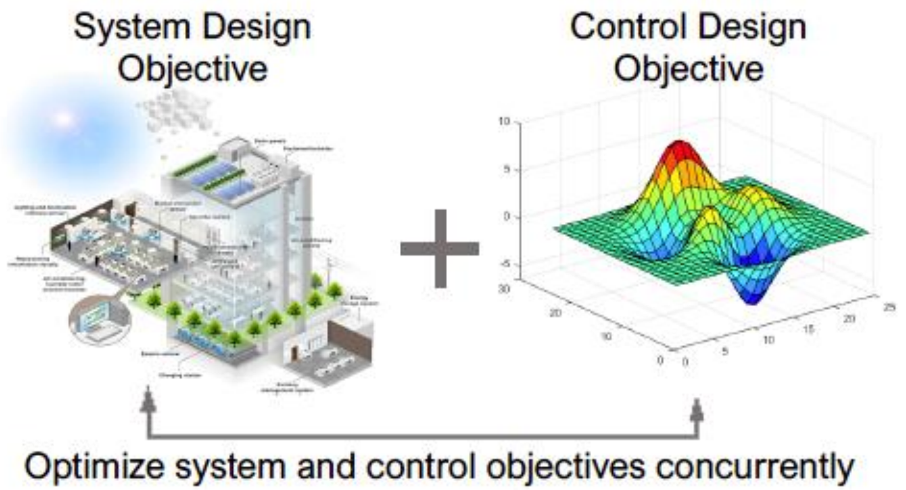
- **Differentiable Programming**
  - M. Innes, et al., *A Differentiable Programming System to Bridge Machine Learning and Scientific Computing*, 2019
- **Physics-informed Neural Networks**
  - M. Raissi, et al., *Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations*, 2019
- **Neural Differential Equations**
  - R. T. Q. Chen, et al., *Neural Ordinary Differential Equations*, 2019
  - C. Rackauckas , et al., *Universal Differential Equations for Scientific Machine Learning*, 2021
- **Differentiable Optimization**
  - A. Agrawal, et al., Differentiable Convex Optimization Layers, 2019
  - P. Donti, et al., *DC3: A learning method for optimization with hard constraints*, 2021
  - S. Gould, et al., *Deep Declarative Networks: A New Hope*, 2020
  - J. Kotary, et al., *End-to-End Constrained Optimization Learning: A Survey*, 2021
- **Differentiable Control**
  - B. Amos, et al., *Differentiable MPC for End-to-end Planning and Control*, 2019
  - S. East, et al., *Infinite-Horizon Differentiable Model Predictive Control*, 2020

Differentiable Programming Enables New Control Paradigms

- **ML Based System & Control Co-Design**

  Systems are becoming more complex with significant intersystem couplings that are less understood

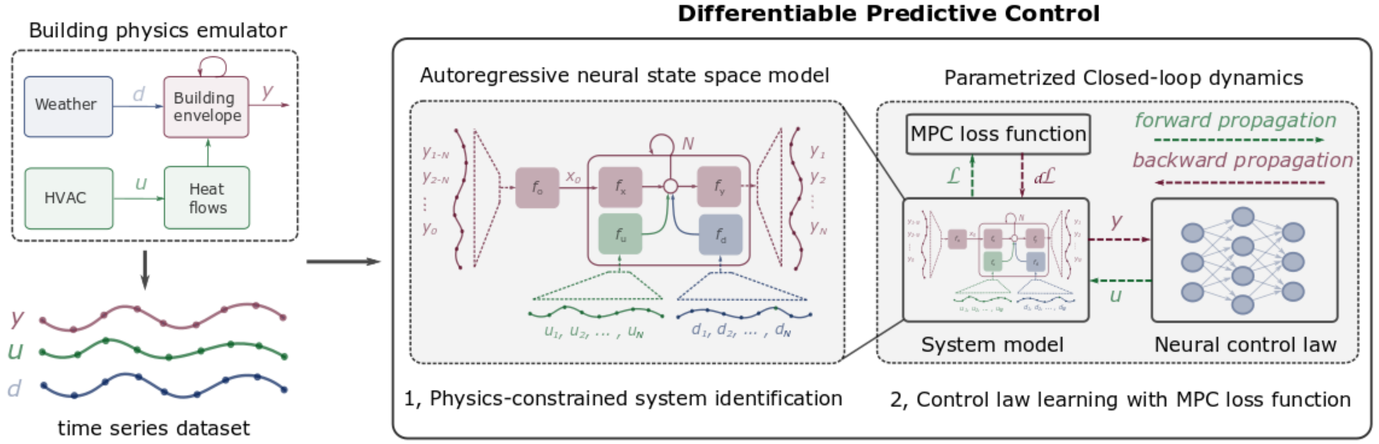
  - Enable design and operation of systems for multiple objectives
  - Address need to incorporate and evaluate control options early in the project design cycle



- **Simulation-based modeling and control**

  Simulations are crucial for decision-making

  - Improve computational efficiency and scalability for heterogenous scientific simulations
  - Use data to optimized explicit predictive control policy



Invited Speakers

Boris Ivanovic
(NVIDIA)

Mario Zanon
(IMT Lucca)

Bingqing Chen
(Bosh AI)

Chris Rackauckas
(MIT)

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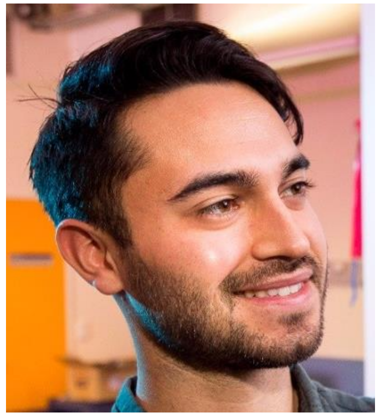
Workshop Organizers

Jan Drgona

Aaron Tuor

Biswadip Dey



Wenceslao Shaw Cortez

Soumya Vasisht

Draguna Vrabie

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SIEMENS

Workshop Schedule

08:30 am - 09:00 am - **Sonja Glavaski-Radovanovic** (PNNL): Opening remarks and overview of differentiable programming

9:00 am - 9:30 am - **Boris Ivanovic** (NVIDIA): Differentiable robotics

9:30 am - 10:00 am - **Biswadip Dey** (Siemens): Learning Hamiltonian dynamics with control

10:00 am - 10:30 am - Coffee break

10:30 am - 11:00 am - **Mario Zanon** (IMT Lucca): Differentiating MPC with applications in Reinforcement Learning

11:00 am - 11:30 am - **Bingqing Chen** (Bosch Center for AI): Towards safe and sample-efficient autonomous energy systems via differentiable programming

11:30 pm - 1:00 pm - Lunch Break

1:00 pm - 2:00 pm - **Chris Rackauckas** (MIT): Code tutorial 1: Julia

2:00 pm - 3:00 pm - **Aaron Tuor** (PNNL): Code tutorial 2: PyTorch

3:00 pm - 3:30 pm - Coffee break

3:30 pm - 5:00 pm - **Jan Drgona** (PNNL): Code tutorial 3: PyTorch

Thank you