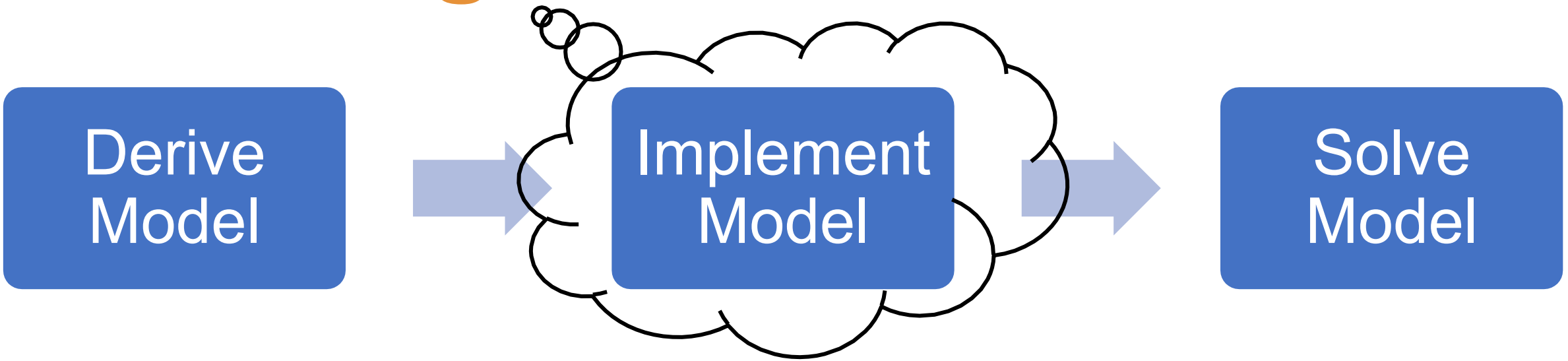
# Open-Source Modeling Platforms

**Bethany Nicholson, Sandia National Laboratories**
**John Hedengren, Brigham Young University**

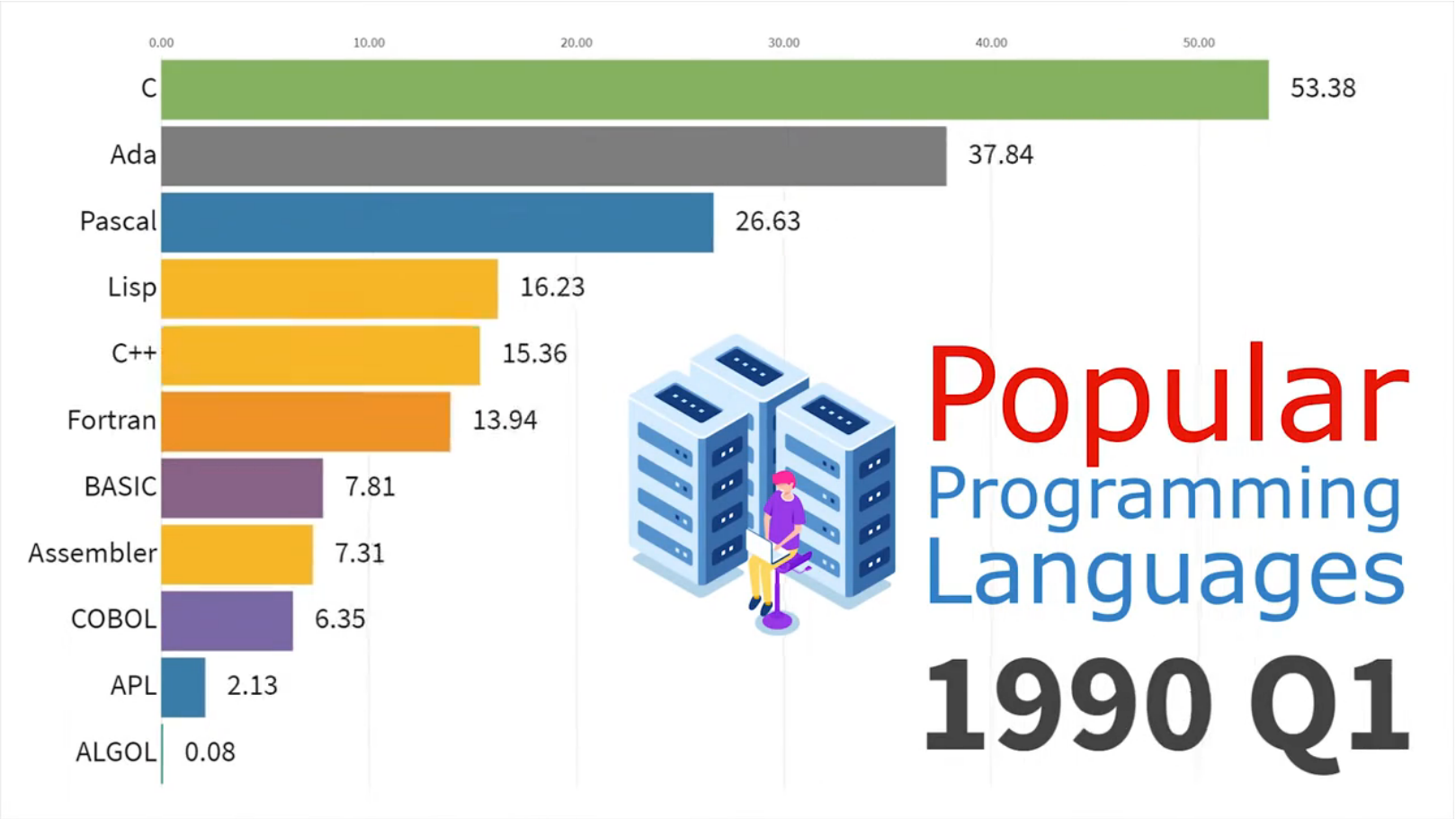
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525


# Open-Source Modeling Platforms



# Current Trends in Programming

- +22% projected growth in programming jobs over next decade
  - Development, QA, Analysis, Testing
- Popular Programming Language Trends




Source: Data is Beautiful
[Most Popular Programming Languages 1965 - 2019]

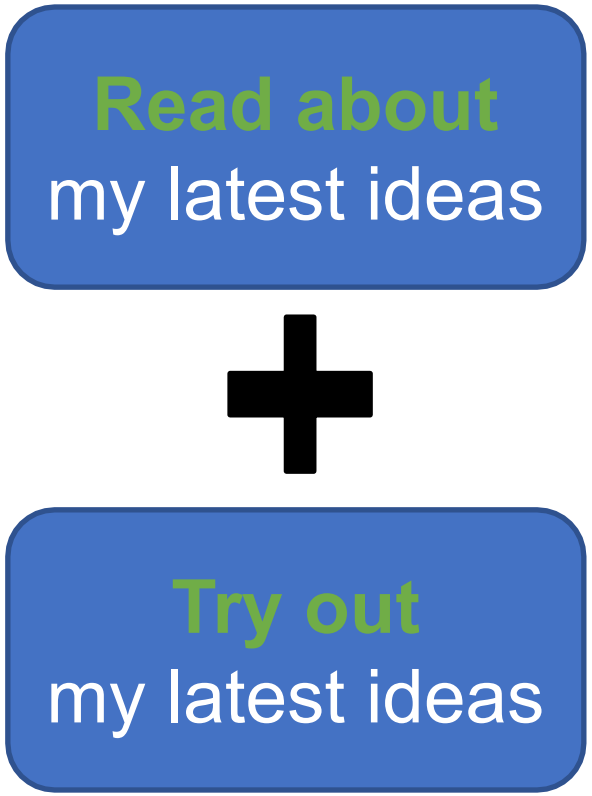
# Overview

- Motivations and Metrics for Open-Source
- Algebraic Modeling Languages
- Data-Driven Modeling Languages
- Speed of Innovation
- Future of Open-Source Tools

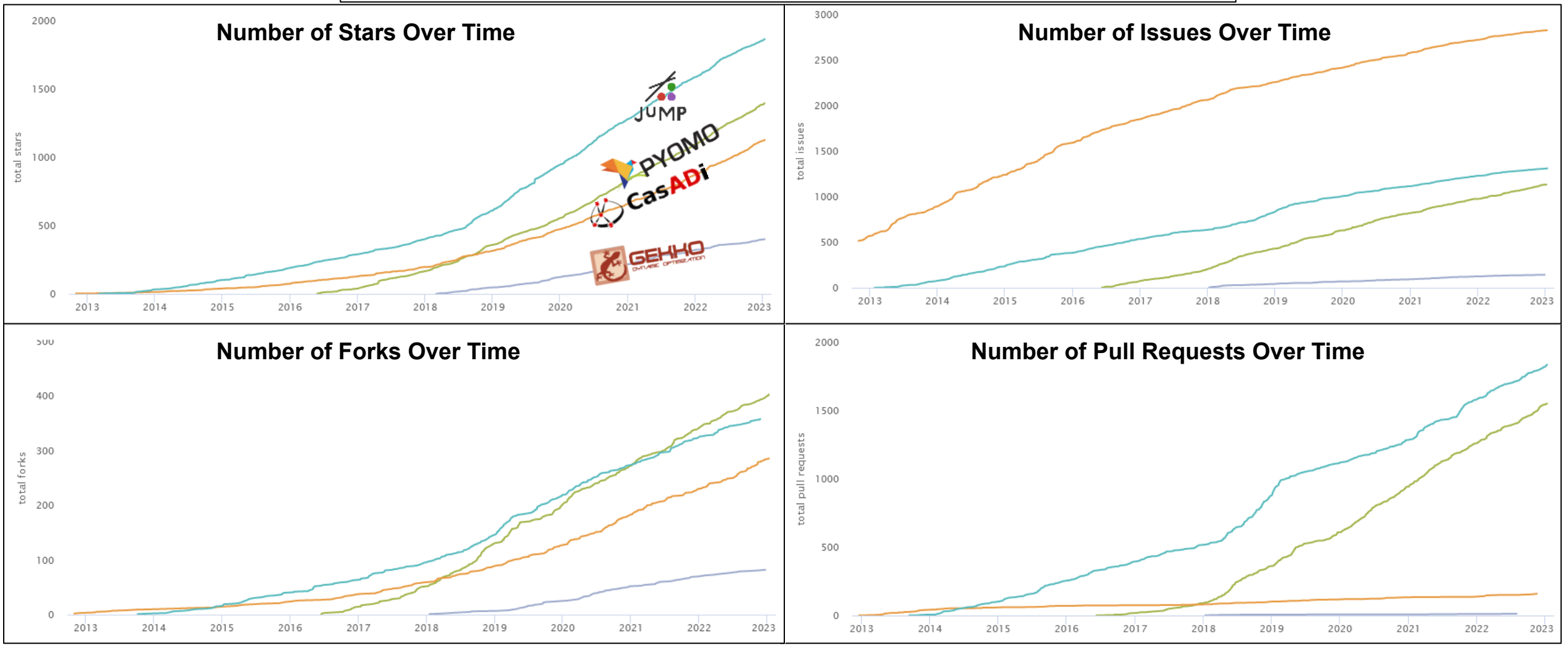
# Motivations and Metrics for Open-Source

- Motivations
  - Sometimes required by sponsoring agency
  - Spread development burden, “mind share”
  - Transparency of results
  - Building a community

- Metrics
  - Install Rate, Q+A Forum Posts, Citations
  - Latest Release, Documentation
  - OS Support, GitHub Insights
  - Ease of installation
  - Extensibility and scalability



# Algebraic Modeling Languages – GitHub Metrics




https://vesoft-inc.github.io/github-statistics/

# History of Pyomo




- First release in 2008 as the Coopr software library
- Rebranded as Pyomo around 2011
- Moved to GitHub in mid-2016
- Pyomo supports a wide range of problem types, including:
  - LP, QP, NLP, MILP, MIQP, MINLP
  - SP, GDP, DAE, Bilevel, MPEC
- Distributed on pypi.org, anaconda.org, and GitHub

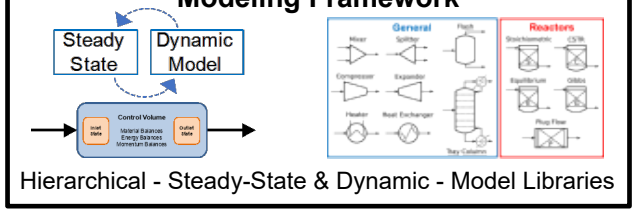
2020 R&D 100 WINNER

# IDAES Integrated Platform

Institute for the Design of Advanced Energy Systems

## IDAES-Core

**Modeling Framework**




Hierarchical - Steady-State & Dynamic - Model Libraries

**Data Management Framework**

**User Interface & Visualization**

**Advanced Equation Oriented Solvers**

PYOMO

**Flexible Programming Foundation**

python

## IDAES-Materials

MatOpt Nanomaterials optimization

## IDAES-UQ

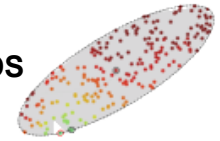
**Data Reconciliation**

**Parameter Estimation**

**K-Aug & sIPOPT**

**Rigorous Model Sensitivity**

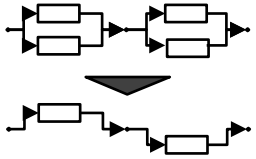
**PyROS**



**Optimization & Uncertainty Quantification**

## IDAES-Design

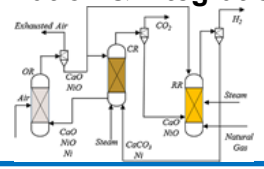
**Conceptual Design via Superstructure Optimization**



PYOMO GDP

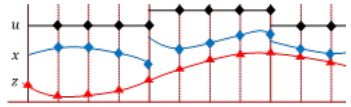
**Pyosyn**

**Process Design, Optimization & Integration**



## IDAES-Operations

**Process Dynamics**




PYOMO DAE

**Trajectory optimization, optimal control, state/parameter estimation**

**Process Control**

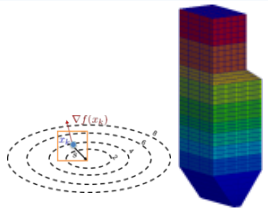
## IDAES-AI

ALAMO a black-box modeling tool

RIPE

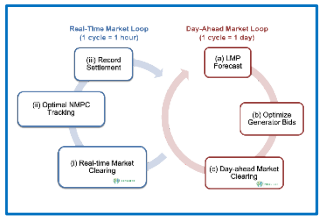
HELMET

PySMO



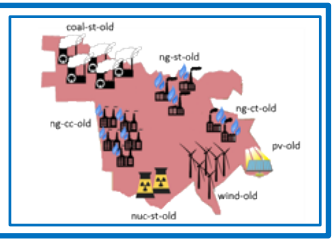
**Multi-Scale Modeling and Optimization**

## IDAES-Enterprise

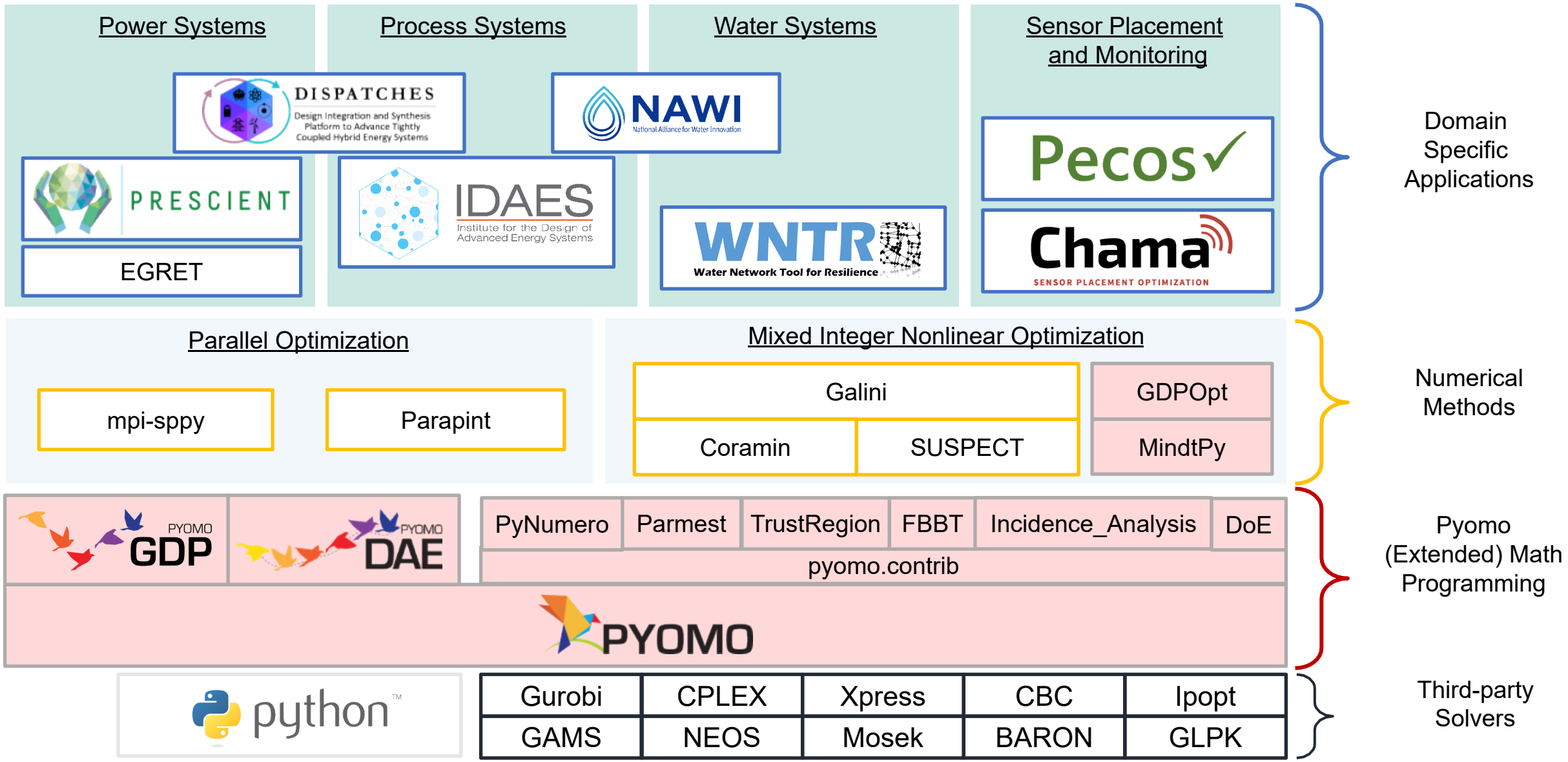



**Electricity Grid Modeling**

**Expansion Planning**



# Optimization software ecosystem



# Benchmark: Energy Storage

$$\min_{g} \quad g \tag{4a}$$

$$\text{s.t.} \quad \frac{de}{dt} = q_{\text{in}} - q_{\text{out}} \cdot \eta \tag{4b}$$

$$q_{\text{in}} = g - d + s_{\text{in}} \tag{4c}$$

$$q_{\text{out}} = d - g + s_{\text{out}} \tag{4d}$$

$$g - d = s_{\text{out}} - s_{\text{in}} \tag{4e}$$

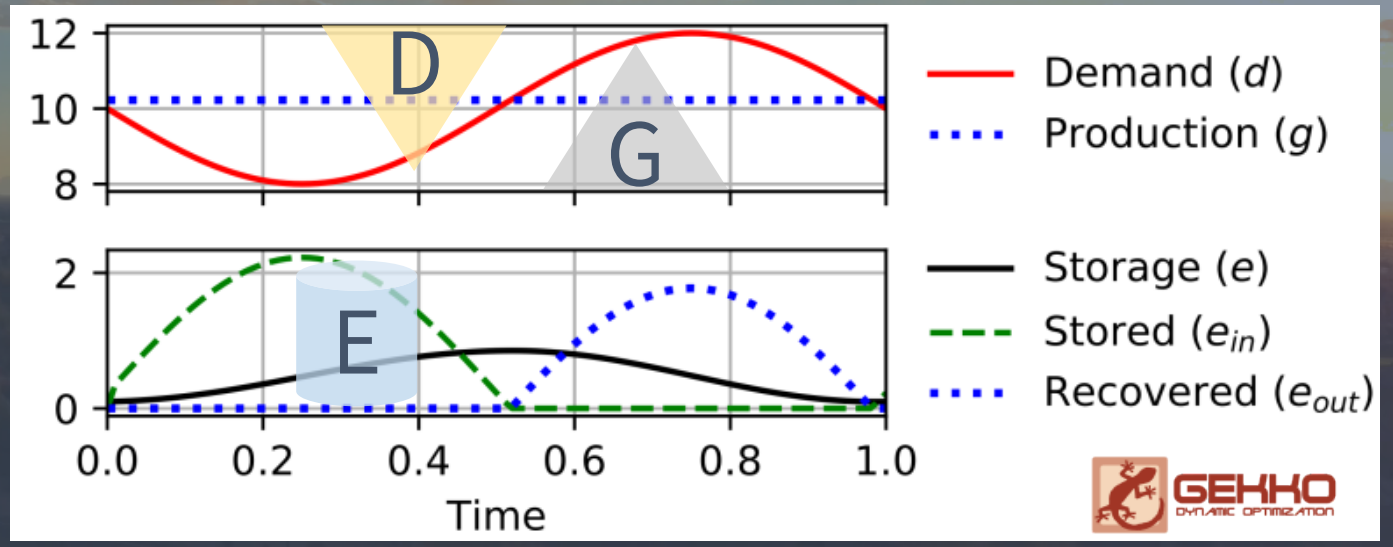
$$s_{\text{out}},\ s_{\text{in}} \geq 0, \quad q_{\text{out}} \times q_{\text{in}} \leq 0 \tag{4f}$$

$$g + q_{\text{out}}/\eta - q_{\text{in}} \geq d \tag{4g}$$

$$e \geq 0, \quad \eta = 0.7 \tag{4h}$$

$$d = 10 - 2\sin(2\pi t) \tag{4i}$$

$$e(0) = e(1) = 0 \tag{4j}$$




Gates, N.S., Hill, D.C., Billings, B.W., Powell, K.M., Hedengren, J.D., Benchmarks for Grid Energy Management with Python Gekko, 60th Conference on Decision and Control (CDC), Austin, TX, USA, December 13-15, 2021.

# Benchmark: Cogeneration

$$\min_{r} \quad J = \sum_{i=1}^{n} \int_{t=0}^{1} \Big[ 1000 \ \max(0,\, d_i - g_i) + \max(0,\, g_i - d_i) \Big] \, dt \tag{2a}$$

$$\text{s.t.} \quad \frac{dg_1}{dt} = r, \quad g_2 = 2g_1 \tag{2b}$$

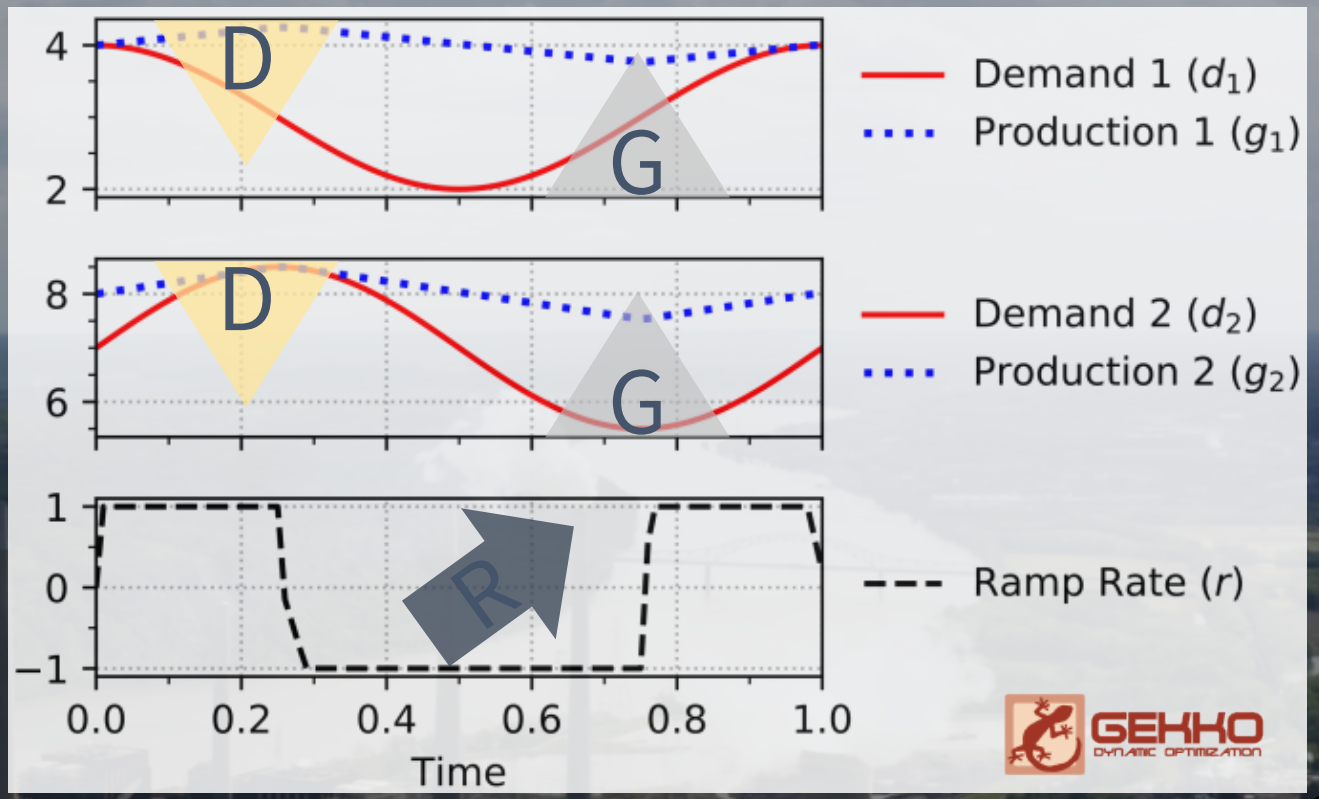
$$d_1 = \cos(2\pi t) + 3 \tag{2c}$$

$$d_2 = 1.5 \sin(2\pi t) + 7 \tag{2d}$$

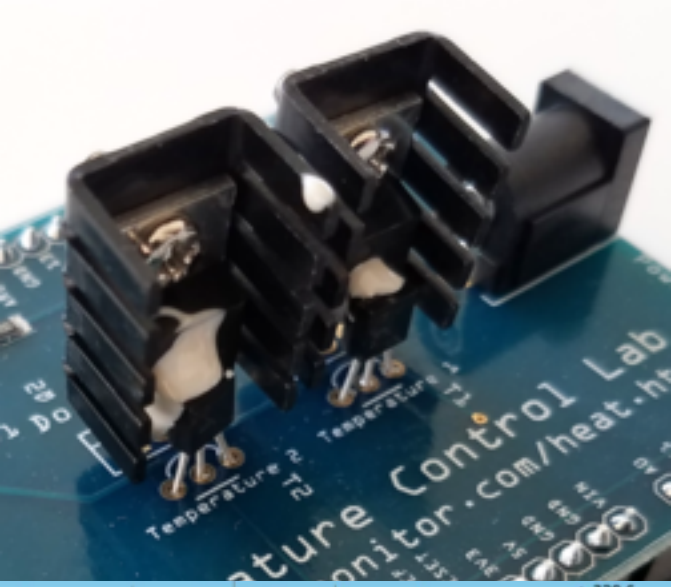
$$-1 \leq r \leq 1 \tag{2e}$$

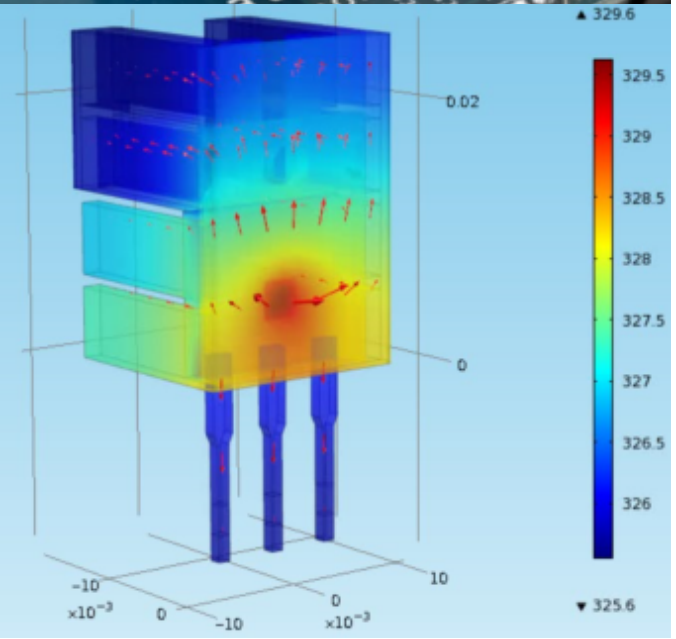
$$g_1(0) = 4 \quad (d_1(0) = 4) \tag{2f}$$

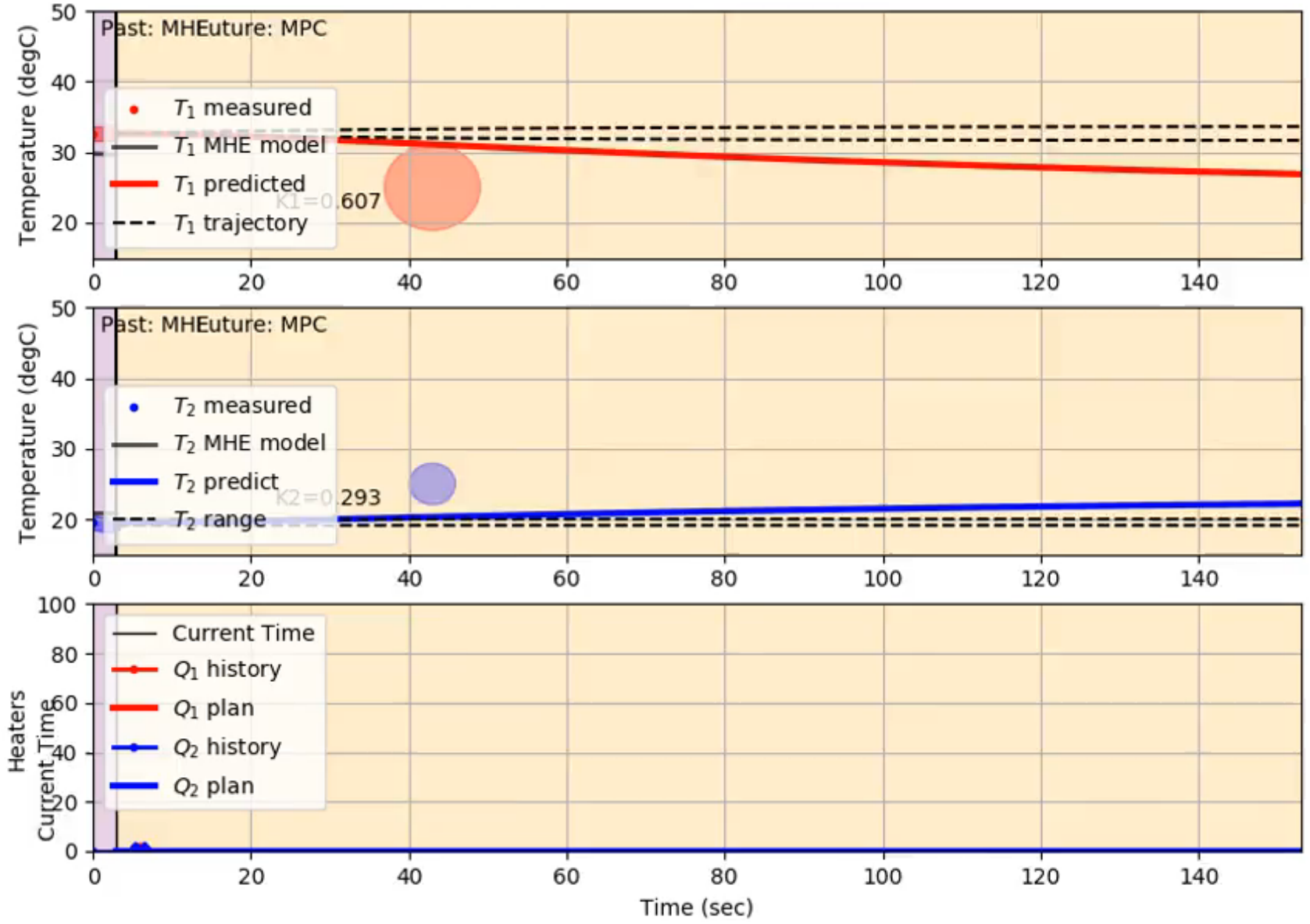
$$g_2(0) = 8 \quad (d_2(0) = 7) \tag{2g}$$



# Benchmark: Temperature Control Hardware





# Application: Flight Optimization

http://prismweb.groups.et.byu.net/360/

Select Variable: Altitude (m)

2D / 3D

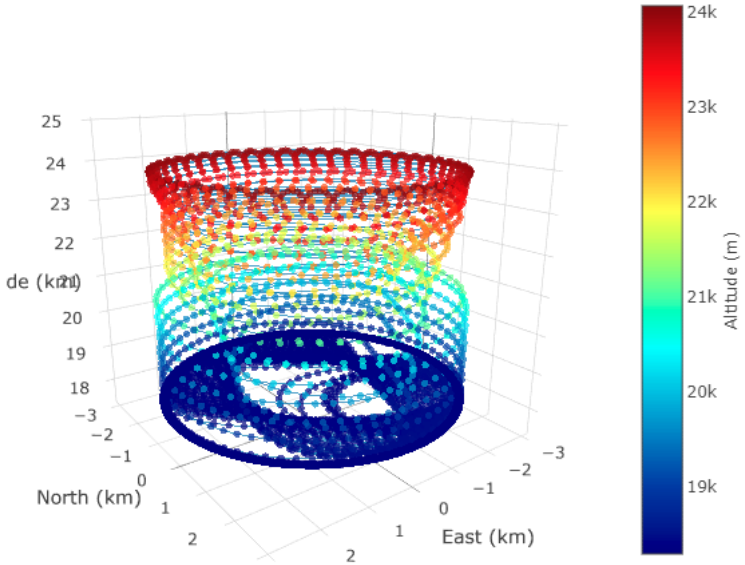
Hide Wind / Show Wind

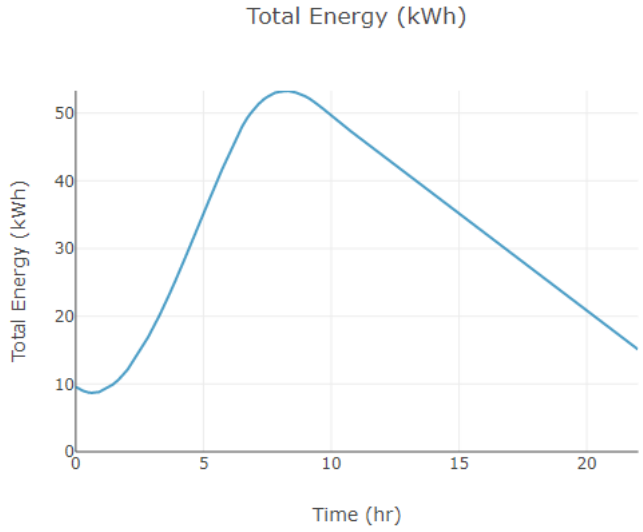
Hide Sun / Show Sun

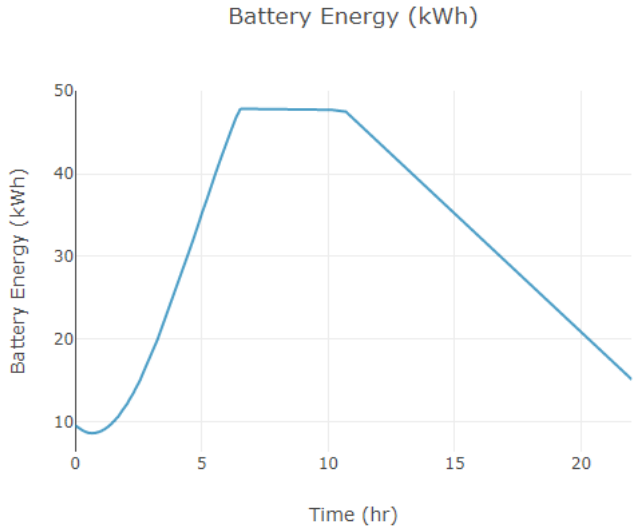
Select Variable: Total Energy (kWh)

Select Variable: Battery Energy (kWh)

https://github.com/BYU-PRISM/hale-trajectory



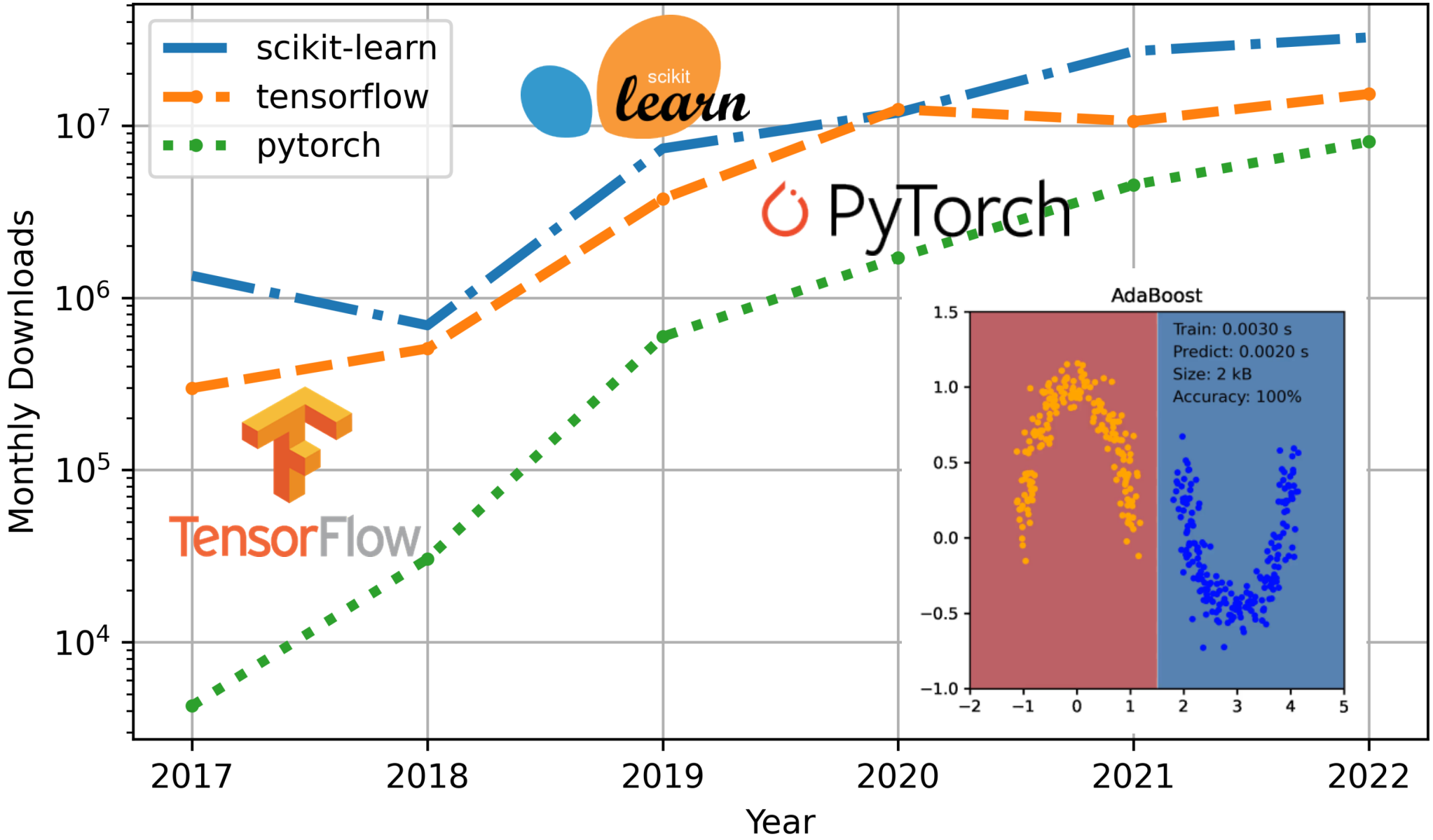



# Application: Drilling Automation

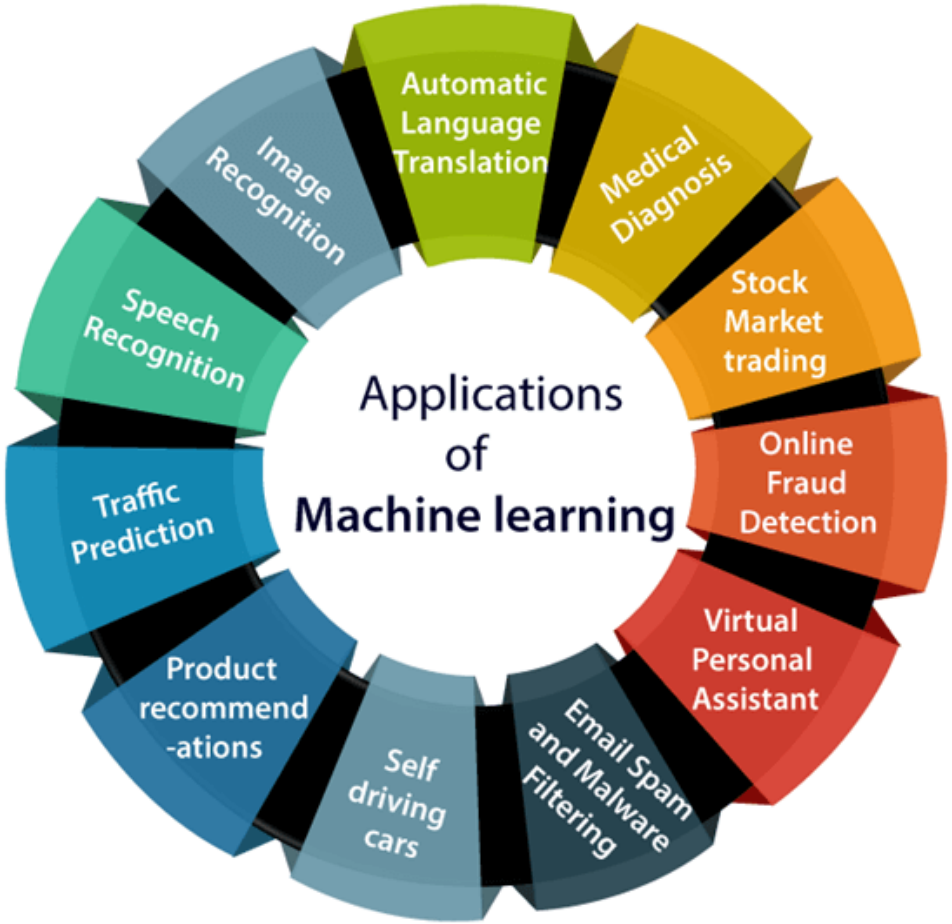

SPE-112109 Courtesy eDrilling

# Data-Driven Modeling Languages



# Data-Driven Applications

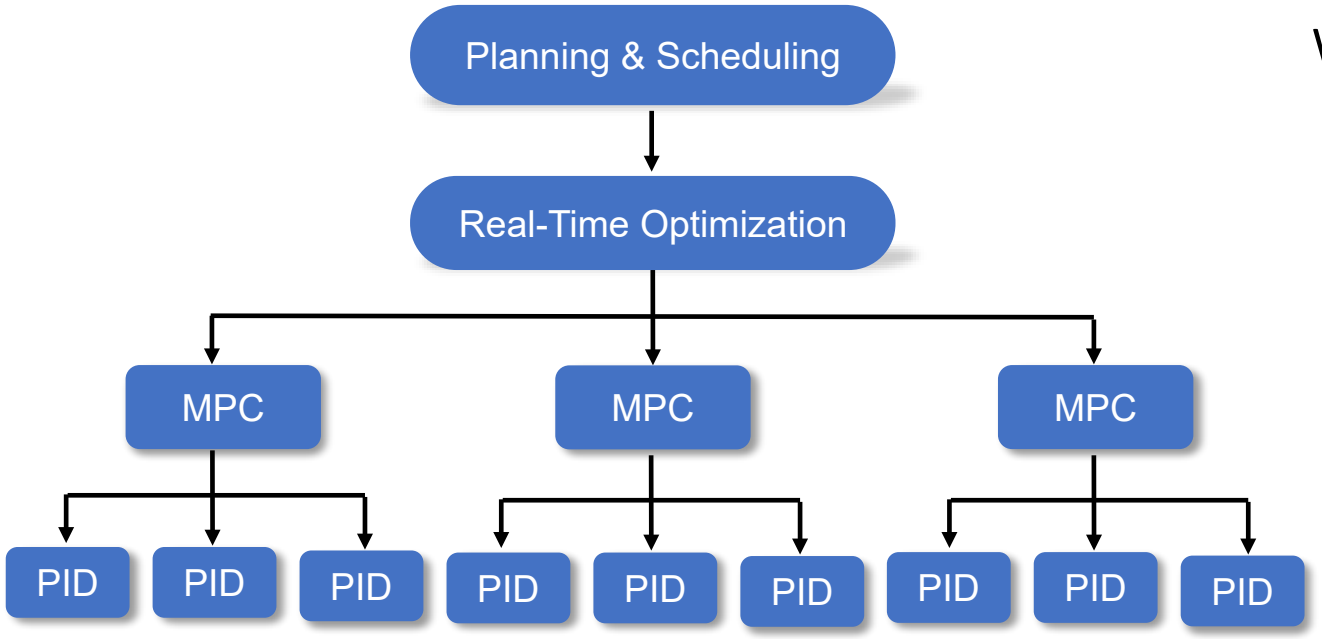





https://www.javatpoint.com/applications-of-machine-learning

# Combined Architectures

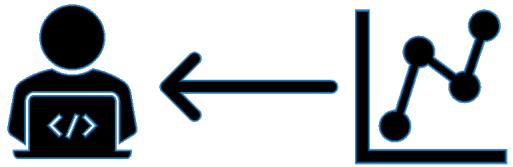
| Model Type | | Execution Interval |
|---|---|---|
| Steady state | Linear | Weeks/Months |
| Steady state | Rigorous | Hours |
| Dynamic | Linear<br>Empirical | Minutes |
| Deterministic control policy | | Seconds |



# Physics-Informed, Data-Driven Modeling

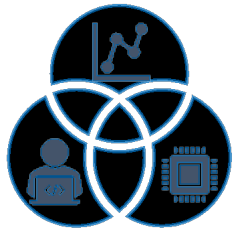
- Option 1: Physics-Based Simulator Provides Data for ML

- Option 2: Adjust Parameters in Physics-Based Simulator to Fit Data

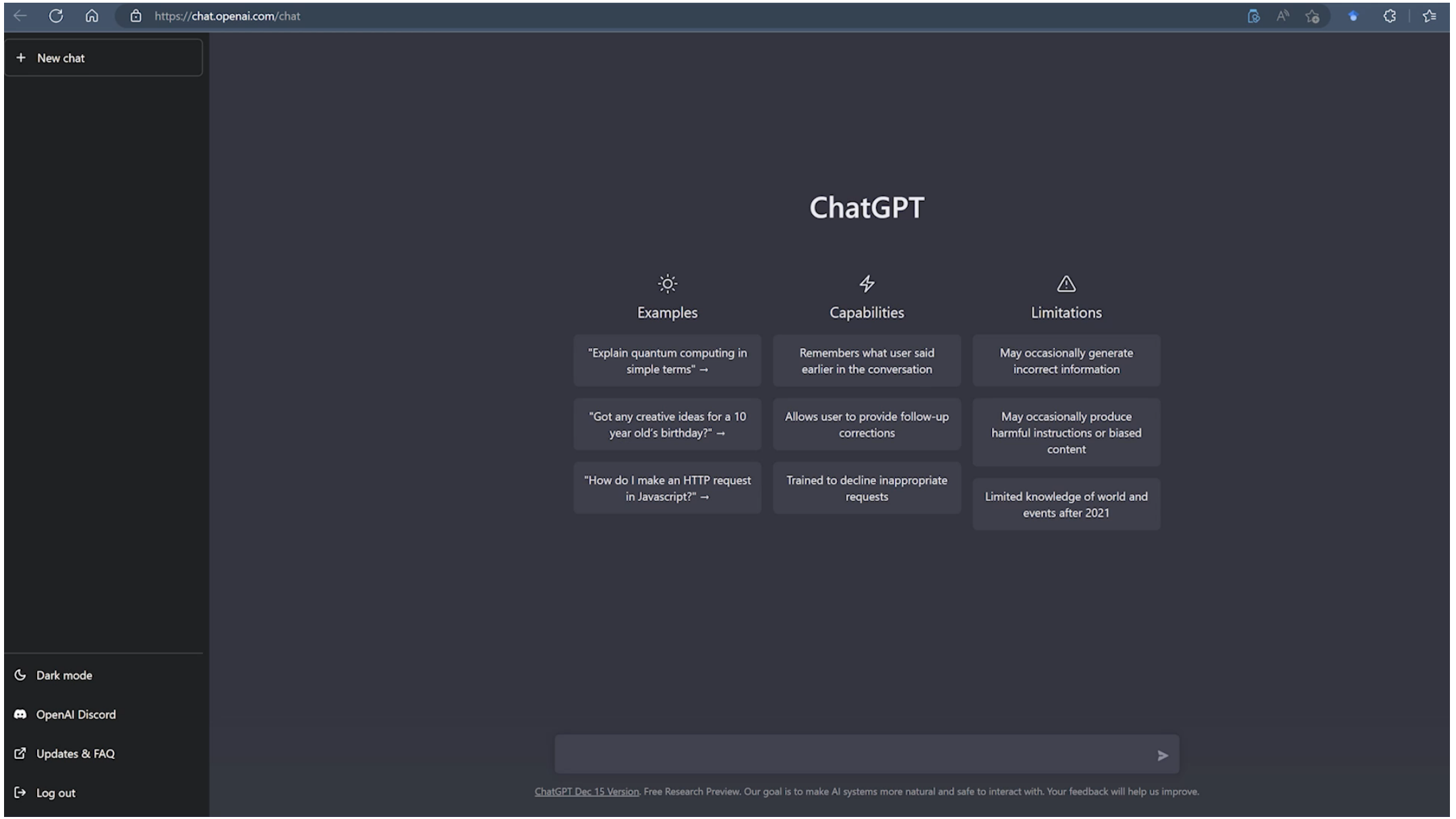


- Option 3: Physics-Based Model + ML for Residual Error

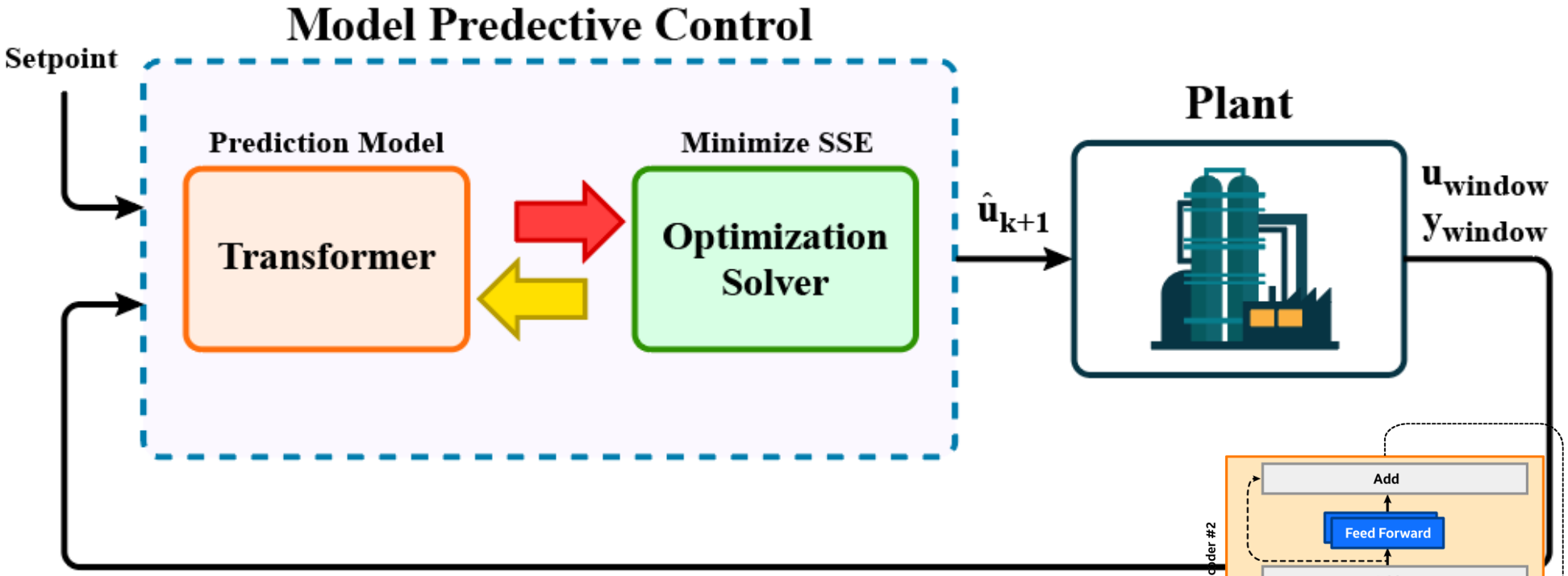
- Option 4: Hybrid Physics-Based and ML Modeling

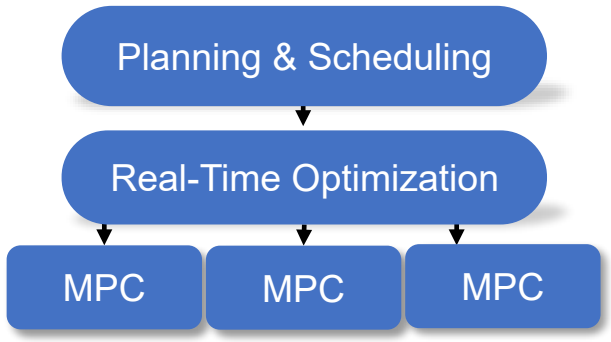


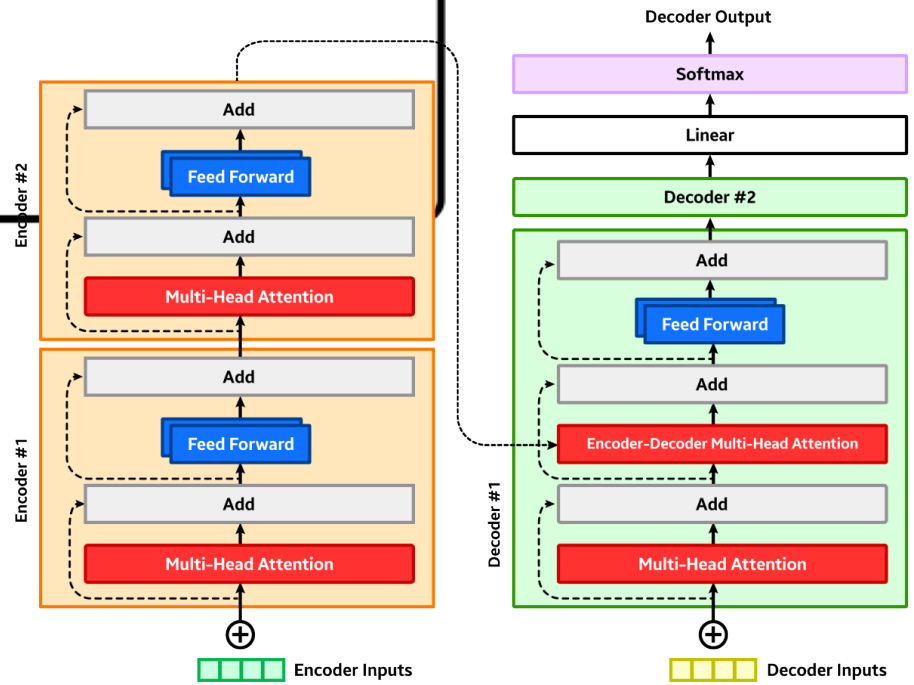
# Speed of Innovation



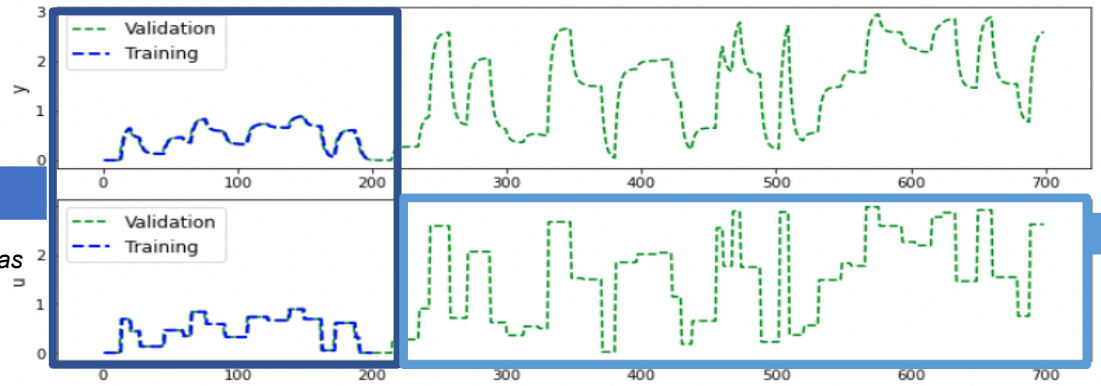
# Future of Open-Source Tools – What's Next



# Physics Informed Neural Network (PINN)

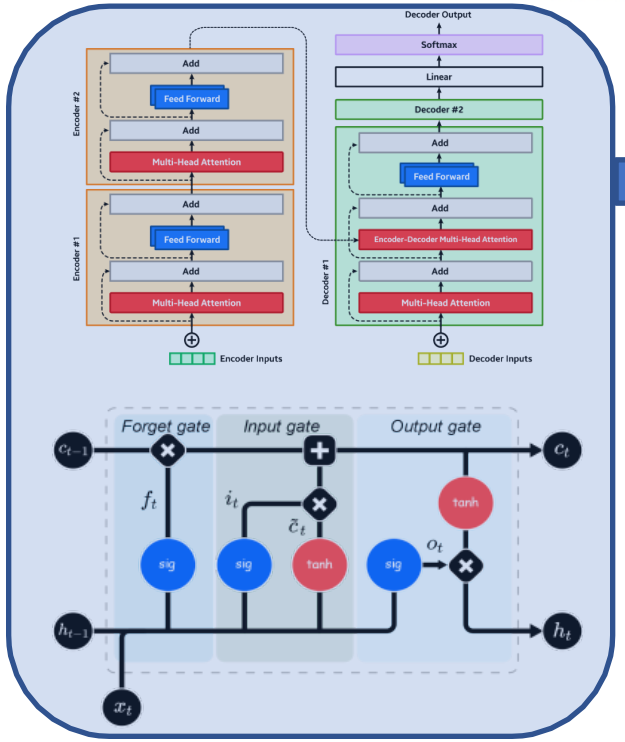



$y_{meas}$, $u_{meas}$

$u_{meas}$

Training

Evaluating

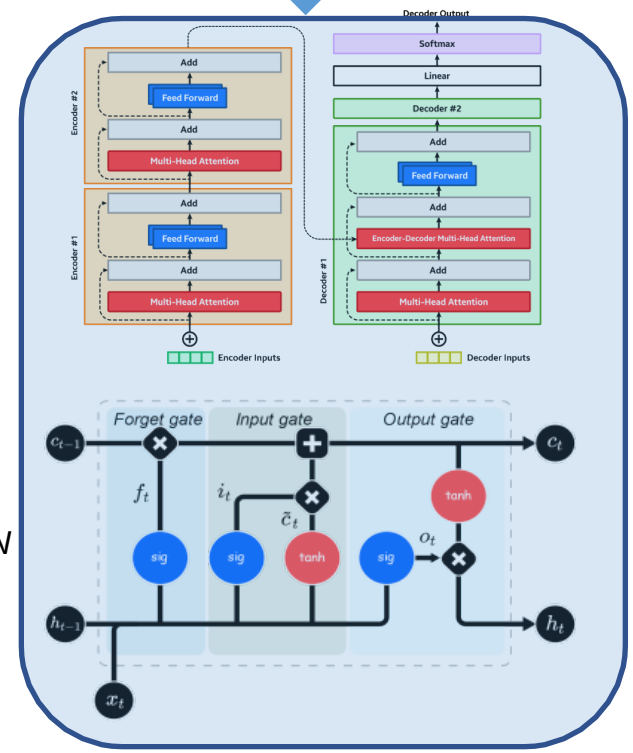



$$MSE_y = \frac{1}{N_y}\sum_{i=1}^{N_y}\left|y_{NN}(t_i,u_i) - y_{meas}\right|^2$$

+

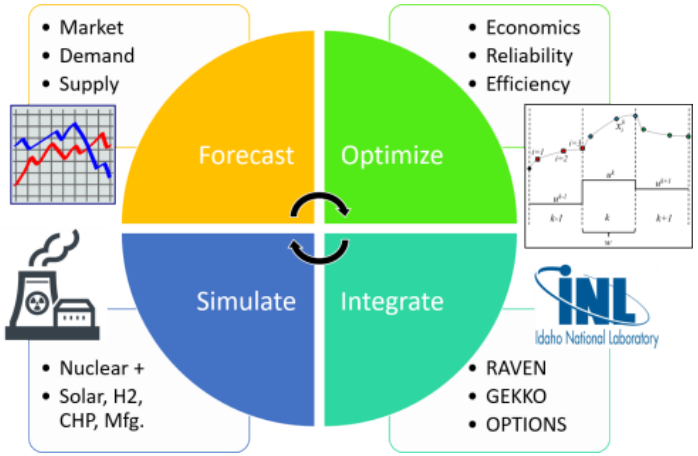
$$MSE_f = \frac{1}{N_f}\sum_{i=1}^{N_f}\left|f(t_i,\dot{y}_{NN},y_{NN},u_{meas})\right|^2$$

$y_{NN}$




Combined Loss function

# Physics-Informed, Data-Driven Modeling

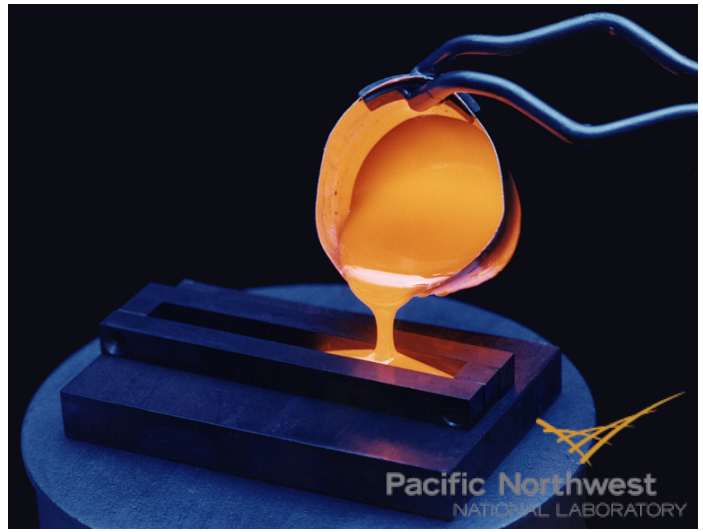

scikit learn

GEKKO DYNAMIC OPTIMIZATION

MLT

PYOMO

TensorFlow




Gunnell, L., Manwaring, K., Lu, X., Reynolds, J., Vienna, J., Hedengren, J.D., Machine Learning with Gradient-based Optimization of Nuclear Waste Vitrification with Uncertainties and Constraints, Processes, 10(11), 2365, Nov 2022, DOI: 10.3390/pr10112365.

# Future of Open-Source Tools – What's Needed

- Long term support and maintenance
  - Stakeholder/project funding dictates priorities
  - Understand development process for the open source tools you rely on
  - Support and coordination of upstream and downstream dependencies
  - Community involvement (bug reports/fixes, feature development, etc.)
- Wider adoption of software engineering practices
  - Lots of free infrastructure for open source
  - Encourage students to get involved in open source
- Recognition of code and software contributions
- Interoperability of existing tools
  - Blending of data-driven and equation-based methods