Open-source high-performance tools for grid modeling, simulation, and learning @ PNNL

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DOE's 17 **national laboratories** tackle critical scientific challenges

A regional, national, and international **scientific resource**

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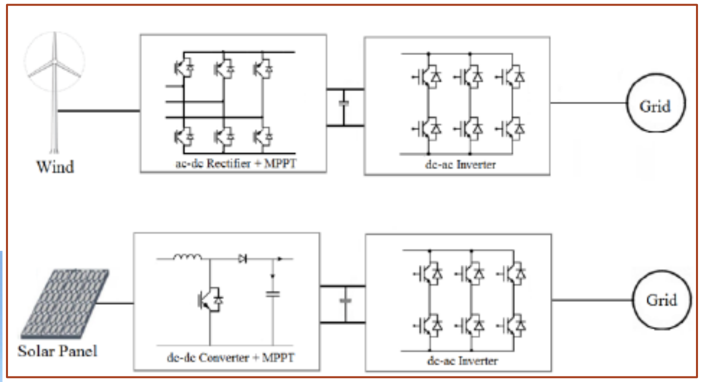
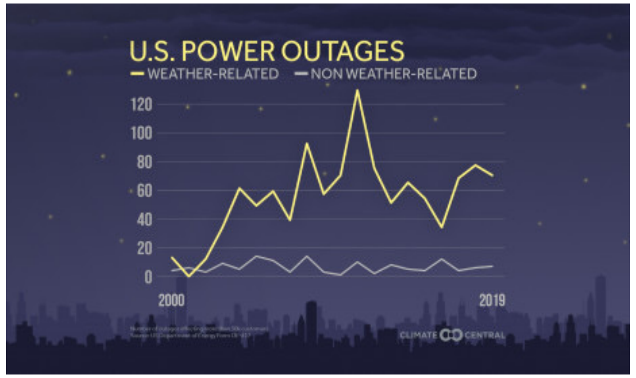
Changing nature of grid

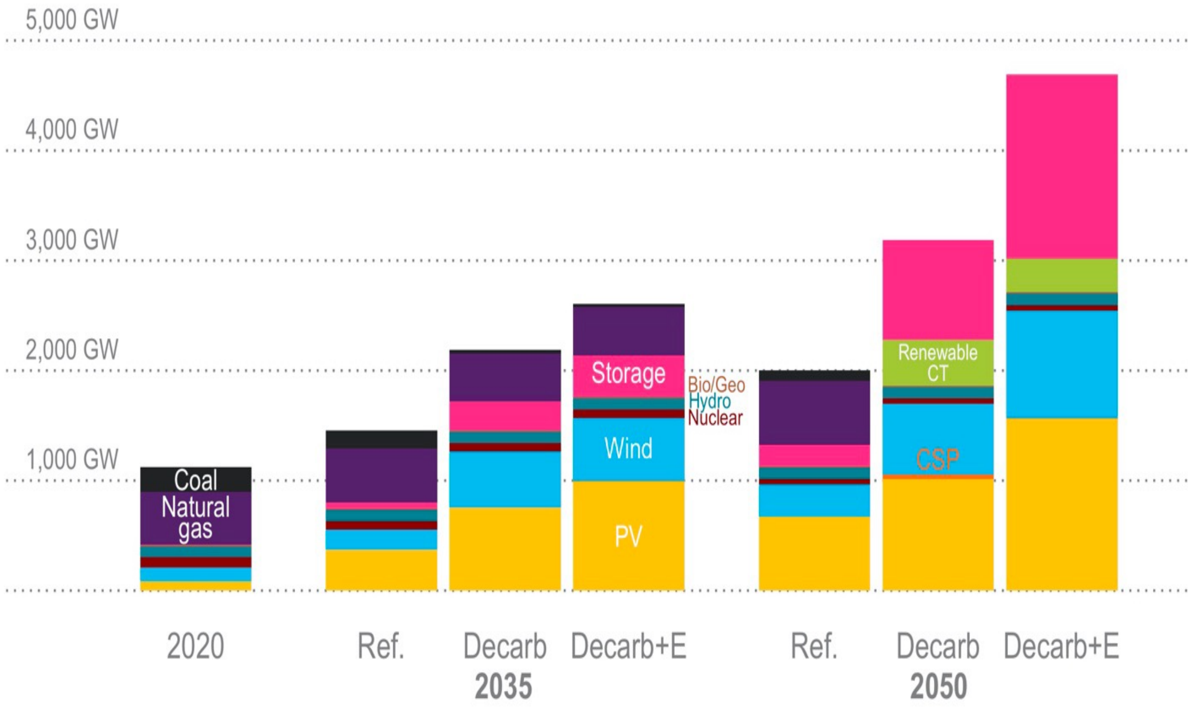
- Move towards 100% renewable penetration
- Inverter-based interfaces (Grid forming/grid following inverters)
- Deployment of distributed generation, storage, flexible load technologies
- Increased visibility (PMU, AMI, …)
- Climate change and increase in number of disruptions





System challenges in clean energy and decarbonization

US Electricity Generation Projection

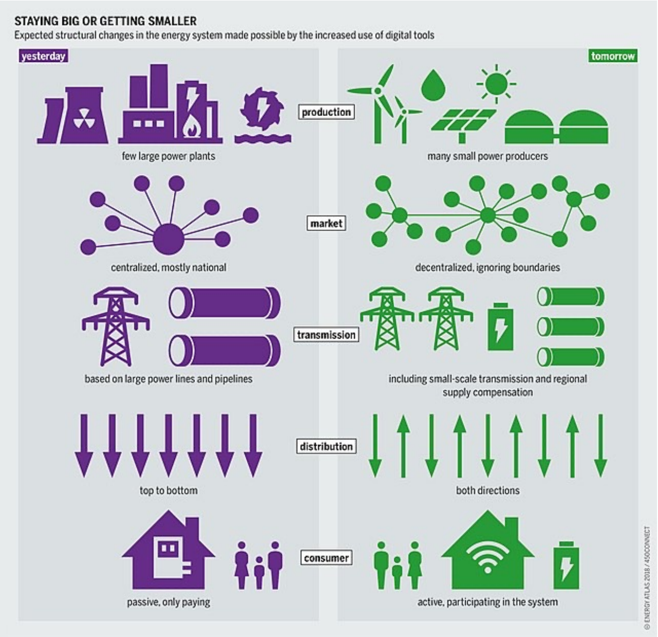


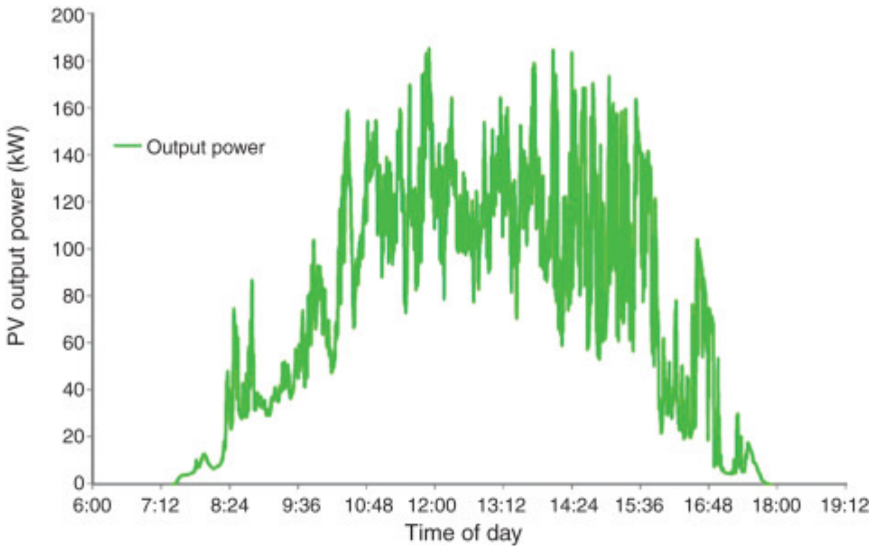
Credit: DOE EERE SETO Solar Futures Study 2021.

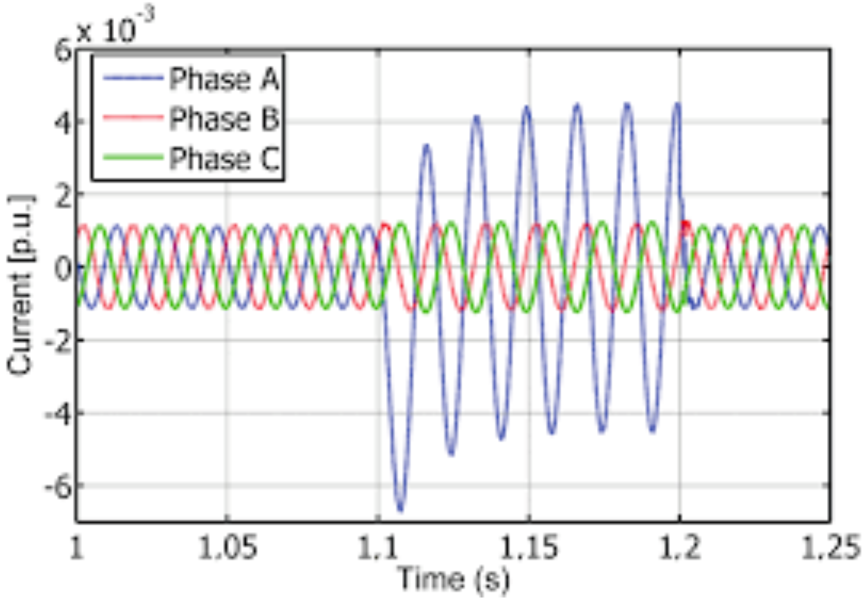
- System trends
  - 3.5X projected capacity increase from 2020
  - Expected retirement of conventional generation sources
- System challenges
  - Increased uncertainty
  - Low-inertia systems with IBRs
  - Power electronics heavy
- Modeling and simulation challenges
  - Large number of scenarios
  - Larger/more complex EMT system model
  - Slow simulation speed

Challenges for analysis tools

- Transmission + distribution
- Handling variability, intermittency, and stochasticity
- Need of faster-scale dynamics (EMT)
- Computational challenges and longer simulation times



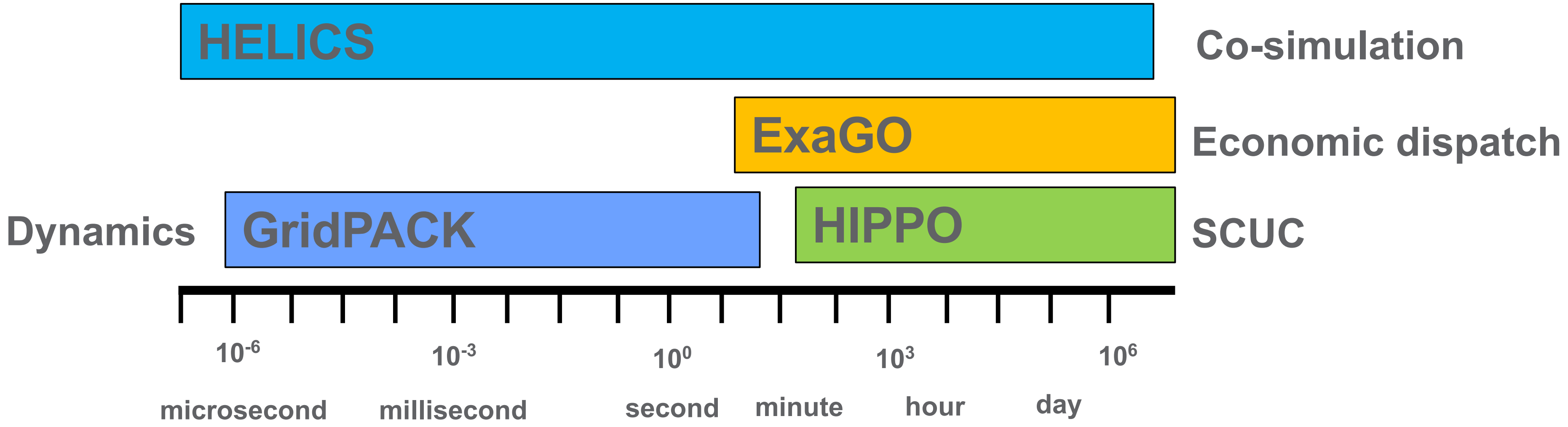




High-performance open power grid analysis tools @ PNNL

- Rich history in development of open-source high-performance tools for grid analysis
- Close linkage with DOE ASCR scientific computing tools

PNNL tools



ASCR tools

MPI

SuiteSparse

PETSc

SuperLU

GlobalArrays

Open-source software @ PNNL

GridLAB-D

- Distribution system analysis
- Power flow, time-series analysis, and dynamics
- Detailed models of end-use loads
- Assess distribution automation design, peak load management, distribution generation and storage, rate structure analysis, etc.

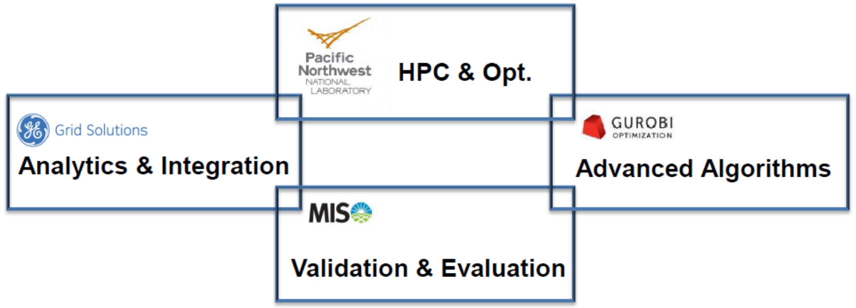
https://www.gridlabd.org/

HELICS

- Co-simulation framework to integrate simulators
- Developed jointly by several national labs
- Transmission-distribution analysis, grid-communications system, gas-electric grid interdependency, large-scale DER market interactions

https://helics.org/

Open-source software @ PNNL



HIPPO

- Accelerate day-ahead SCUC
- High-performance computing
- Advanced algorithms for solving mixed-integer problems
- Close collaboration with MISO

HIPPO info

GridPACK™

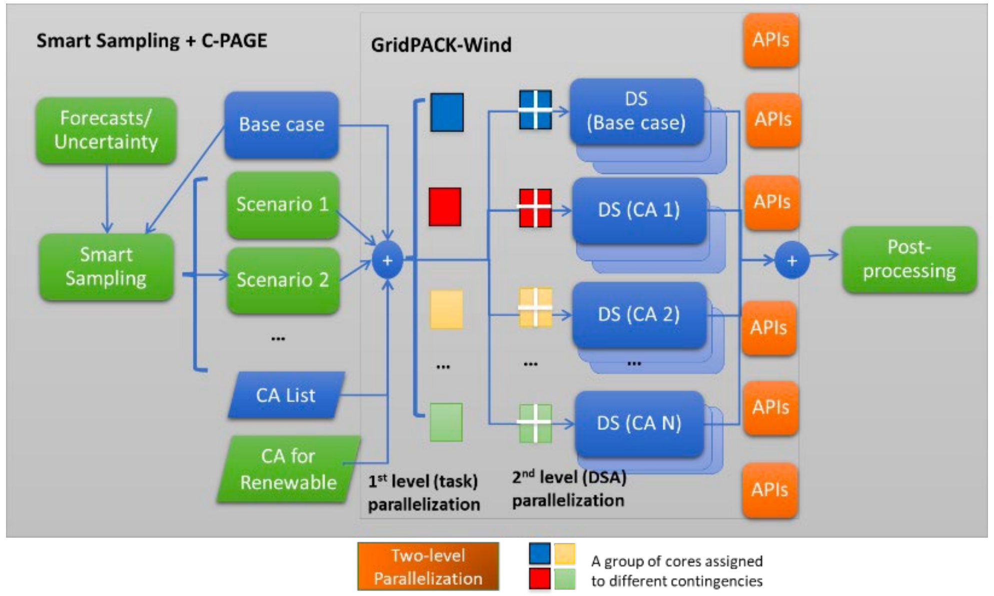
- High-performance framework for application development
- Interface with state-of-the-art open source numerical solvers
- Power flow, state estimation, contingency analysis, and dynamics

https://www.gridpack.org/

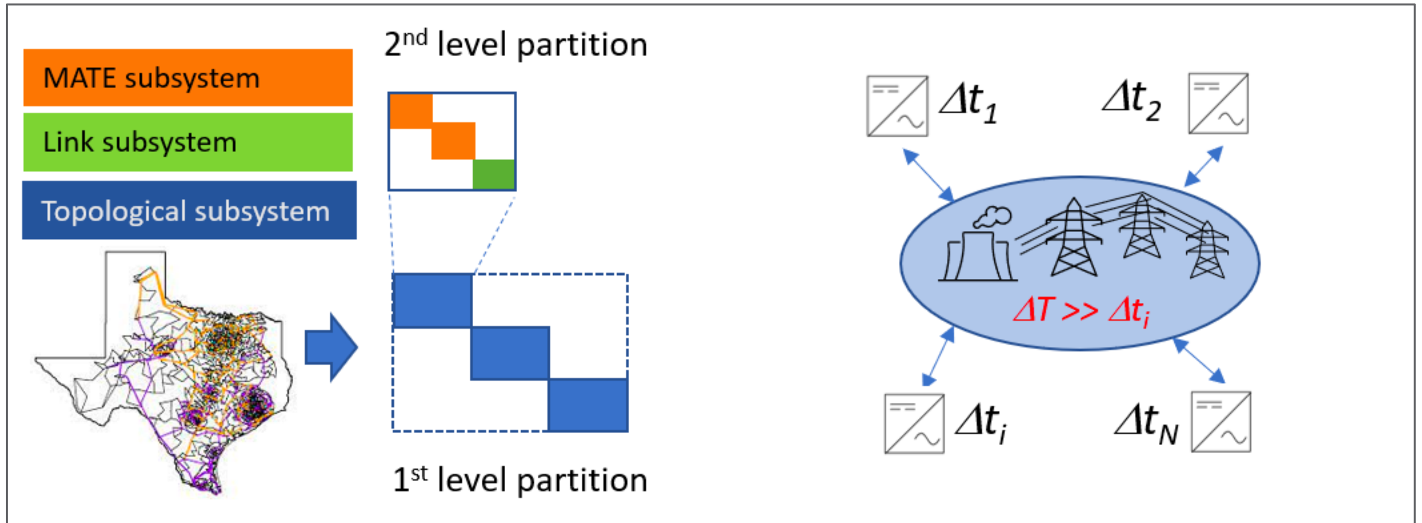
New additions to GridPACK

- High-performance dynamics simulation of wind-heavy systems

Dynamic security assessment for uncertainty quantification



HPC-enabled EMT simulation engine

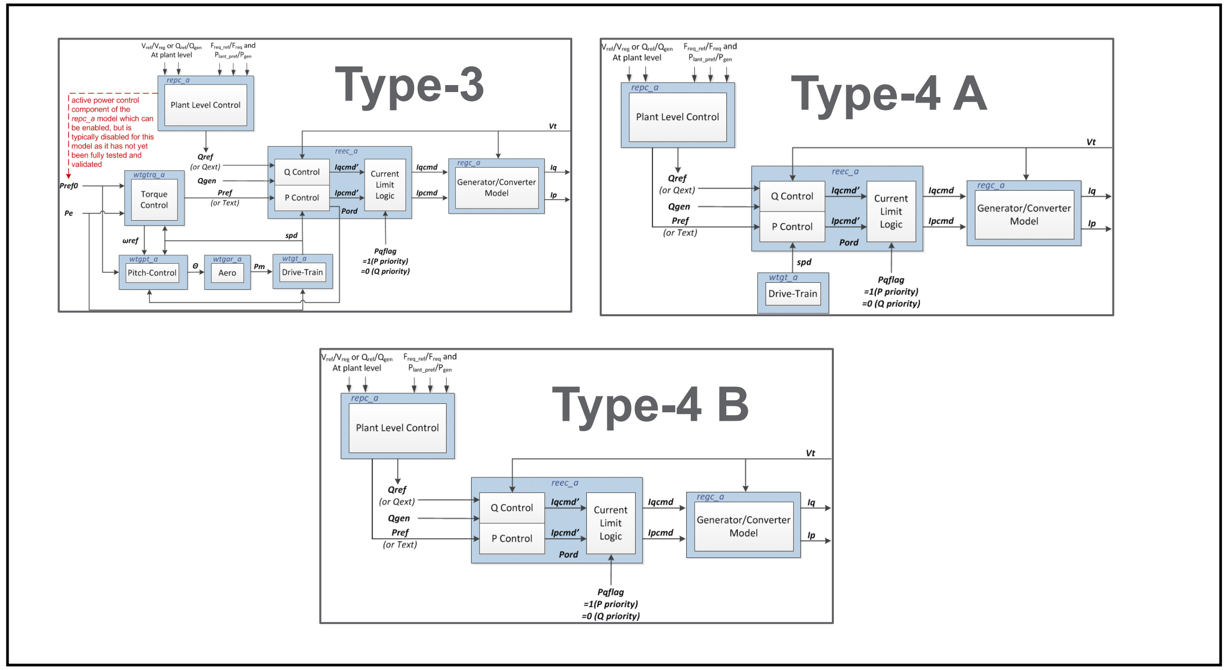


(a) A two-level partitioning scheme (b) multi-rate EMT simulation

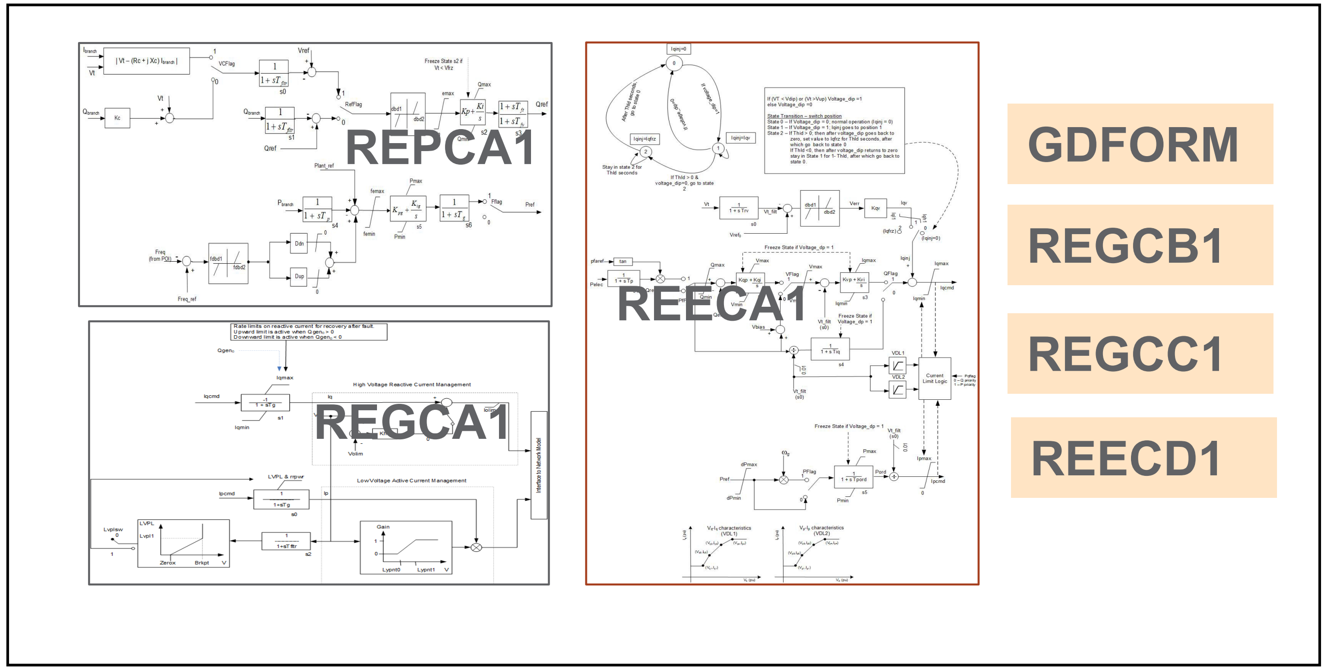
Wind integration modeling in GridPACK

- Validated detailed models of wind turbines with complex power electronics
- WECC generic models plus grid forming inverter model

Wind plant models

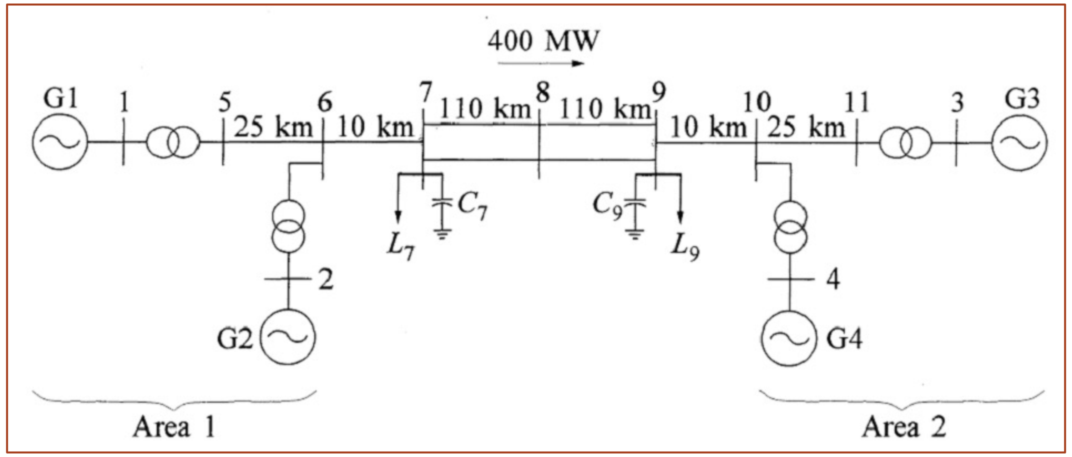


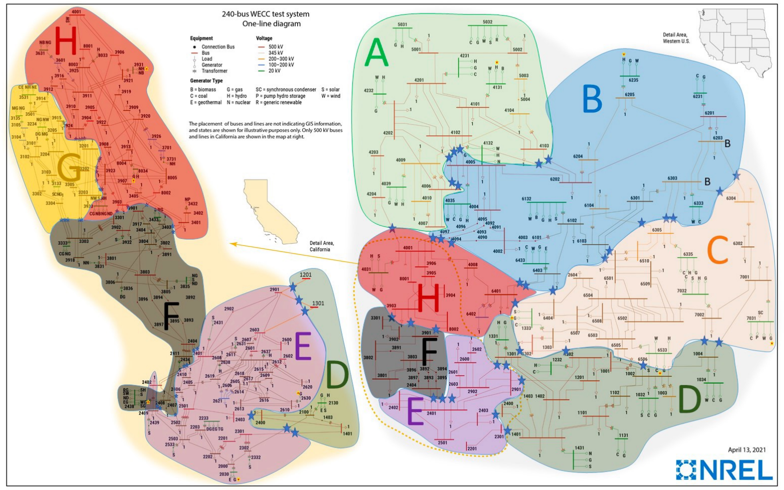
WECC generic models++

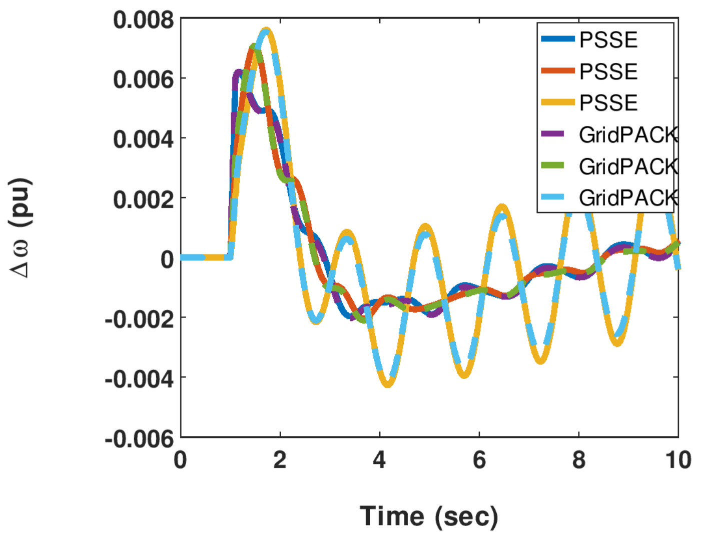


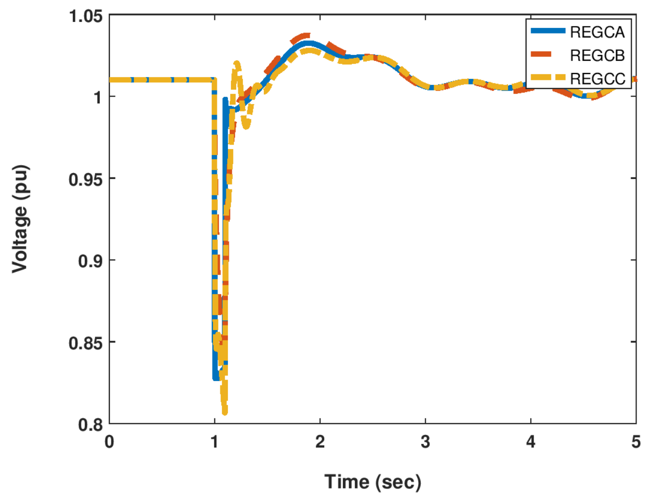
Wind Integration simulation with GridPACK

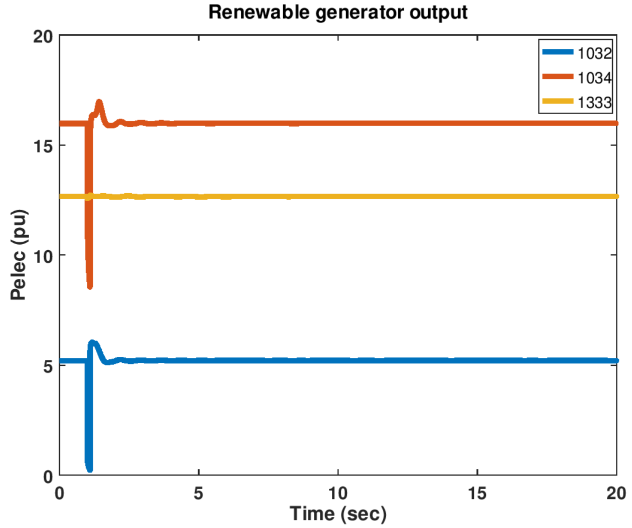
- Validation, comparison, and analysis

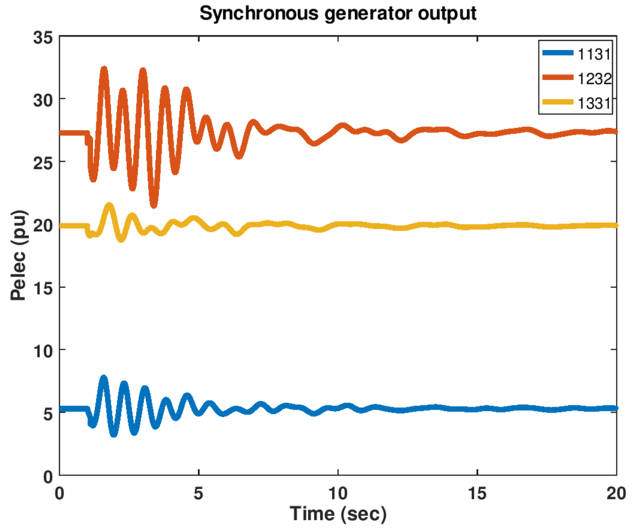






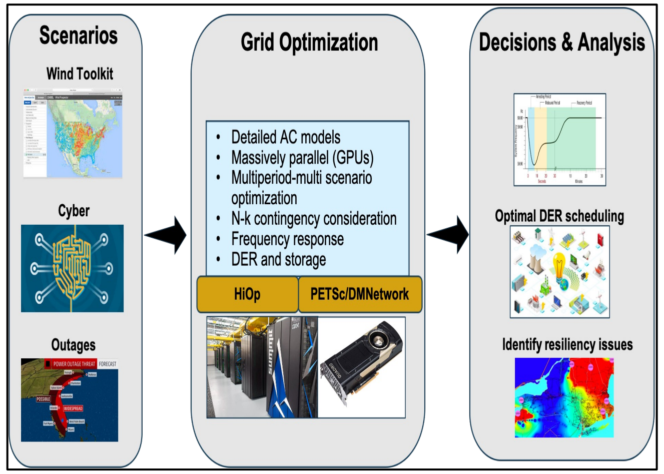


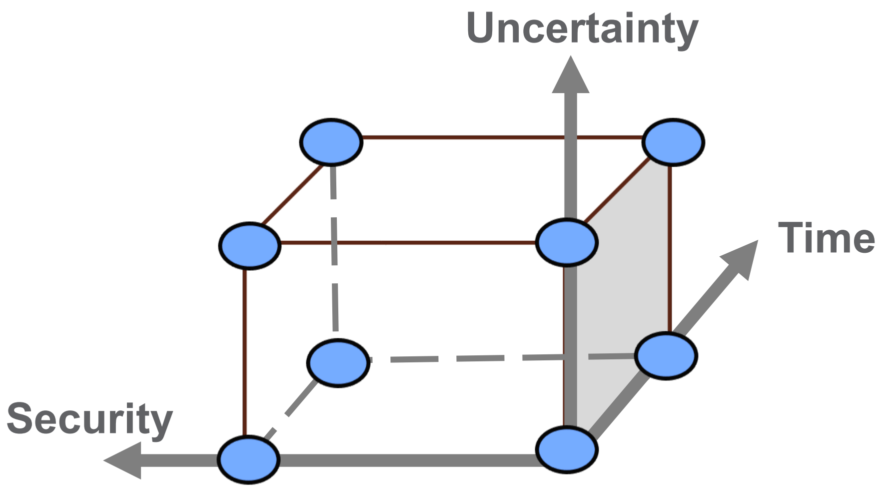


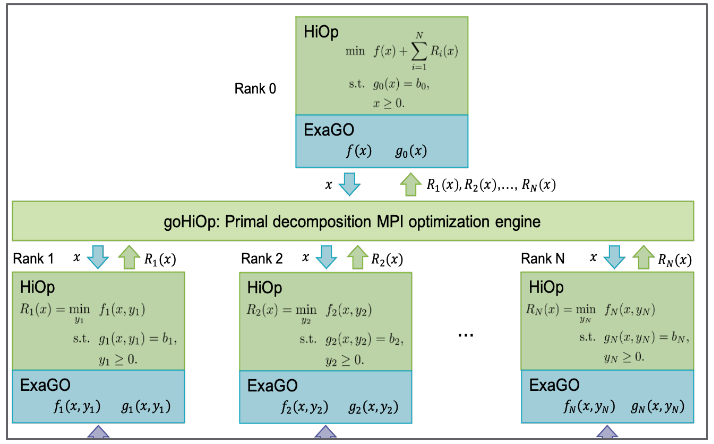


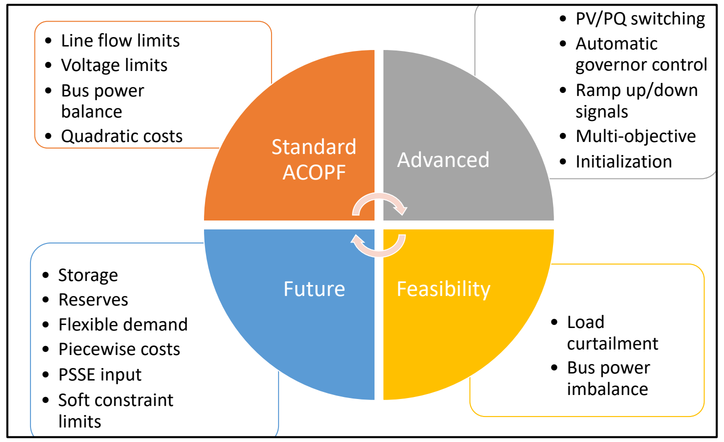
Exascale Grid Optimization (ExaGO) toolkit

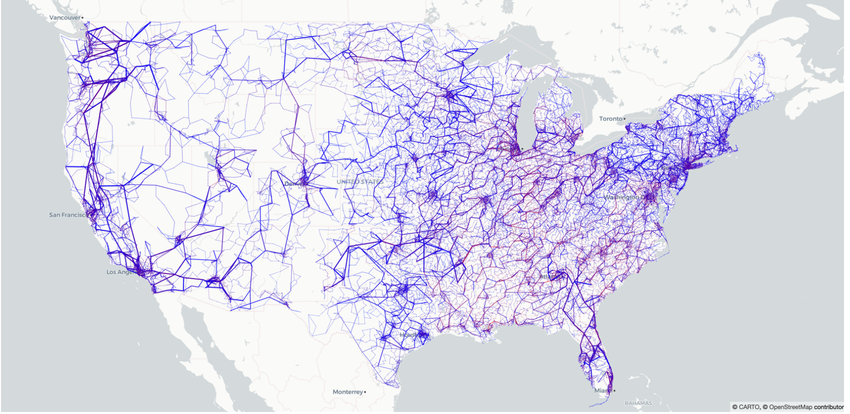
- Open-source software tool for large-scale ACOPF optimization with
  - Renewable integration (uncertainty)
  - Outages (security)
  - Scheduling (time)
- High-performance heterogenous (CPU-GPU) computing
- (Exa)scalable algorithms
- Software sustainability/adoption
  - Python API
  - Visual front-end

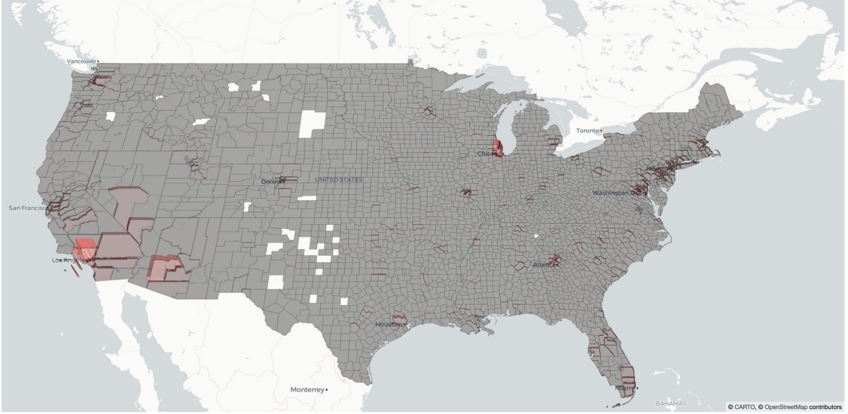


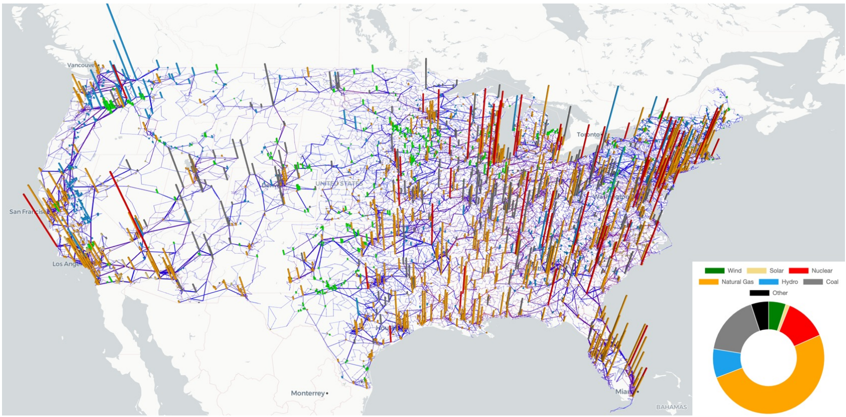




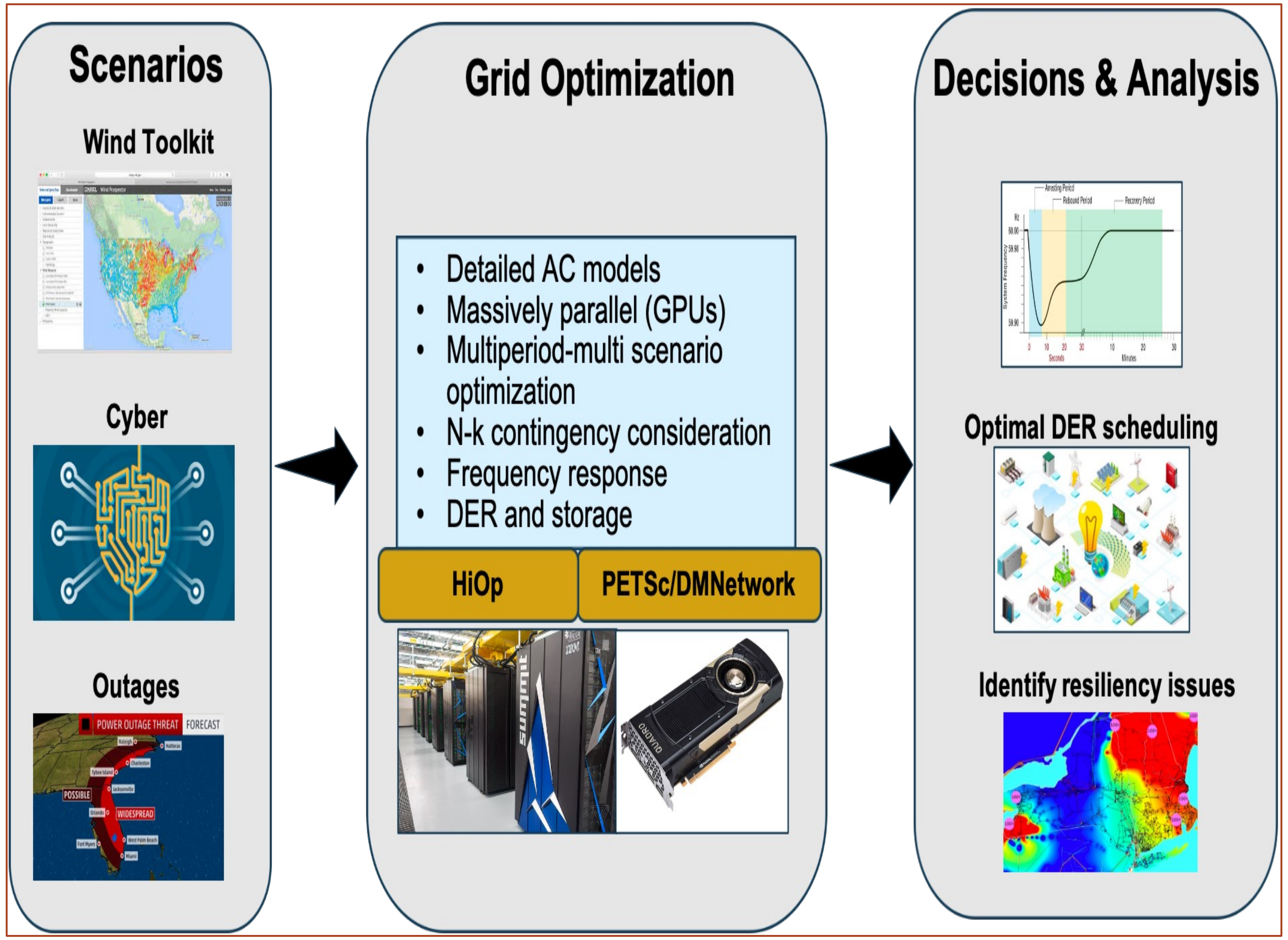








Exascale Grid Optimization (ExaGO^{TM}) toolkit



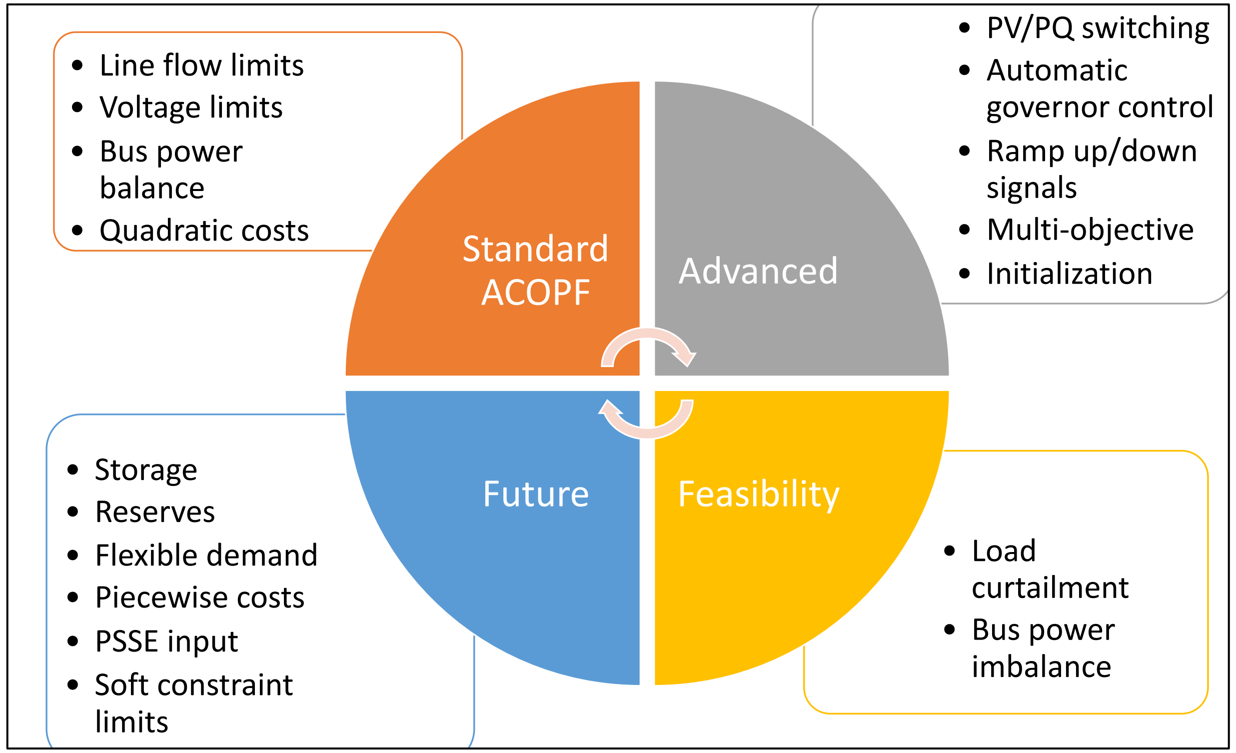
- Large-scale ACOPF-based grid optimization
- Planning, reliability, and resiliency analysis
- Incorporate stochastic (wind forecast, load variations), security (contingencies), and multi-period (ramping) constraints
- High-performance solvers
- CPU and mixed CPU-GPU

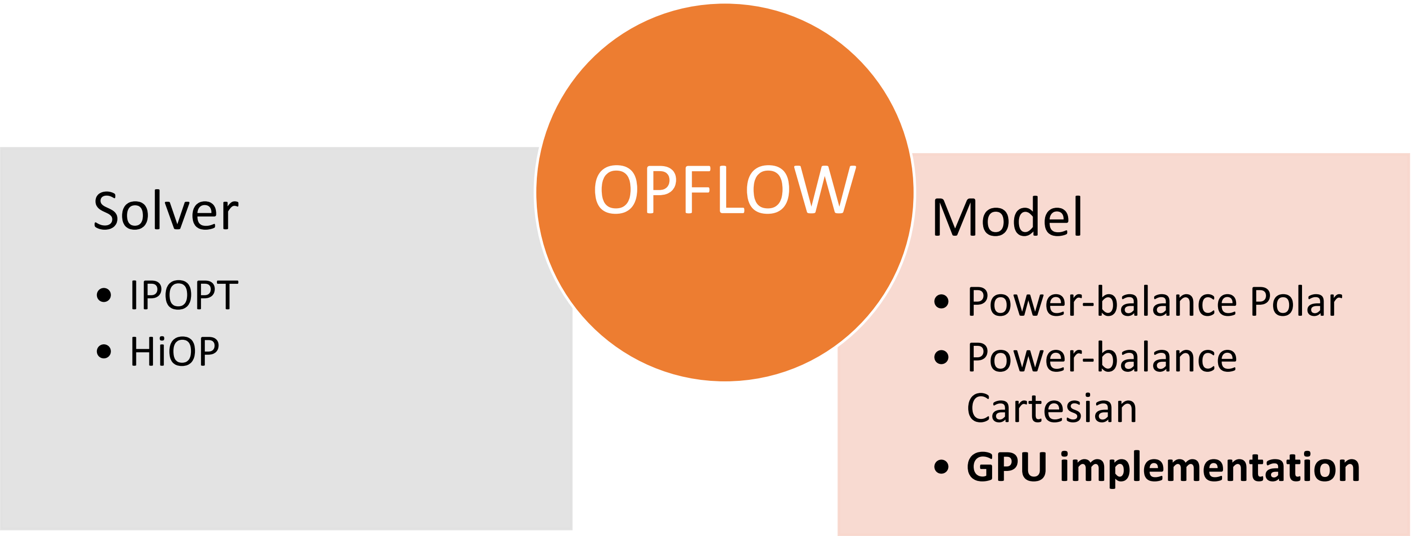
Download: https://gitlab.pnnl.gov/exasgd/frameworks/exago

ExaGO AC Optimal Power Flow (OPFLOW)

- Implements nonlinear AC optimal power flow
- Models: Power-balance-polar, power-balance-cartesian, GPU-based ones

$$
\begin{aligned}
\min\ & f(x) \\
& \text{s.t.} \\
& g(x) = 0 \\
& h(x) \le 0 \\
& x^- \le x \le x^+
\end{aligned}
$$

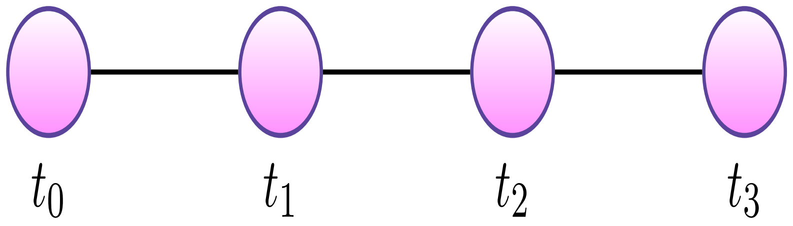


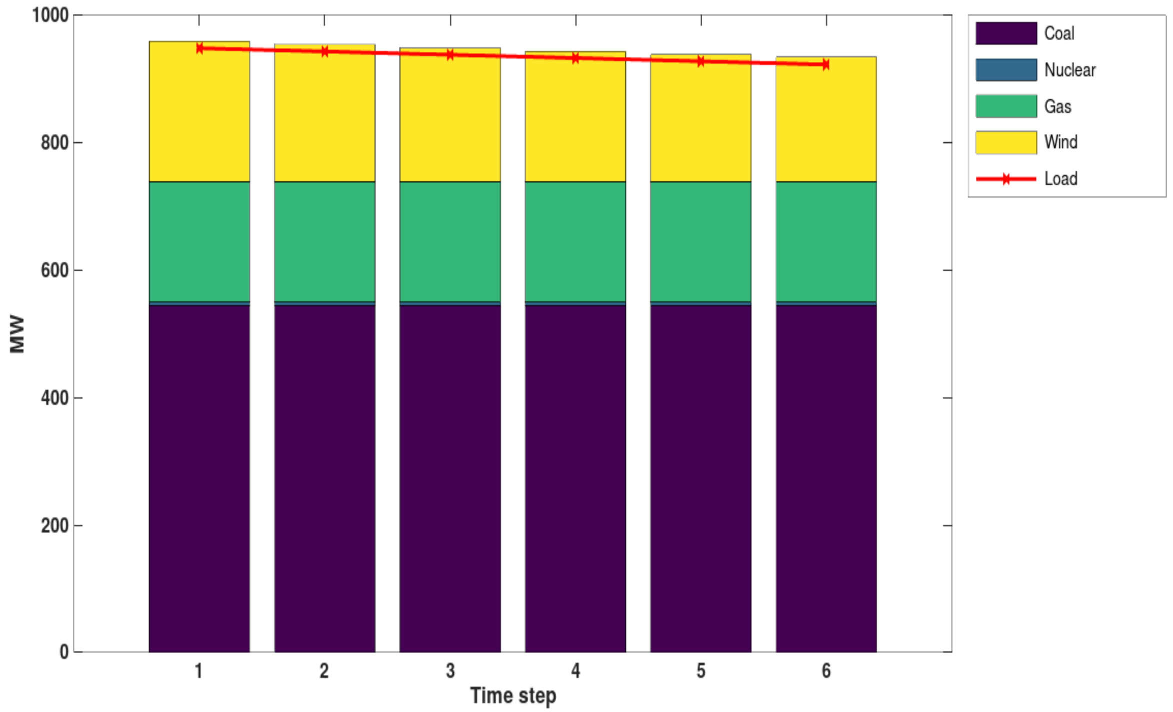


ExaGO multi-period optimal power flow (TCOPFLOW)

- For economic dispatch problems over a given time horizon
- Multiperiod constraints (generator ramping)

$$
\begin{aligned}
\min.\ & \sum_{t=0}^{N_t-1} f_t(x_t) & \\
\text{s.t.} & & \\
& g_t(x_t) = 0, & t \in [0, N_t - 1] \\
& h_t(x_t) \le 0, & t \in [0, N_t - 1] \\
& x^- \le x_t \le x^+, & t \in [0, N_t - 1] \\
& -\delta_x \le x_t - x_{t-\Delta t} \le \delta_x, & t \in [1, N_t - 1]
\end{aligned}
$$

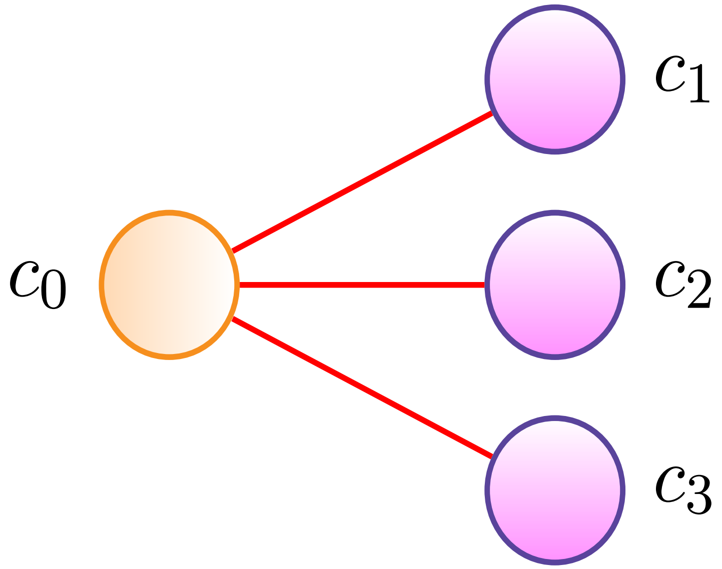


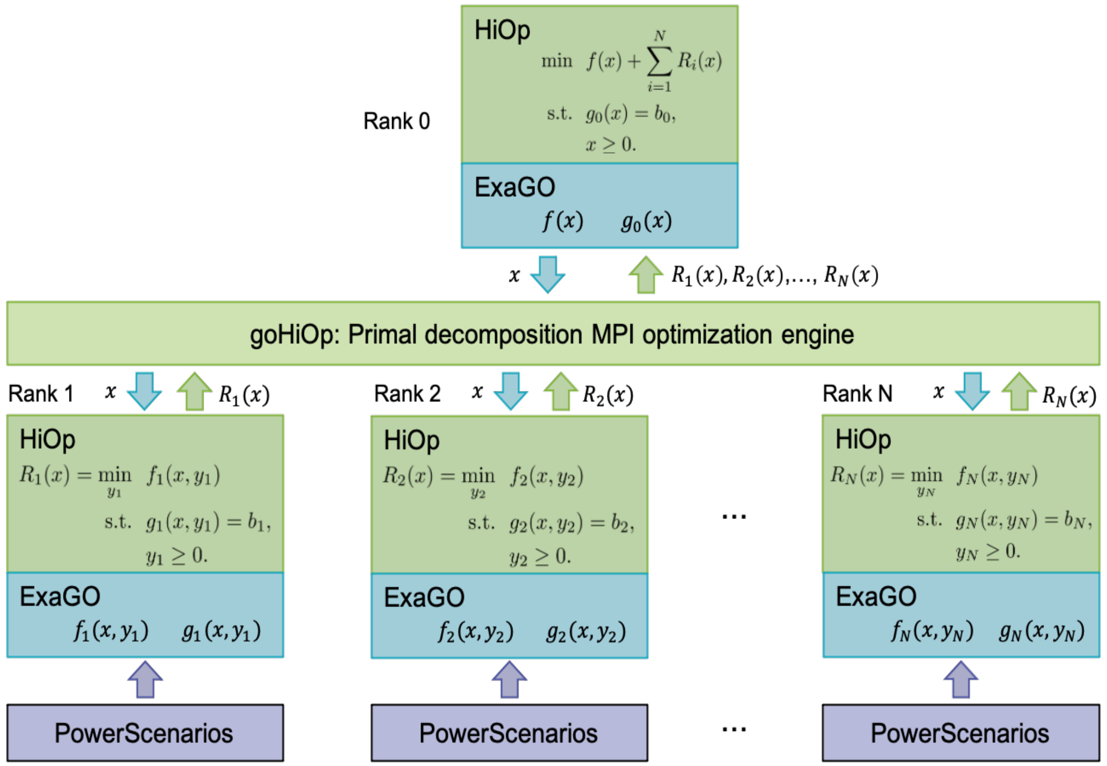


ExaGO security-constrained optimal power flow (SCOPFLOW)

- Secure operation under contingencies
- “ What should be the dispatch such that if any of the contingencies do occur then the system will be secure”

$$
\begin{aligned}
\min.\ & \sum_{c=0}^{N_c-1} f_c(x_c) \\
\text{s.t.}\ & \\
& g_c(x_c) = 0, && c \in [0, N_c - 1] \\
& h_c(x_c) \le 0, && c \in [0, N_c - 1] \\
& x^- \le x_c \le x^+, && c \in [0, N_c - 1] \\
& -\delta_x \le x_c - x_0 \le \delta_x, && c \in [1, N_c - 1]
\end{aligned}
$$

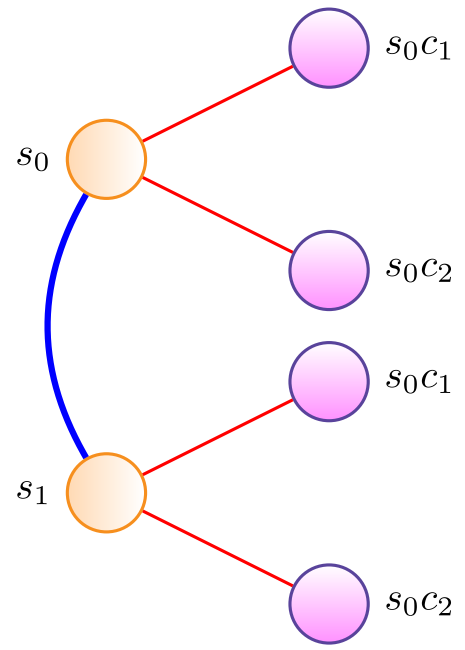


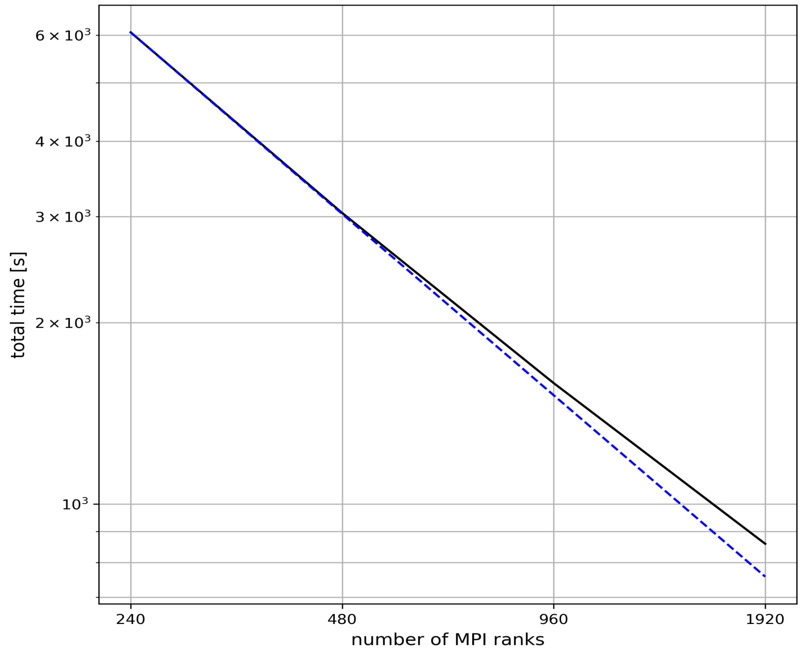


ExaGO Stochastic Security-Constrained Optimal Power Flow (SOPFLOW)

$$
\begin{aligned}
\min \sum_{s \in \mathrm{S}} \pi_s \sum_{c \in \mathrm{C}} & f_{sc}(x_{s,c}) \\
\text{s.t.} & \\
g_{sc}(x_{s,c}) &= 0, \\
h_{sc}(x_{s,c}) &\leq 0, \\
x^- \leq x_{s,c} &\leq x^+, \\
-\Delta x_s \leq x_{s,0} - x_{0,0} &\leq \Delta x_s \\
-\Delta x_c \leq x_{s,c} - x_{0,0} &\leq \Delta x_c
\end{aligned}
$$

- Secure operation under contingencies and wind forecasts
- " What should be the dispatch such that if any of the contingencies in any of the wind forecast scenarios do occur then the system will be secure"





Largest run on Summit with 10 scenarios and 1000 contingencies on TAMU 2k case on 1920 ranks.
Credits: Jingyi Wang (LLNL)

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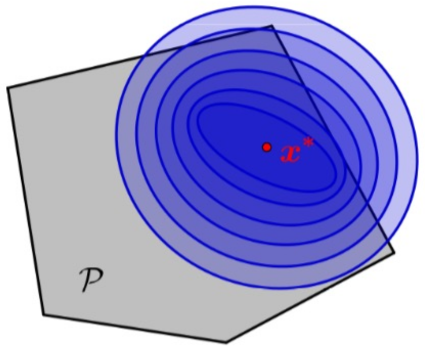
Landscape of Solution Methods

Online optimization

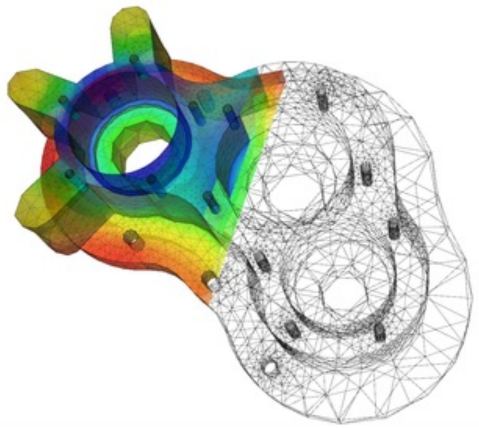
$$
\begin{aligned}
\min_{x} \quad & f(x) \\
\text{subject to} \quad & b(x) \geq 0 \\
& c(x) = 0.
\end{aligned}
$$



- Requires prior knowledge

Differential equations

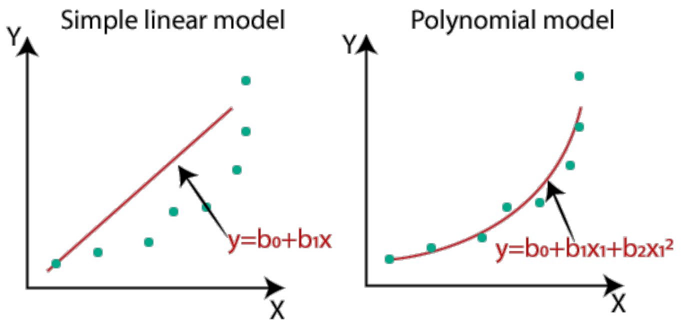
$$\frac{dy}{dx} = f(x)$$



- Requires prior knowledge

Supervised Learning

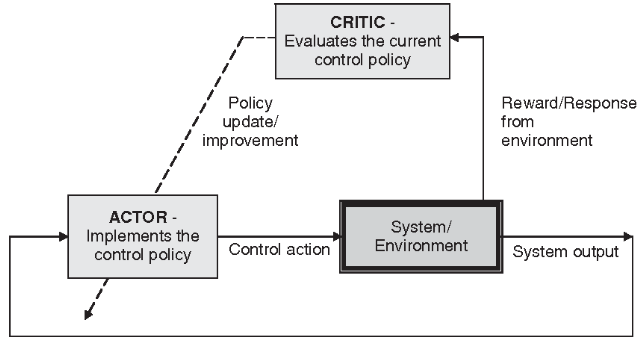
$$\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} L(y^i, f(x^i, \theta))$$



- Requires large labeled datasets

Reinforcement Learning

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



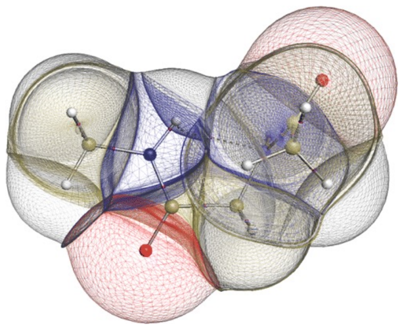
- Requires environment model to sample

More domain knowledge

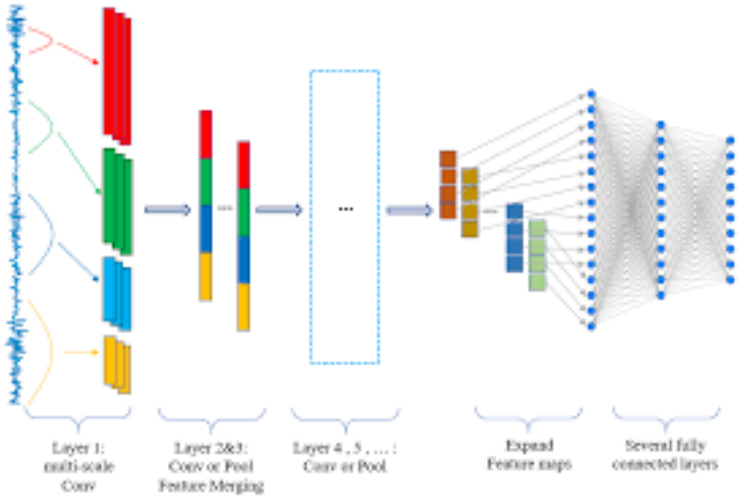
Less domain knowledge

Data-driven Modeling

Models

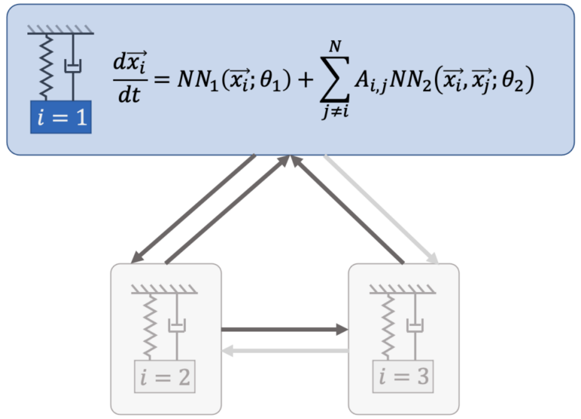


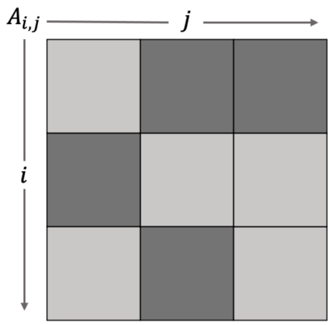
White-box	Gray-box	Black Box
$\frac{dx}{dt} = \alpha x - \beta xy$ $\frac{dy}{dt} = \delta xy - \gamma y$	$\frac{dx}{dt} = \alpha x - 0.75xy$ $\frac{dy}{dt} = NN(x, y)$	$\frac{d\boldsymbol{X}}{dt} = NN(\boldsymbol{X})$

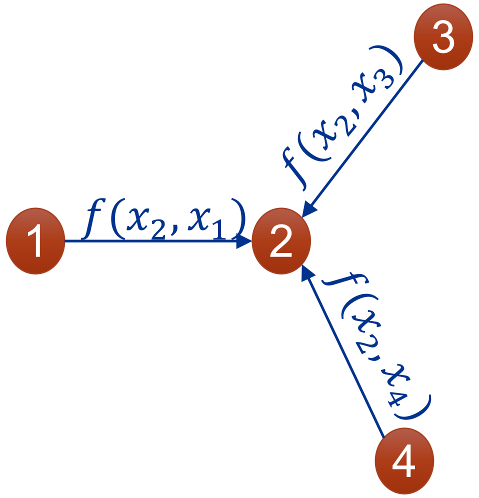


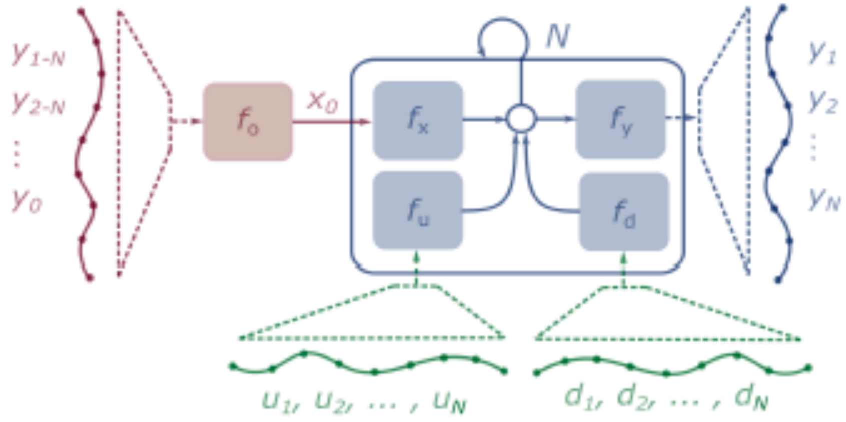
More domain knowledge ⟷ Less domain knowledge

- physics-based
- physics priors
- networked neural ODEs
- graph neural networks
- neural differential equations
- state space models









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Landscape of Solution Tools

Online optimization

- PYOMO
- JUMP
- GEKKO DYNAMIC OPTIMIZATION
- CVXPY
- CasADi
- GUROBI OPTIMIZATION

Differential Equations

- DifferentialEquations.jl
- MATLAB
- SciPy
- PETSc TAO
- NWCHEM

Supervised Learning / **Reinforcement Learning**

- PyTorch
- TensorFlow
- flux
- JAX
- Gym

More domain knowledge

Less domain knowledge

Landscape of Solution Tools

Online optimization	Differential Equations	Supervised Learning	Reinforcement Learning
PYOMO	DifferentialEquations.jl	PyTorch	
JUMP	MATLAB	TensorFlow	
GEKKO DYNAMIC OPTIMIZATION	SciPy	flux	
CVXPY	PETSc TAO		
CasADi	NWCHEM	JAX	Gym
GUROBI OPTIMIZATION			

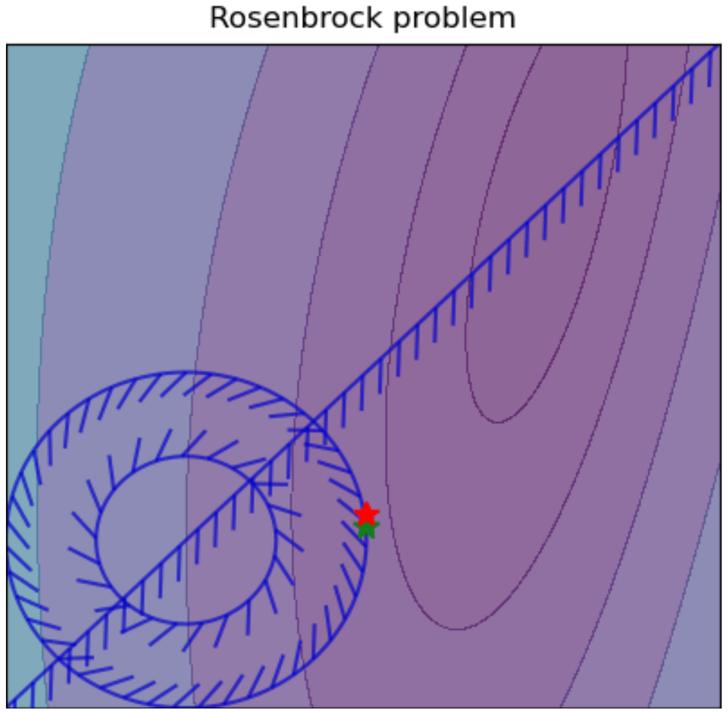
What comes next? … Differentiable programming (DP): a unifying approach for data-driven modeling and optimization of complex systems based on automatic differentiation (AD)

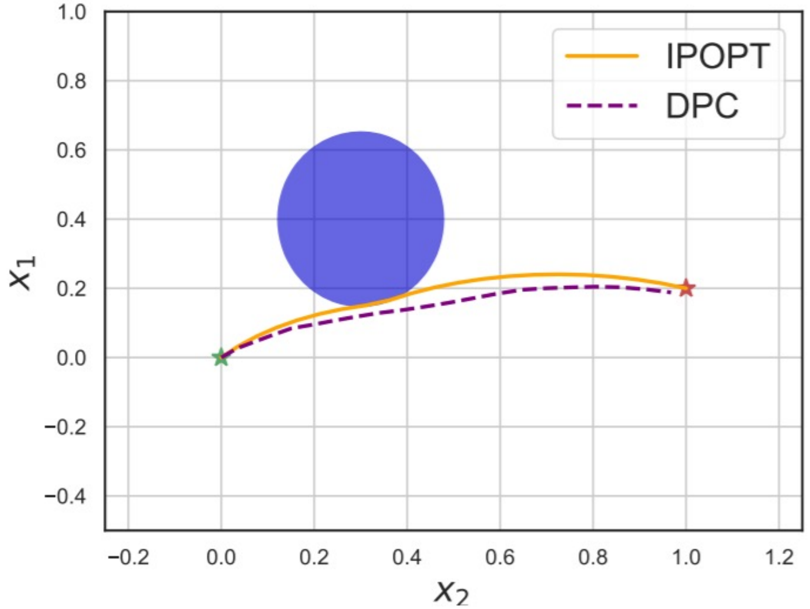
NeuroMANCER

Open-source scientific machine learning (SciML) toolbox in PyTorch for integrating deep learning, constrained optimization, and physics-based modeling

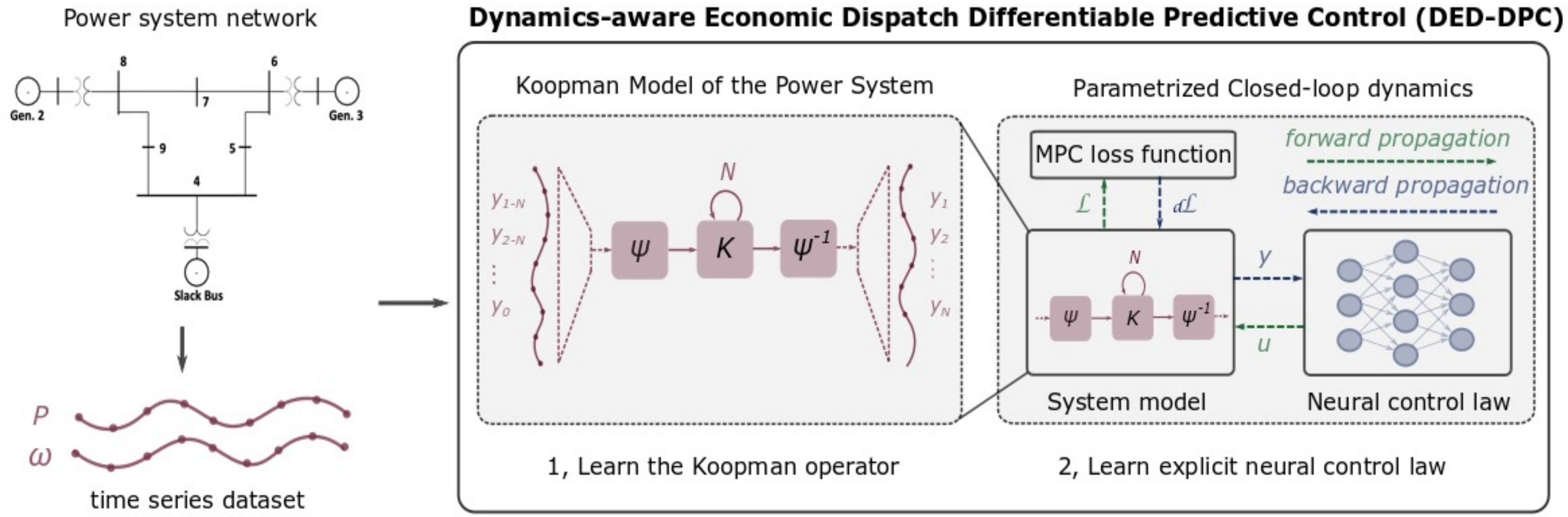
- **Differentiable constrained optimization**
  - Parametric nonlinear programs (pNLP)
- **Constrained machine learning**
  - Classical deep learning (RNN, MLP, ResNet)
  - Graph neural nets (GNNs)
- **Physics-informed modeling of dynamic systems**
  - Neural state space models (NSSM)
  - Neural ordinary differential equations (NODE)
- **Constrained control of dynamic systems**
  - Differentiable predictive control (DPC)

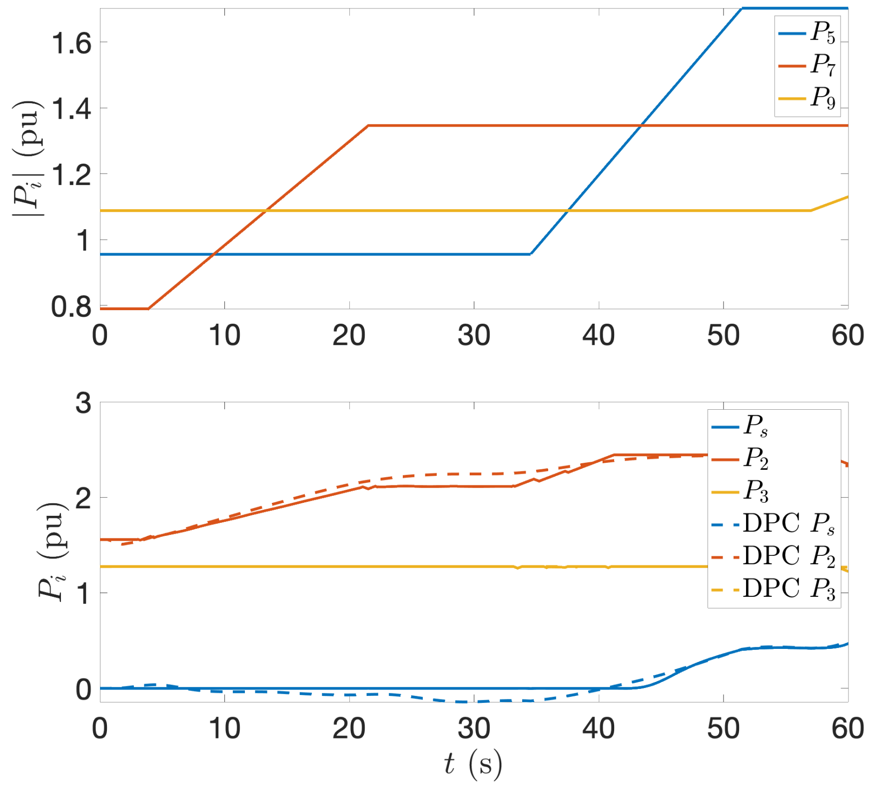
https://github.com/pnnl/neuromancer





Dynamics-Aware Economic Redispatch via Differentiable Predictive Control





Problem: Current redispatch processes do not incorporate system dynamics concerns. Incorporating dynamics in redispatch is too complex and/or time-consuming
Solution: Machine-learning based dynamics-aware redispatch. Learn system dynamics for faster assessment.

Ethan King, Ján Drgoňa, Aaron Tuor, Shrirang Abhyankar, Craig Bakker, Arnab Bhattacharya, Draguna Vrabie, **Koopman-based Differentiable Predictive Control for the Dynamics-Aware Economic Dispatch Problem**, 2022 American Control Conference

Architectures
- Koopman dynamics model
- CNN control policy

Results
- **5 orders of magnitude speed-up**
- Near optimal performance

PNNL open-source tools for grid modeling, simulation, and learning

- GridLab-D
  - https://github.com/gridlab-d/gridlab-d
- HELICS (co-developed with other national labs)
  - https://github.com/GMLC-TDC/HELICS
- GridPACK
  - https://github.com/GridOPTICS/GridPACK
- ExaGO
  - https://gitlab.pnnl.gov/exasgd/frameworks/exago
- NeuroMancer
  - https://github.com/pnnl/neuromancer

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Thank you

Future outlook and needs for grid analysis tools

- Deeper penetration of IBRs will require larger emphasis on **EMT** analysis
- Handling increased variability with large-scale renewable deployment – **deterministic to stochastic**
- Additional considerations for reliability and resiliency analysis
- Computer architecture keeps on changing – CPUs, GPUs, Quantum computers, …
- AI/machine learning tools will be a key!