SYNERGIZING MODEL-BASED AND DATA-DRIVEN METHODS FOR CPS DESIGN

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Source: Sanjai Narain, Peraton
"AIMED: AI-Mediated Exploration of Design – An experience report," in DESTION/CPS Week 2023, May 09-12, San Antonio, TX

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OUTLINE

- CPS design
- Model-based design & design automation
- Data-driven augmentation
- Takeaways

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WHAT IS CPS DESIGN?

CPS Systems Engineer

Components & Subsystems

Motors
ESC
Propellers
Batteries
Mission Sensors & Payload
Chassis
Linkages

System Architecture & Topology

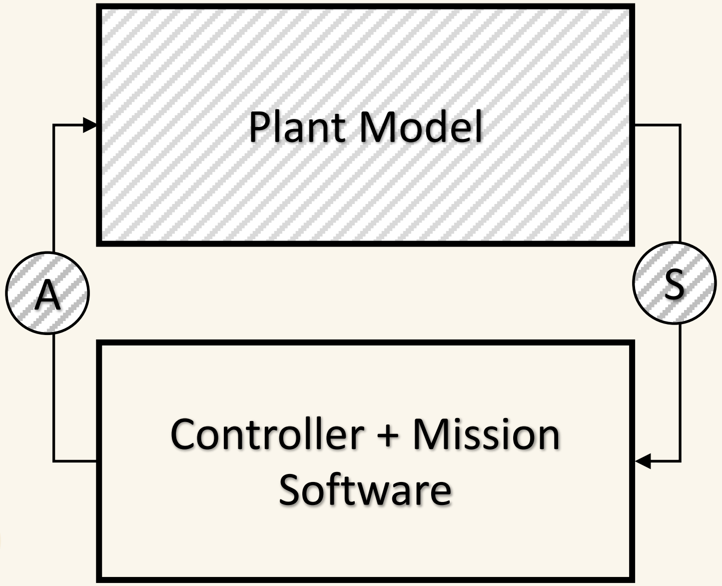
Quadcopters
Hexacopters

Planar
Articulated
Fixed-wing
Hybrid

Design Concerns

- Mission and System Requirements
- Structural integrity
- Thermal management
- Manufacturing
- + CPS/SW concerns …

CPS Researcher



Design Concerns
- SW/Process requirements
- Safety
- Real-time
- Cyber Security
- +ilities …

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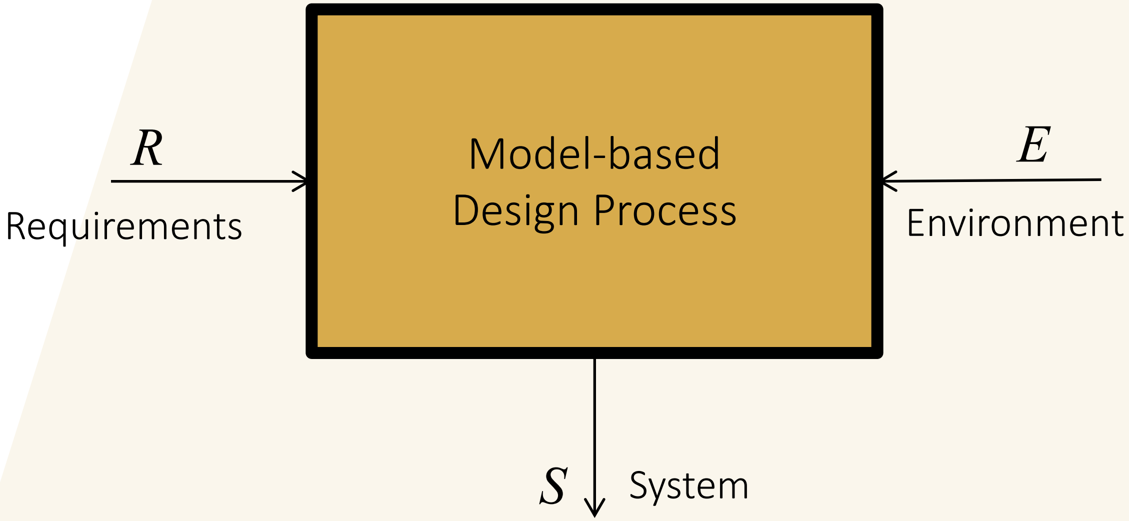
MODEL-BASED DESIGN … FORMALIZED



Design goal: $S \parallel E \vDash R$

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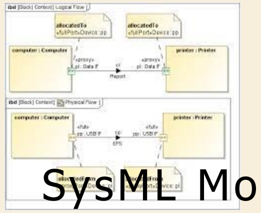
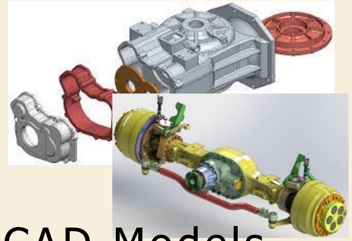
HOW MANY MODELS TO DESIGN A CPS?

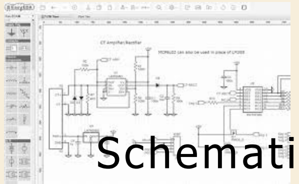
Architecture Models



SysML Models

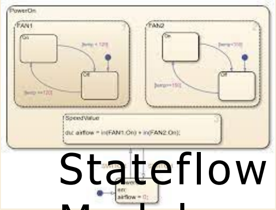


CAD Models
(components & systems)

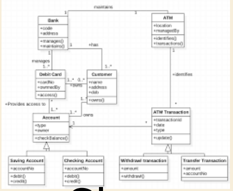


Schematic
Models

Implementation Models



Stateflow
Models



Class
diagrams

VHDL
Models

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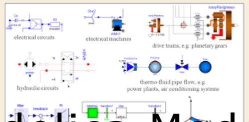
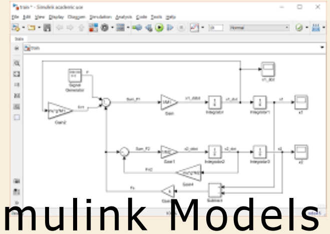
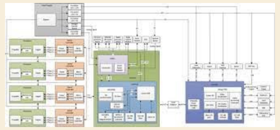
Analysis Models



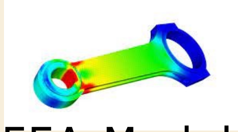
Modelica Models



Simulink Models



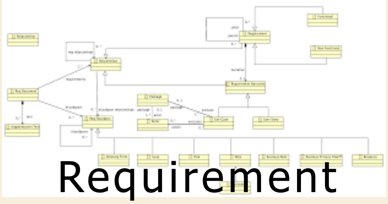
AADL Models



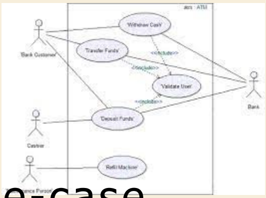
FEA Models

...

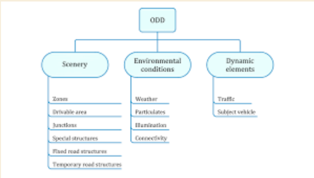
Context Models



Requirement
Models



Use-case
Models



Environment
Models

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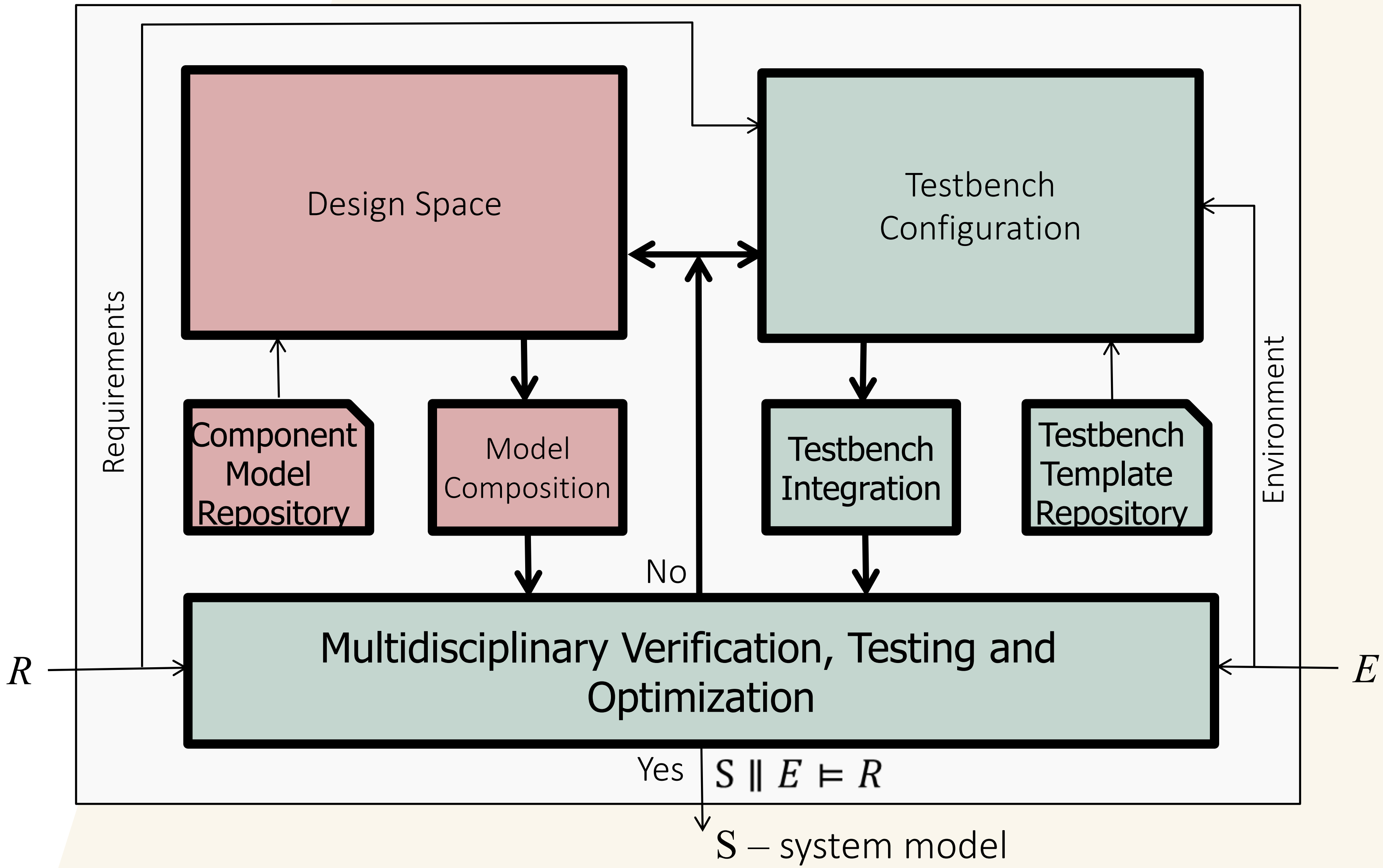
DESIGN AUTOMATION FOR CPS

Product

Design process



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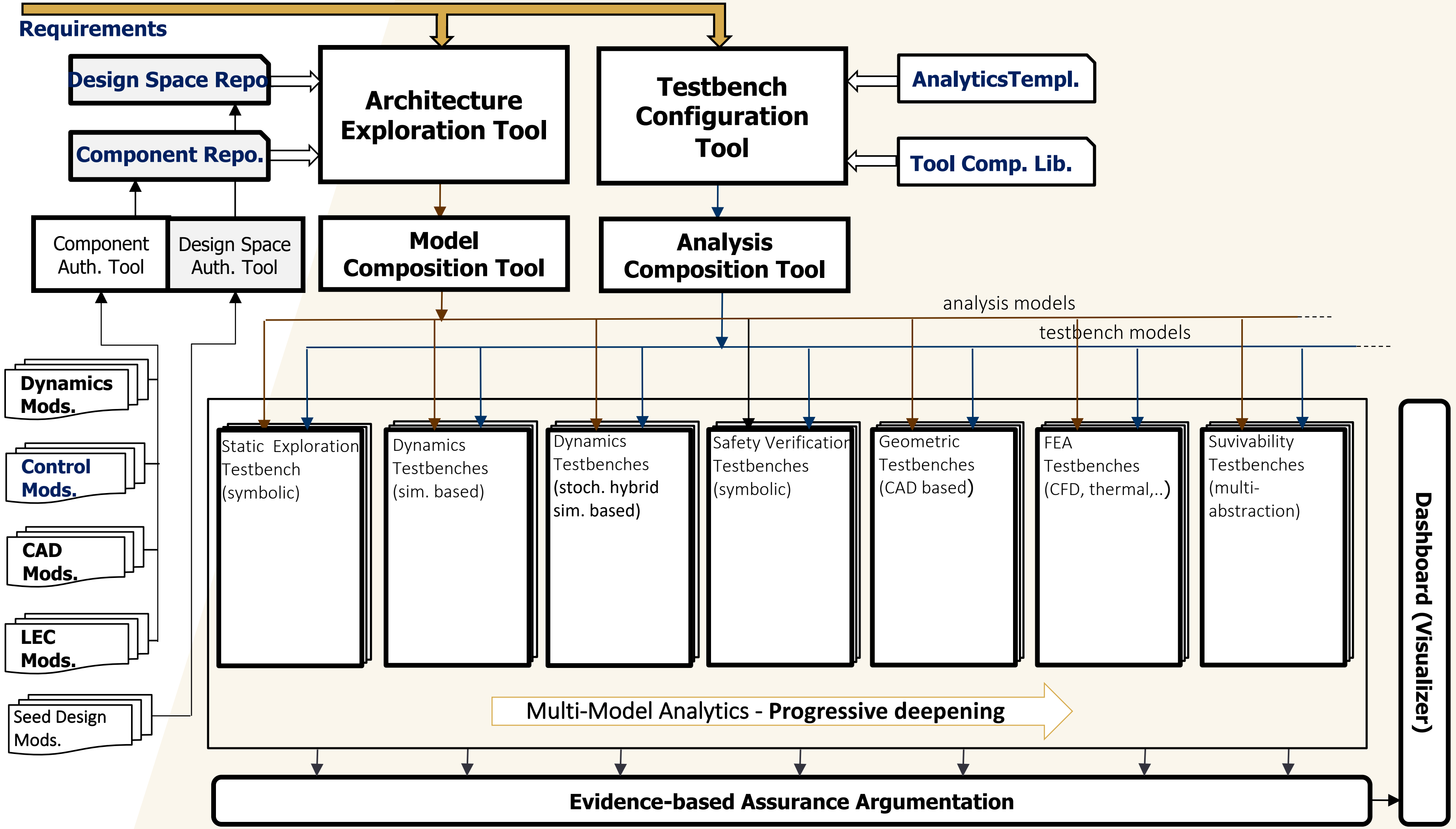
OPEN-META TOOL CHAIN



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MIND THE GAP …

- First-principles based models not always available or accurate

- High-fidelity analysis is cost prohibitive

- Design space exploration and optimization not tractable in high-dimensional spaces

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DATA-DRIVEN AUGMENTATION

- First-principles based models not always available
  - Data-driven models to bridge the epistemic gap
- High-fidelity analysis is cost prohibitive
  - Data-driven surrogate models of high-fidelity analysis for performing design trades
- Design space exploration and optimization not tractable in high-dimensional spaces
  - Sample-efficient exploration strategies utilize learned representation of design/performance space

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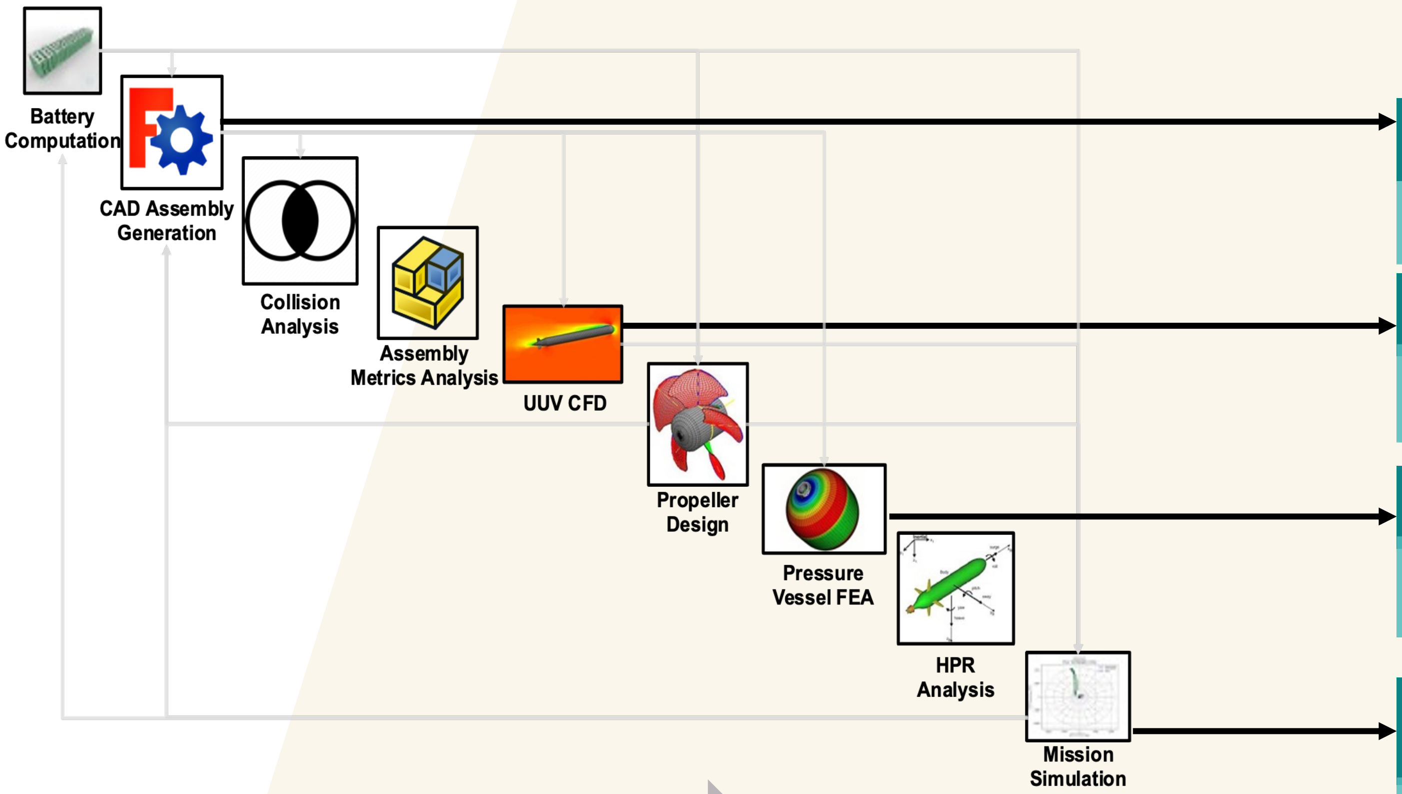
ACCELERATED ANALYSIS THROUGH SURROGATE MODELS

Accelerated design evaluation through use of AI-based (neural networks) surrogate models which once trained provide comparable result at a fraction of computational cost



CAD: Manual Generation

SymCPS CAD: AI–generated

CFD: ~5 hours

SymCPS CFD: <1 second (AI-acceleration)

FEA: ~1 hour

SymCPS FEA: <1 second (AI-acceleration)

Mission: Uncertain Operations

SymCPS Mission: Robust Design

6 hours per design → **18 seconds** per design

Source: Arun Ramamurthi, Siemens

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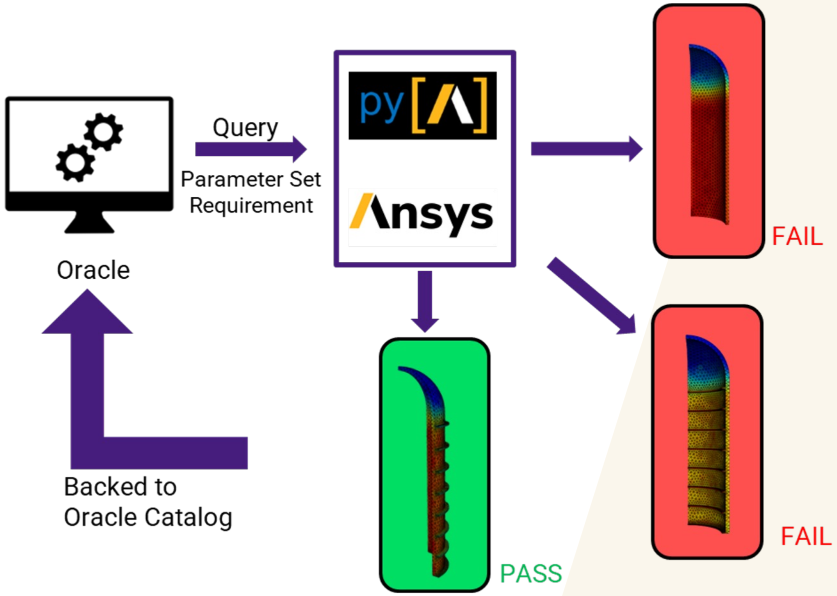
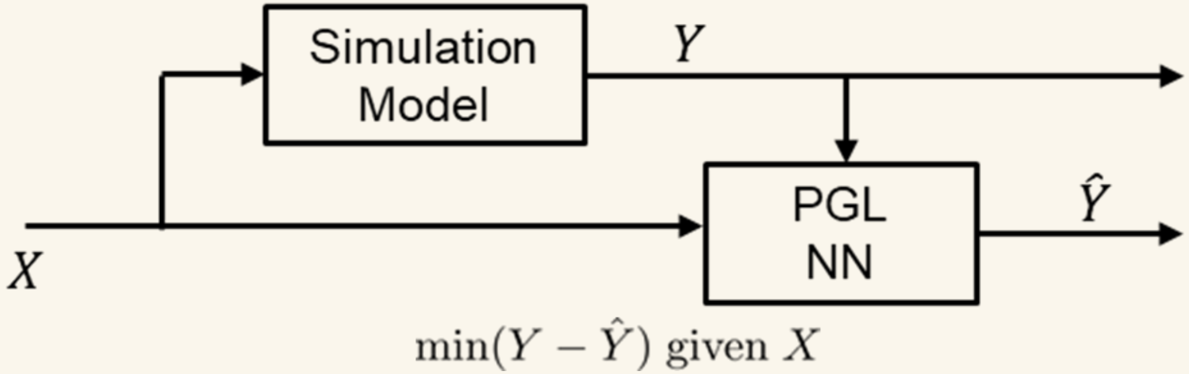
PHYSICS GUIDED SURROGATE MODELING





FEA to understand structural feasibility of a design

$$\text{ratio}_{\text{feasibility}} = \sigma_{max} / \sigma_{nominal}$$

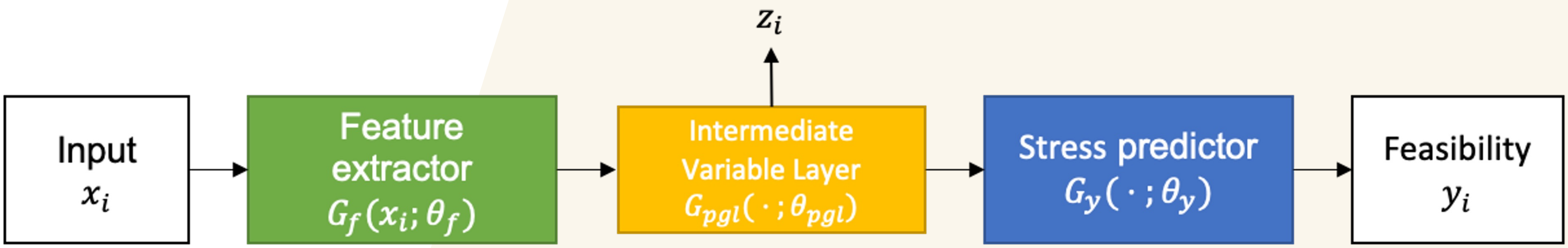
Challenges

- High accuracy and low computation cost
- Generalization, especially, for the design space we don't have training data
- Interpretability for understanding and explaining results

Introduce intermediate physics-based variables in loss functions

Source: Peter Volgyesi, Vanderbilt

PHYSICS GUIDED SURROGATE MODELING



- Set of neural network layers that extract latent features: G_f
- Set of neural network layers that generates feasibility ratio: G_y *(also blackbox loss function)*

$$\mathcal{L} = \frac{1}{n}\sum \mathcal{L}_y(y_i, \hat{y}_i)$$

- Set of neural network layers associated with physics-based parameters: G_{pgl}

$$\mathcal{L} = \frac{1}{n}\sum \mathcal{L}_y(y_i, \hat{y}_i) + \frac{\lambda_{pgl}}{n}\sum \mathcal{L}_{pgl}(z_i, \hat{(z)}_i)$$

- z_i and $\hat{z}_i$ are the physics-related true and predicted parameters

Source: Peter Volgyesi, Vanderbilt

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EXAMPLE – UUV HULL DESIGN

INPUTS

- ***E* : Material Elasticity**
- **σ : Material Strength**
- **ν : Poisson Ratio**
- **ρ : material density**
- r_i : inner diameter
- t : thickness
- l : cylinder length
- p_{hyd} : hydraulic pressure

EXPECTED OUTPUT

- $\text{Ratio}_{\text{Feasibility}} = \sigma_{max} / \sigma_{nominal}$

INTERMEDIATE PHYSICS-BASED VARIABLES

- $\sigma_{1,2,3}$: maximum principal stresses
- $\sigma_{x,y,z}$: maximum directional stresses
- $\sigma_{xy,yz,xz}$: maximum plane stresses

In total, **9 intermediate PGL variable stresses**

Source: Peter Volgyesi, Vanderbilt

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RESULTS – PLAIN CAPSULE MODEL

Design Space	Black-box Avg MSE	Black-box Avg AE in %	Black-box MAE 5%	Black-box MAE	PGL Avg MSE	PGL Avg AE in %	PGL MAE 5%	PGL MAE
Regions with Traning Data	0.0001395	2.2088	**0.0750**	9.4272	**0.0000967**	**2.1767**	0.0850	**8.9565**
Regions without Traning Data	0.0005468	8.6550	0.91	16.1248	**0.0000684**	**3.0105**	**0.09**	**6.3226**

- *Better performance for PGL, for original and less explored design spaces*

	$\text{Ratio}_{\text{Feasibility}}$	σ_{xy-max}	$\hat{\sigma}_{xy-max}$	Err_{Expl} %	σ_{yz-max}	$\hat{\sigma}_{yz-max}$	Err_{Expl} %	σ_{xz-max}	$\hat{\sigma}_{xz-max}$	Err_{Expl} %
Feasible Example	0.24	2522.07	2522.07	4.01	2512.36	2512.36	1.85	4861.82	4861.82	0.37
Non-feasible Example	1.82	18619.95	17919.50	3.76	18653.14	17955.92	3.74	37760.57	36176.86	4.19

*All units in psi

- *Interpretability, because of physics-based intermediate variables*

Source: Peter Volgyesi, Vanderbilt

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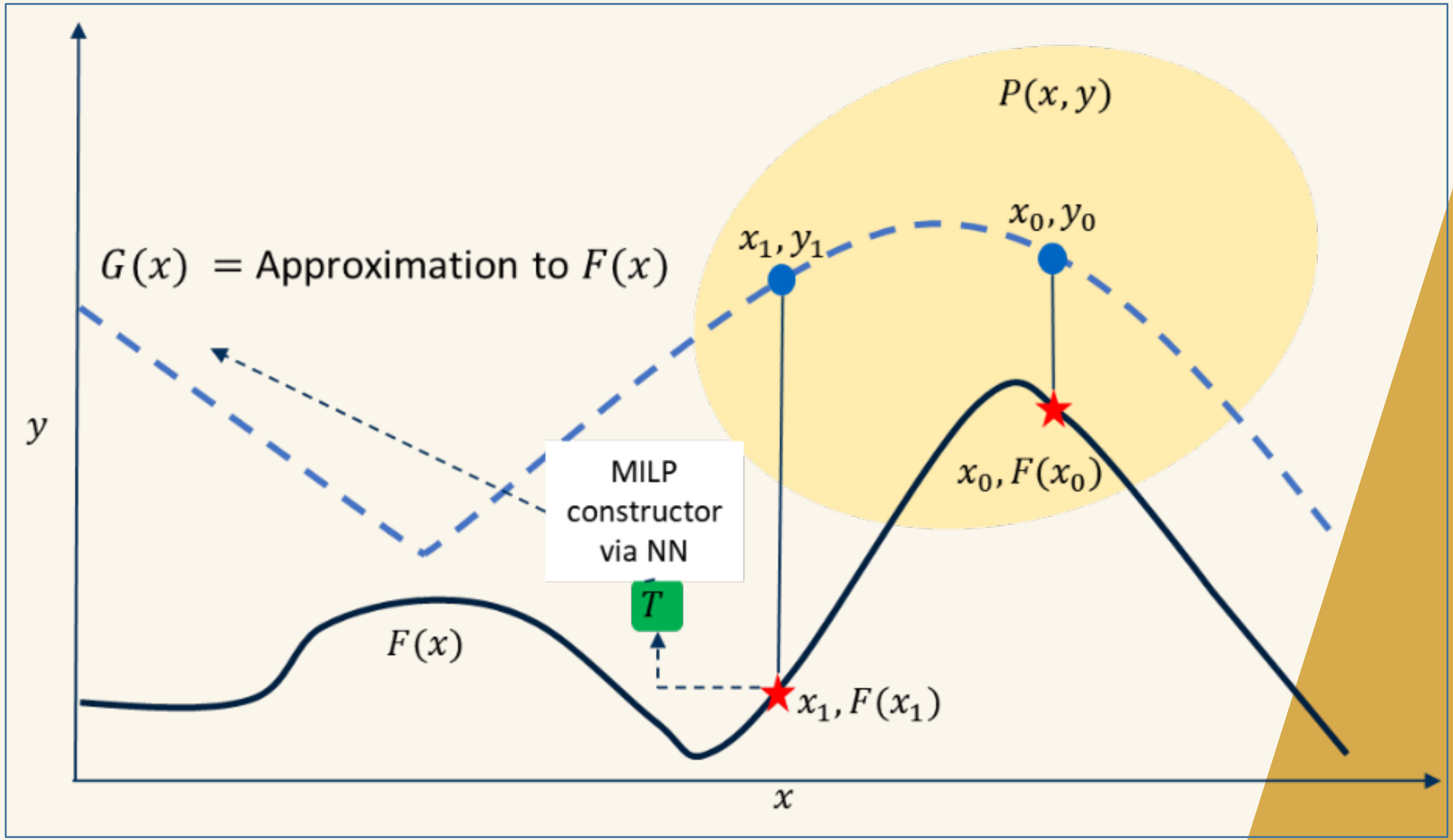
CONSTRAINED OPTIMIZATION WITH NN, MLP, AND ACTIVE LEARNING

Optimize $\phi(x, y)\ s.t.\ F(x) = y \wedge P(x, y)$

- x, y are vectors of discrete and continuous variables
- F is a **blackbox** function e.g., a simulator or evaluator
- ϕ is an objective function and P is a constraint.
- P can model recursive and fixed-point constraints
- ϕ, F and P can be nonlinear

Conservative in number of function evaluations

- Learns F in the part of its domain relevant to solving the problem
- Outperforms Bayesian optimization in sample efficiency



Source: Sanjai Narain, Peraton

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TAKEAWAYS

- What makes CPS design hard?
  - Heterogeneous domains, multiple models, intractably large design spaces
  - Multiple performance objectives, multiple constraints

- Synergizing model-based and data-driven approaches
  - Automate synthesis for evaluation of design candidates
    - Model-based design automation
  - Accelerate high-fidelity analyses through surrogate modeling techniques
    - CFD, FEA – physics guided learning
  - Scale design space exploration with data-driven ML
    - Constraint guided optimization with NN, MILP, and active learning

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THANK YOU!

UNDERPINNINGS

Model-based Design

Computational models that predict properties of cyber-physical systems "as designed" and "as built".

Challenge: Develop **domain-specific abstraction layers** for complex CPS that are evolvable, heterogeneous, yet semantically sound and supported by tools.

Research directions:
- Domain-Specific Modeling Languages (DSML)
- Metamodeling
- Model-Integrated Computing tools

– Component-based Design

Reusable units of knowledge (models) about CPS components.

Challenge: Understand **composition of heterogeneous systems** where system-level properties can be computed from the properties of components.

Research directions:
- Formal semantics of DSMLs
- Model Integration Languages
- Component models and composition semantics

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MODEL- AND COMPONENT-BASED DESIGN PROCESS

- Component Repository:

$A = \pi r^2 \; C = \{C_i(x, p)\}$

- For a system model *S:*

  $C_S = comptypes(S)$ denotes the set of component model types instantiated in S

- The architecture of a system S is a labelled graph G_S, which is well formed if it satisfies a set of constraints Φ over G_S derived from the semantics of the interaction types

- The set of component types and composition constraints define a design space:

$$D \stackrel{\text{def}}{=} \{S \mid G_S \vDash \Phi, comptypes(S) \subseteq C\}$$

- The goal of the design process is to synthesize $S \in D$ *such that* $S \parallel E \vDash R$

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