INL/CON-21-64861-Revision-0

From Machine Learning to Nuclear Digital Twins

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Changing the World's Energy Future

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Idaho National Laboratory

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From Machine learning to Nuclear Digital Twins

Consultancy Meeting on Applications of AI and Pattern Recognition Techniques for Uncertainty Quantification in Nuclear Power Modelling and Simulation

October 21- 22, 2021

Mohammad G. Abdo, Ph.D.

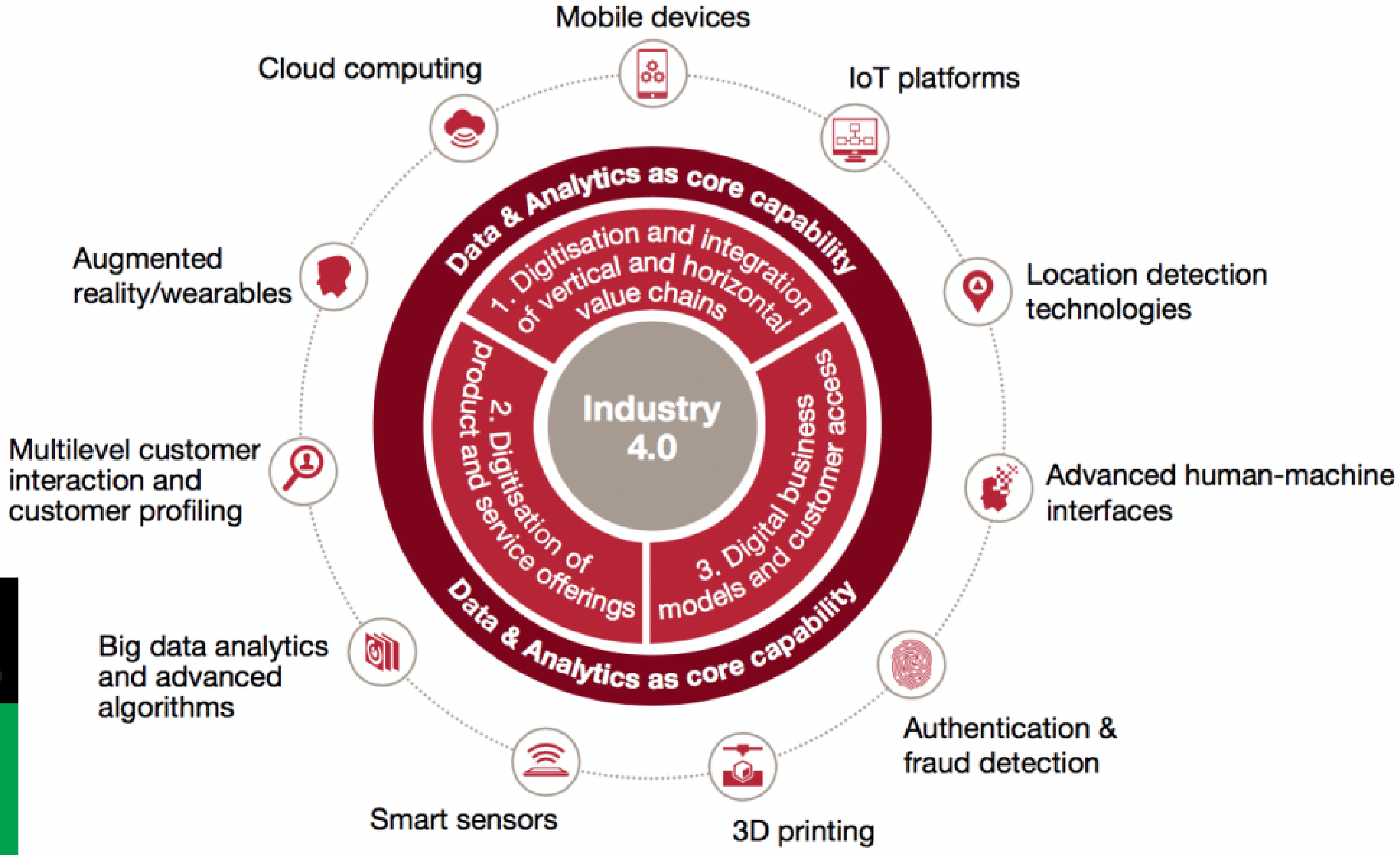
Modeling and Simulation Specialist, Digital Reactor Technology and Development, NS&T, INL

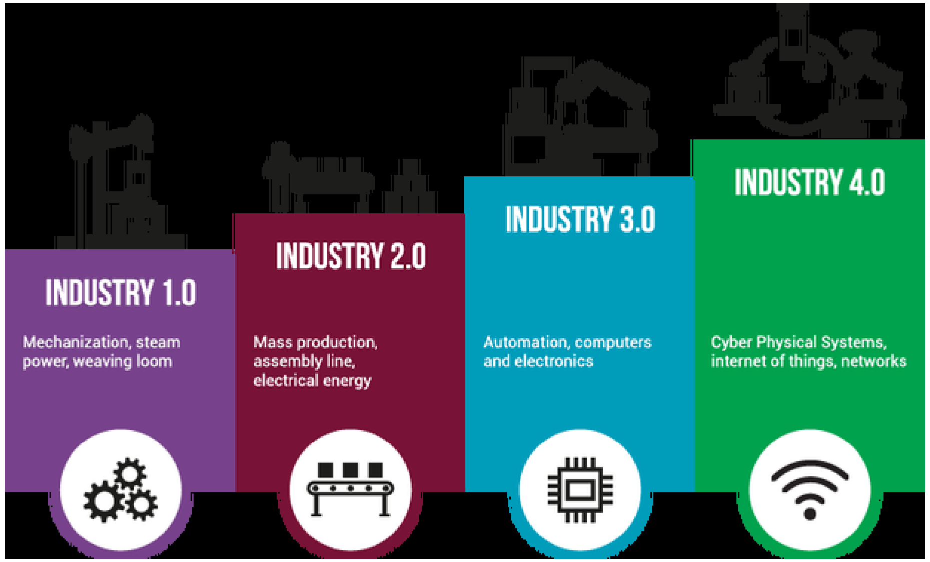
About the Presenter

- Mohammad G. Abdo, Ph.D. (INL)
  - Title: Modeling and Simulation Specialist
  - Department: Digital Reactor Technology and Development (C160) .
  - Division: Reactor Systems Design and Analysis | NS&T

- Research areas of interest and Highlights:
  - LWRS-RISA pathway: Fuel reload pattern Optimization.
  - Sensitivity-informed ROM-based preconceptual design of a TREAT Sodium Loop experiment.
  - Validation, Scaling, and Interpolation of experiments for representativity of full plants.
  - Optimal Sparse Sensing and Sparse Signal Recovery Capability for Nuclear Digital Twins.
  - Integrated Energy Systems: Gap analysis for digital transformation and grid twinning.
  - Areas of interest: Machine Learning, Deep Learning, Reduced Order Modeling, SA/UQ, Sparse Sensing/learning, Digital Twinning, Koopman theory, time delayed embeddings for digital signal processing.

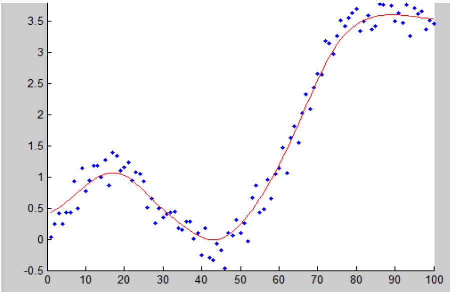
Industry 4.0 framework and contributing digital technologies

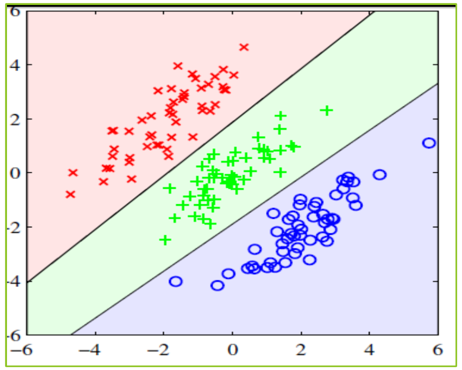


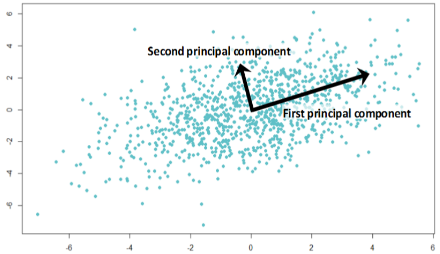


Methods and Taxonomy

'Field of study that gives computers the ability to learn without being explicitly programmed' – Arthur Samuel 1959







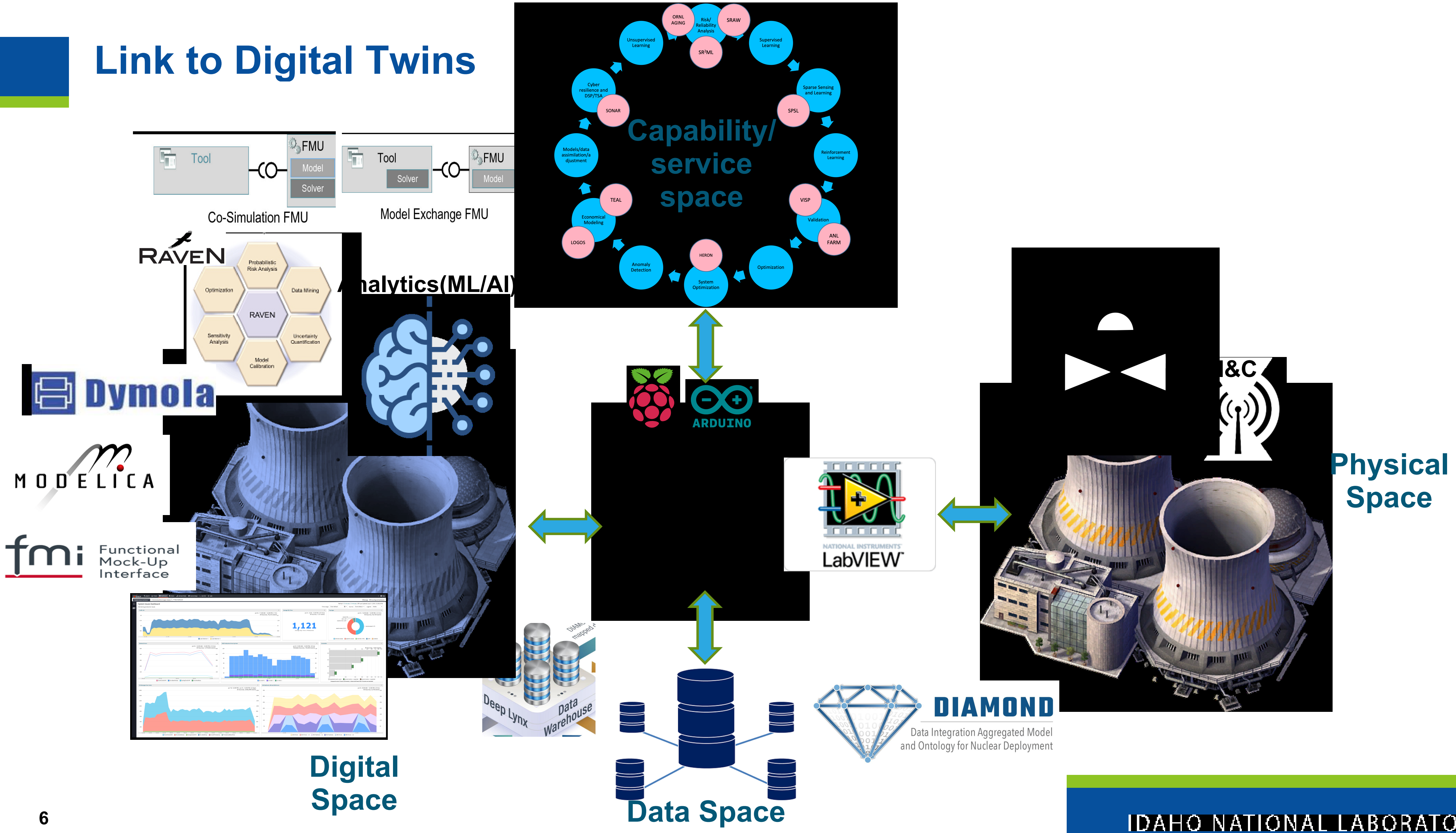
Link to Digital Twins

- Digital Twin definition:

A digitized replica of a physical component, system, or process rendering its whole lifecycle utilizing connectivity to real-time sensory data alongside with deep analytics to enable adaptive learning, inference, reasoning, and decision making with minimal human intervention to achieve the ultimate goal of facilitating the real, continuous, and dynamic communication between design, manufacturing, and quality.

5

Link to Digital Twins



Components of the

1. Physical Space

(ASI, P&ID, BOM, Actuators)

2. Digital/Virtual Space

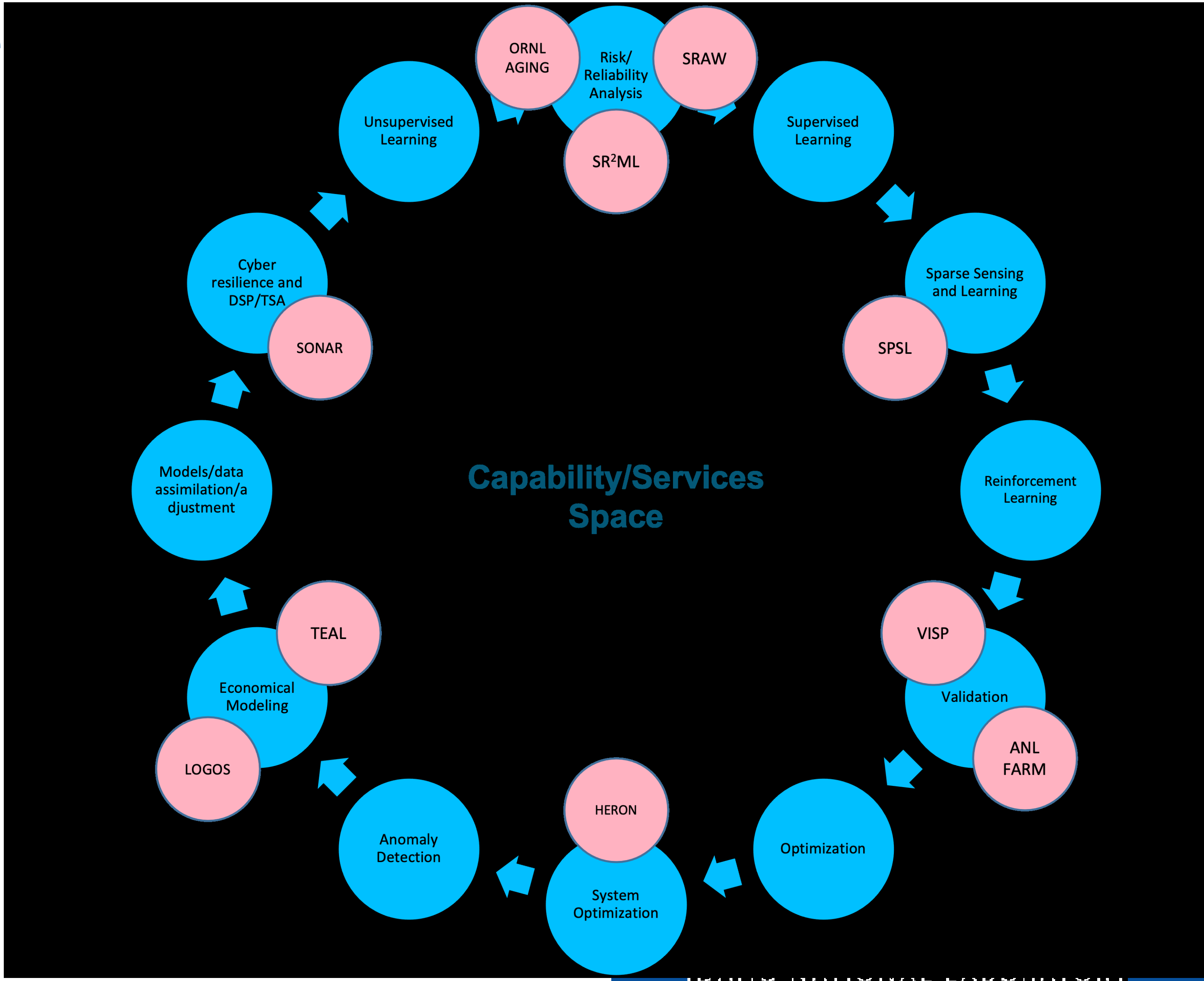
(CAD/GUIs/Analytics)

3. Data Space

(Storage, Connectivity, IIoT)

4. Services Space

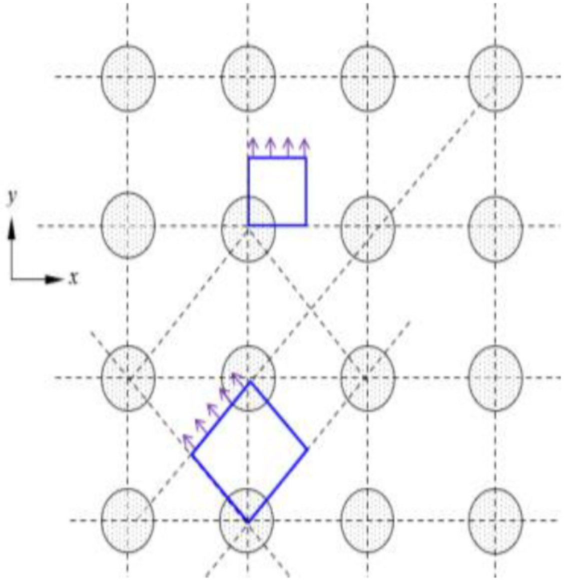
(Prediction/Monitoring/Control)



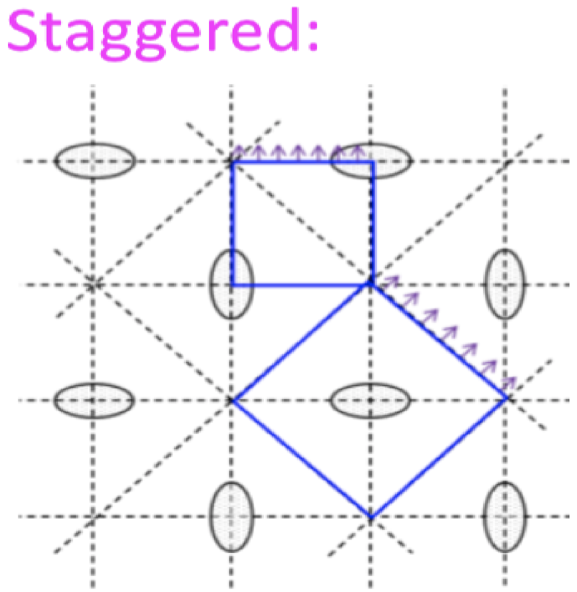
Application1: Thermal modeling of porous materials

Mohammad Abdo, Yu-Lin Shen (UNM), and Isabella Von Rooyen

- Uncertain Parameters:
  - a, b (Major and Minor axes).
  - C_x, C_y (Coordinates of the center of the elliptical pore).
  - Phi (Orientation of the pore)
  - K_{Matrix} (K_{AL})
  - K_{Pore} (K_{AIR})

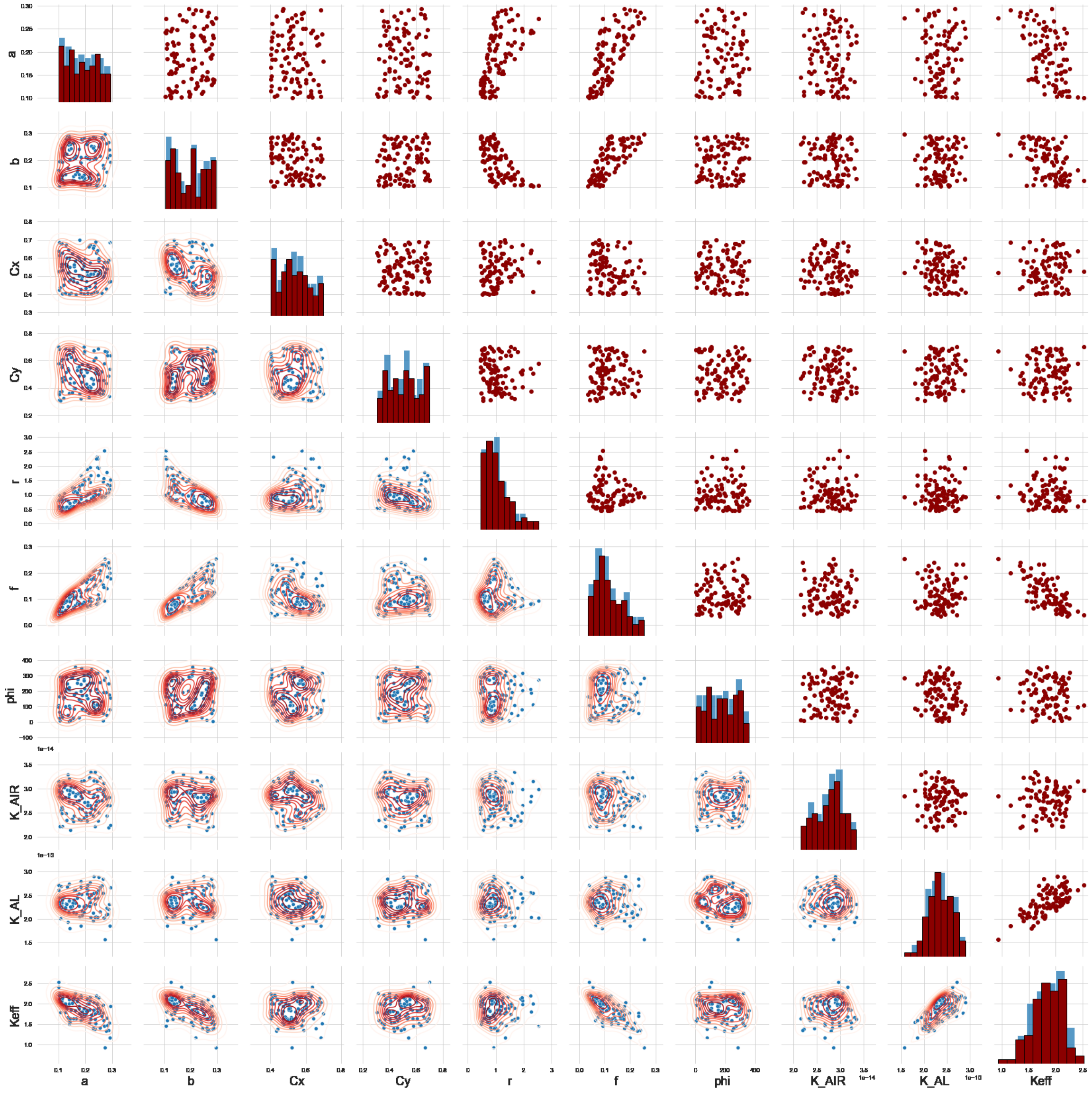


Spherical Model



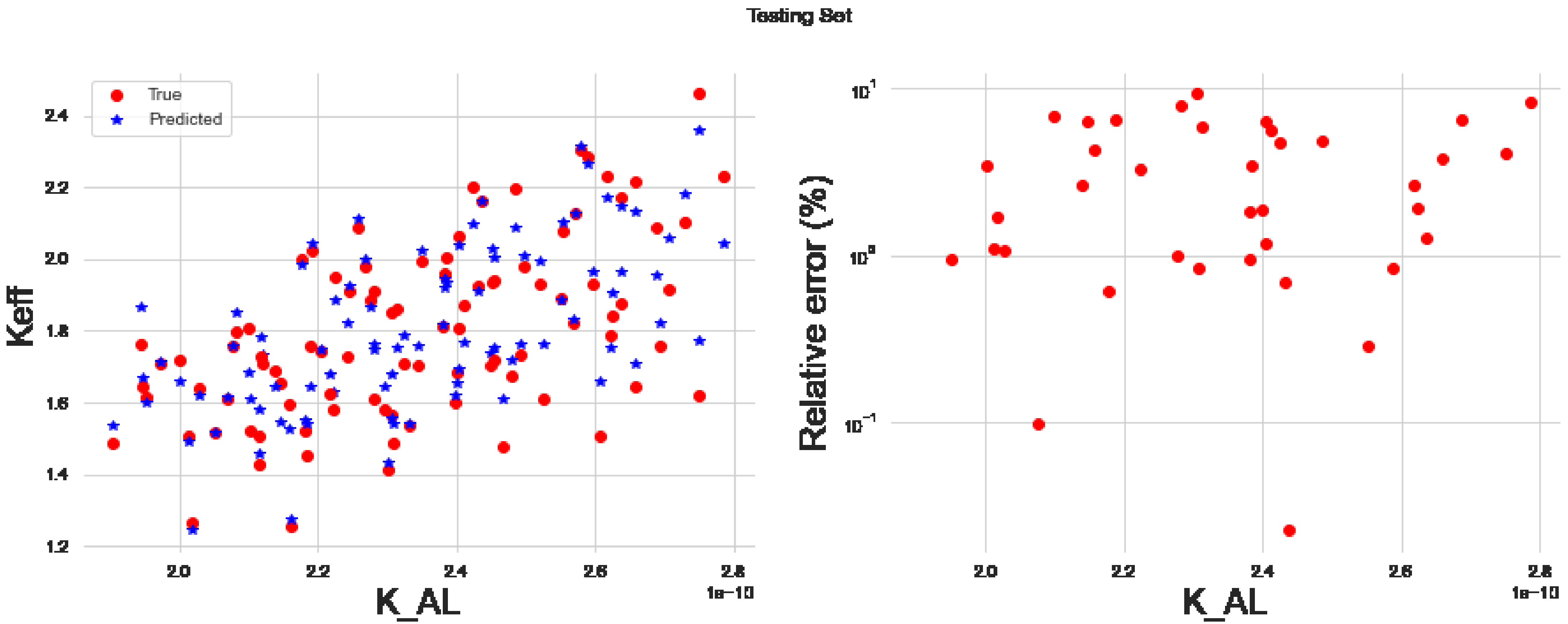
Elliptical Model

DATA Exploration Pair Plots

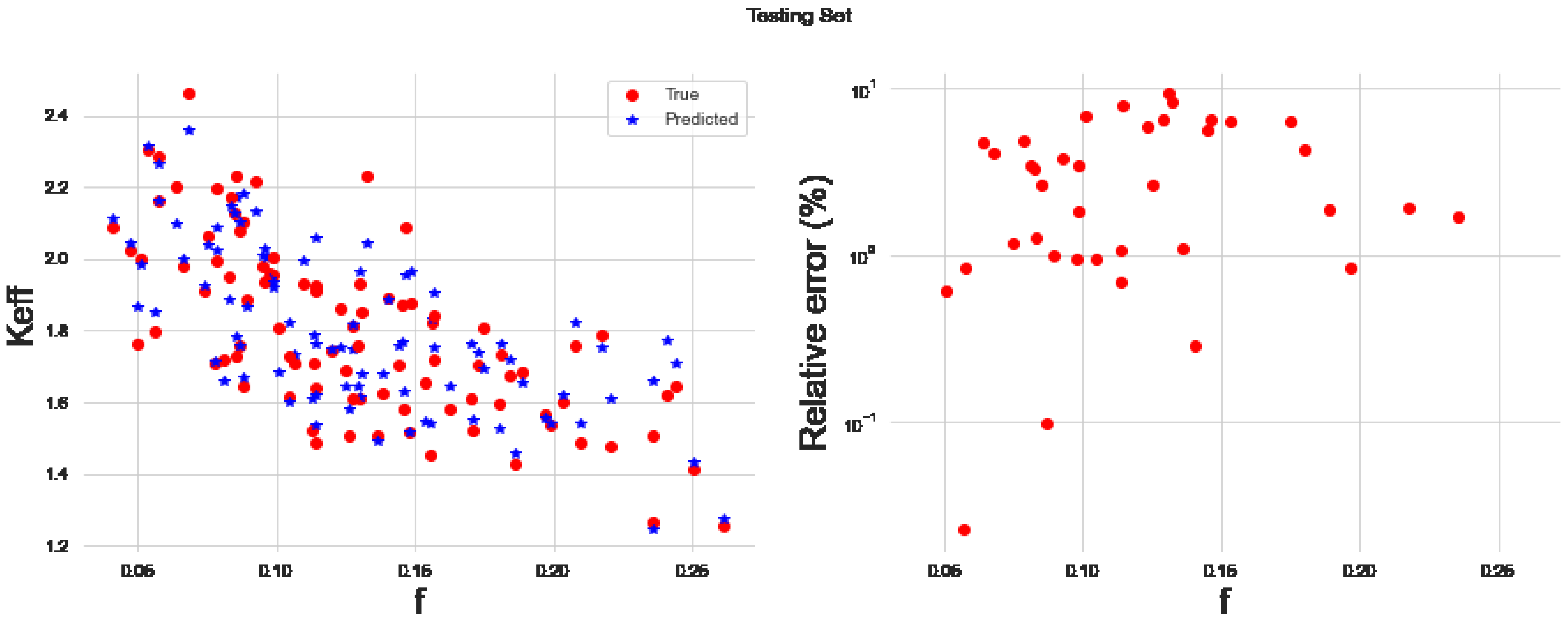


Mathematics of Linear Regression (LR)

LR - Surrogate Validation



LR – Surrogate Validation



ROM vs. Literature

For Spherical Pores Model

Analytical models

Maxwell: $\frac{K_{eff}}{K_m} = 1 - \frac{3p}{2+p}$ (spherical pores)

Rayleigh: $\frac{K_{eff}}{K_m} = 1 - \frac{3p}{2 + p - 0.3923p^{\frac{10}{3}} + \cdots}$ (3D, aligned spherical pores)

$\frac{K_{eff}}{K_m} = 1 - \frac{2p}{1 + p + (0.30584p^4 + 0.013363p^8 + \cdots)}$ (2D, aligned circular pores)

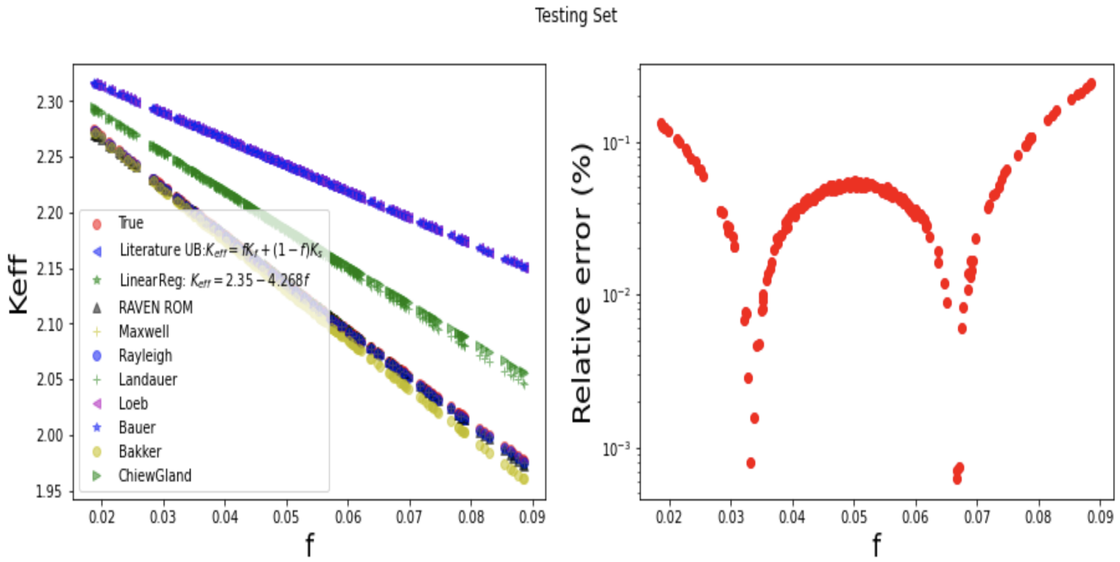
Landauer: $\frac{K_{eff}}{K_m} = 1 - \frac{3}{2}p$ (effective medium percolation theory)

Loeb: $\frac{K_{eff}}{K_m} = 1 - p$

Bauer: $\frac{K_{eff}}{K_m} = (1-p)^{3\varepsilon/2}$ ε : fitting parameter (random pores of arbitrary shape)

Bakker et al.: $\frac{K_{eff}}{K_m} = (1-p)^{1.5}$ (3D, spherical porosity)

$\frac{K_{eff}}{K_m} = (1-p)^2$ (2D, circular porosity)



SA: Sobol Indices

Main effect:

$$S_i = \frac{\mathbb{V}_{X_i}(\mathbb{E}_{X_{\sim i}}(Y|X_i))}{\mathbb{V}(Y)}$$

Interactive effect:

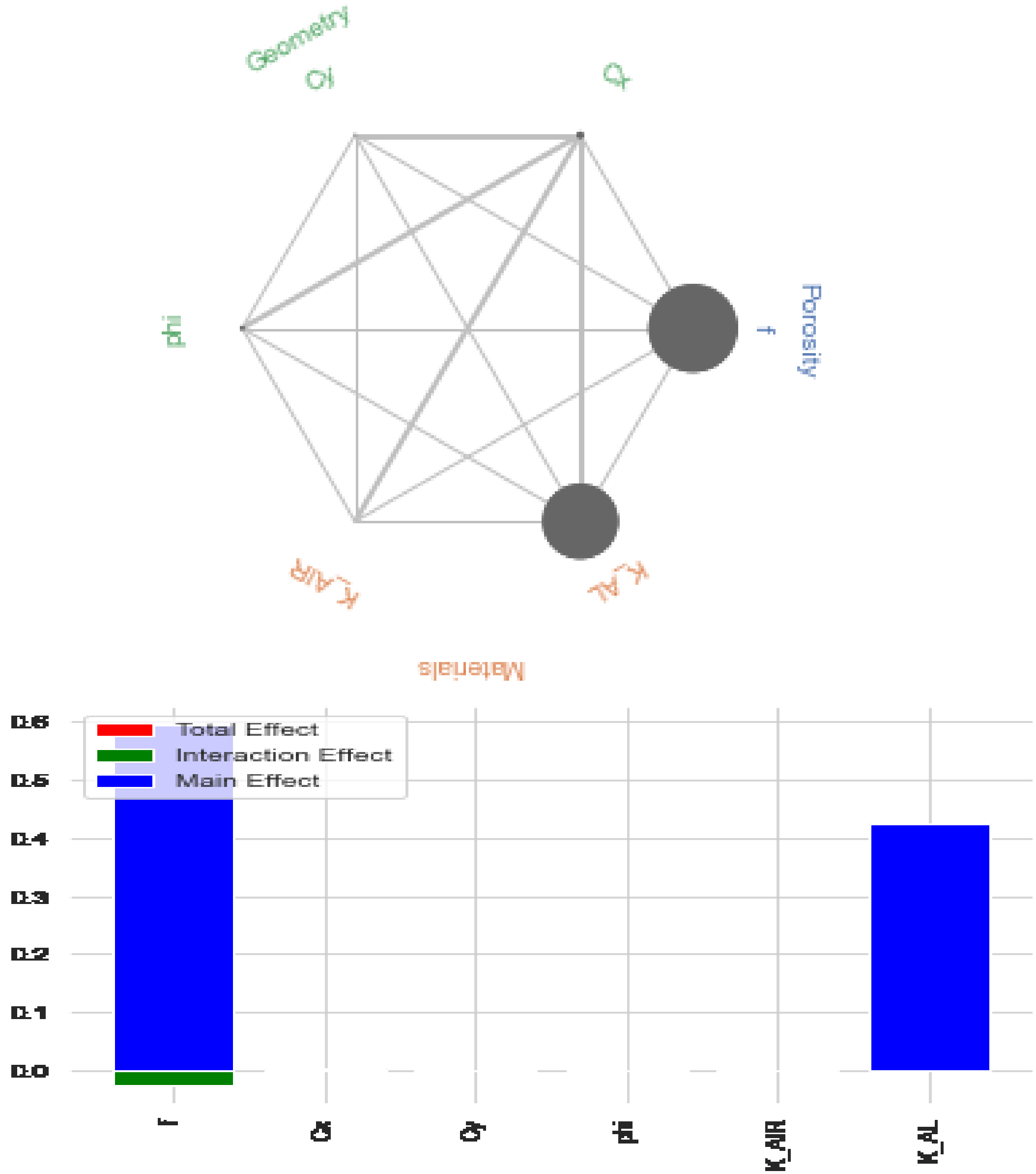
$$S_{ij} = \frac{\mathbb{V}_{X_{ij}}(\mathbb{E}_{X_{\sim ij}}(Y|X_i, X_j)) - \mathbb{V}_{X_i}(\mathbb{E}_{X_{\sim i}}(Y|X_i)) - \mathbb{V}_{X_j}(\mathbb{E}_{X_{\sim j}}(Y|X_j))}{\mathbb{V}(Y)}$$

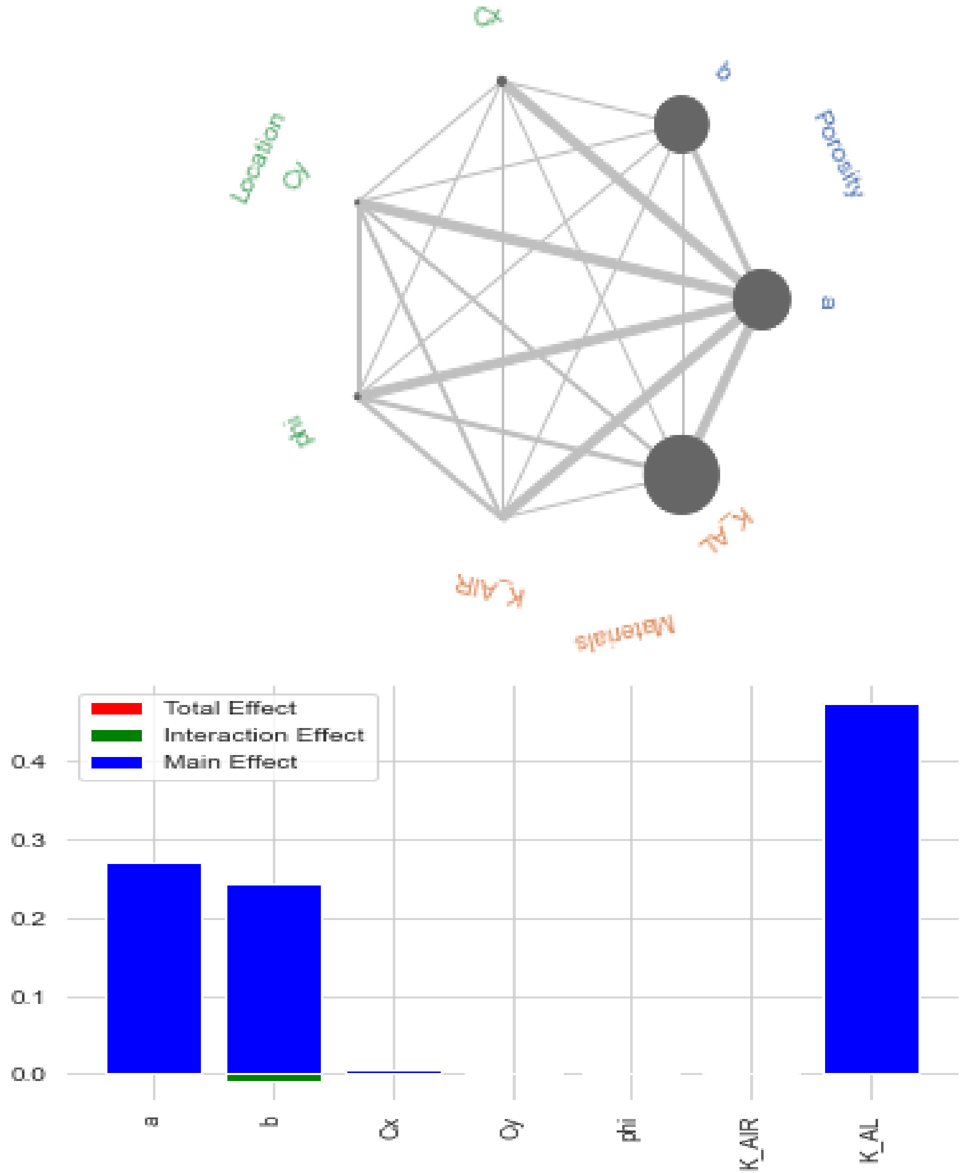
Total effect:

$$S_i^T = \frac{\mathbb{E}_{X_{\sim i}}(\mathbb{V}_{Xi}(Y|X_{\sim i}))}{\mathbb{V}(Y)} = 1 - \frac{\mathbb{V}_{X_{\sim i}}(\mathbb{E}_{X_i}(Y|X_{\sim i}))}{\mathbb{V}(Y)}$$

Uncertainty Propagation

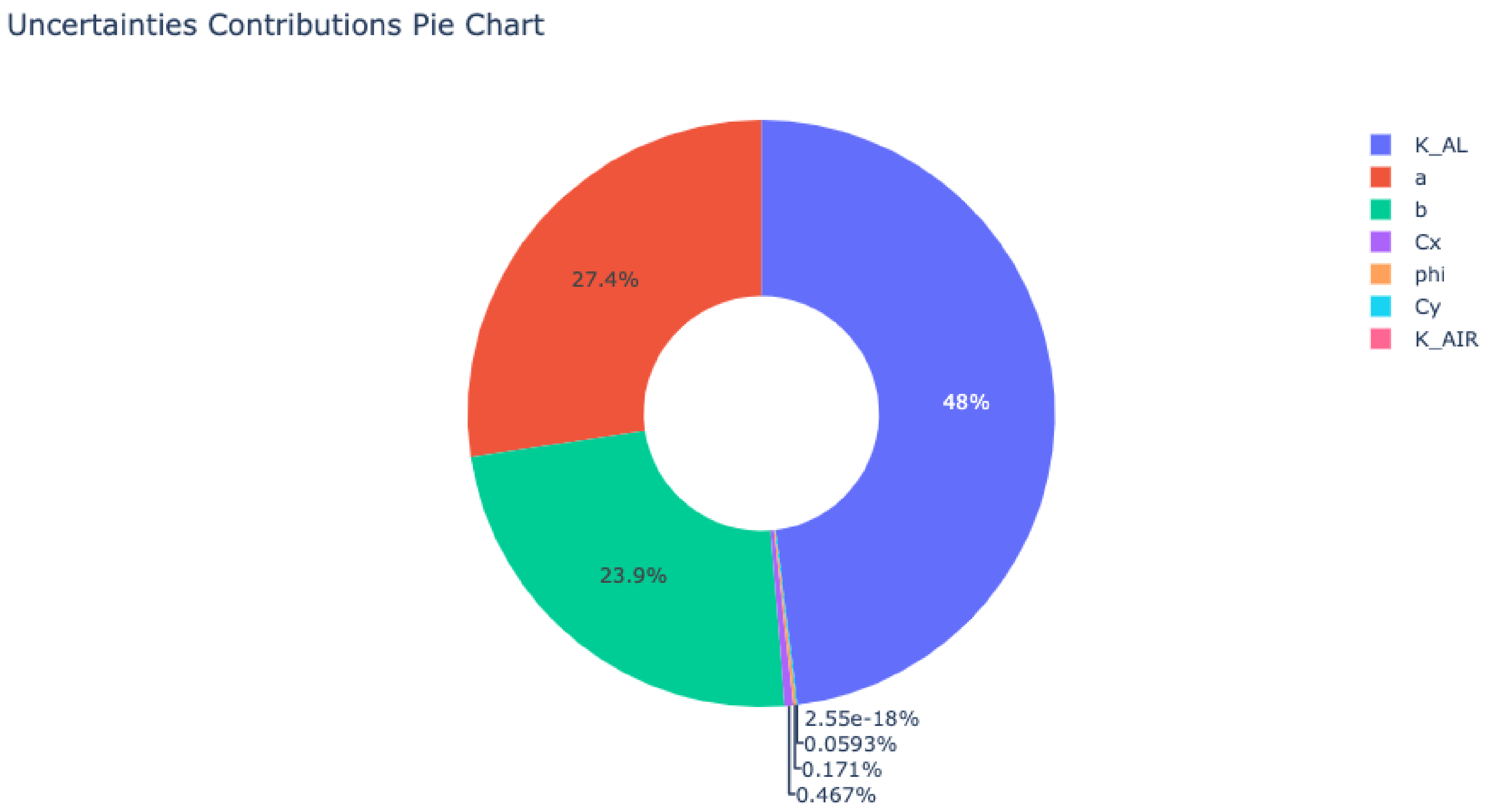
- **For Linear models:**





Sensitivities

Uncertainties

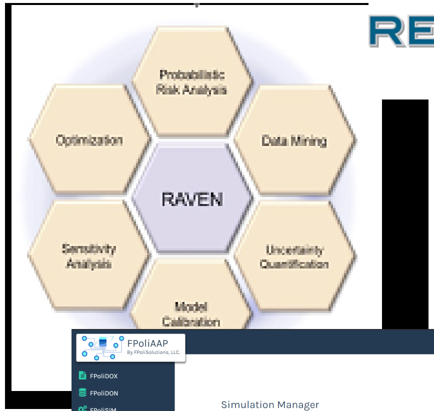


Application 1 Conclusion and Summary

- Influential parameters are local conductivities, and porosity.
- For structured distribution of pores, geomatical parameters (i.e., Cx, Cy, phi, clustering) have minor effect compared to local conductivities and porosity.
- For structured pores, all patterns are linear and hence a linear model can predict the effective thermal conductivity with a mean error of ~2% and a max error of 10%. Higher accuracies can be achieved using more complex models such as Polynomial Regressors, Support Vector Machines (SVMs), Decision Trees (DTs), High Dimensional Model Representation (HDMR), and Artificial Neural Networks (ANNs, CNNs, RNNs, LTSMs).
- For unstructured distribution of pores, X-ray Computed Tomography (XCT) will inform the model about the pore distribution and hence build more accurate models.
- The sparse data coming from experiments can be used for validation and if the required accuracy is not met, a multi-fidelity Gaussian process can be used to incorporate the experimental data with the simulation data from the ROMs and hence build a more accurate. This mitigates the problem of sparsity of the experimental data while leverages insights from the finite element modeling and machine learning models.

Application 2: LWRS-RISA pathway: Fuel pattern optimization

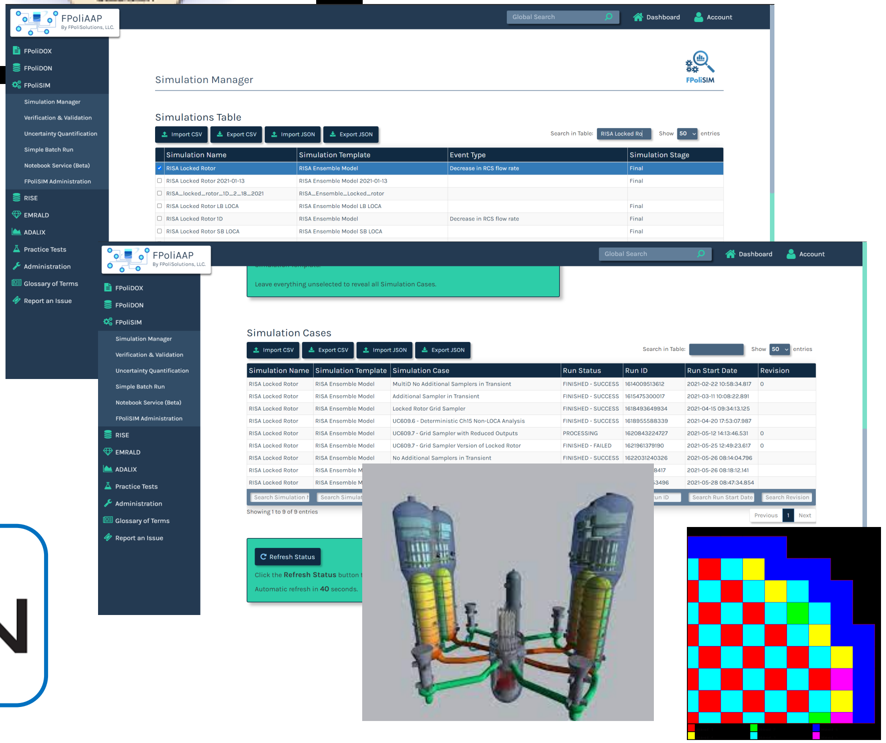
Mohammad Abdo, Yong-Joon Choi



RELAP5-3D

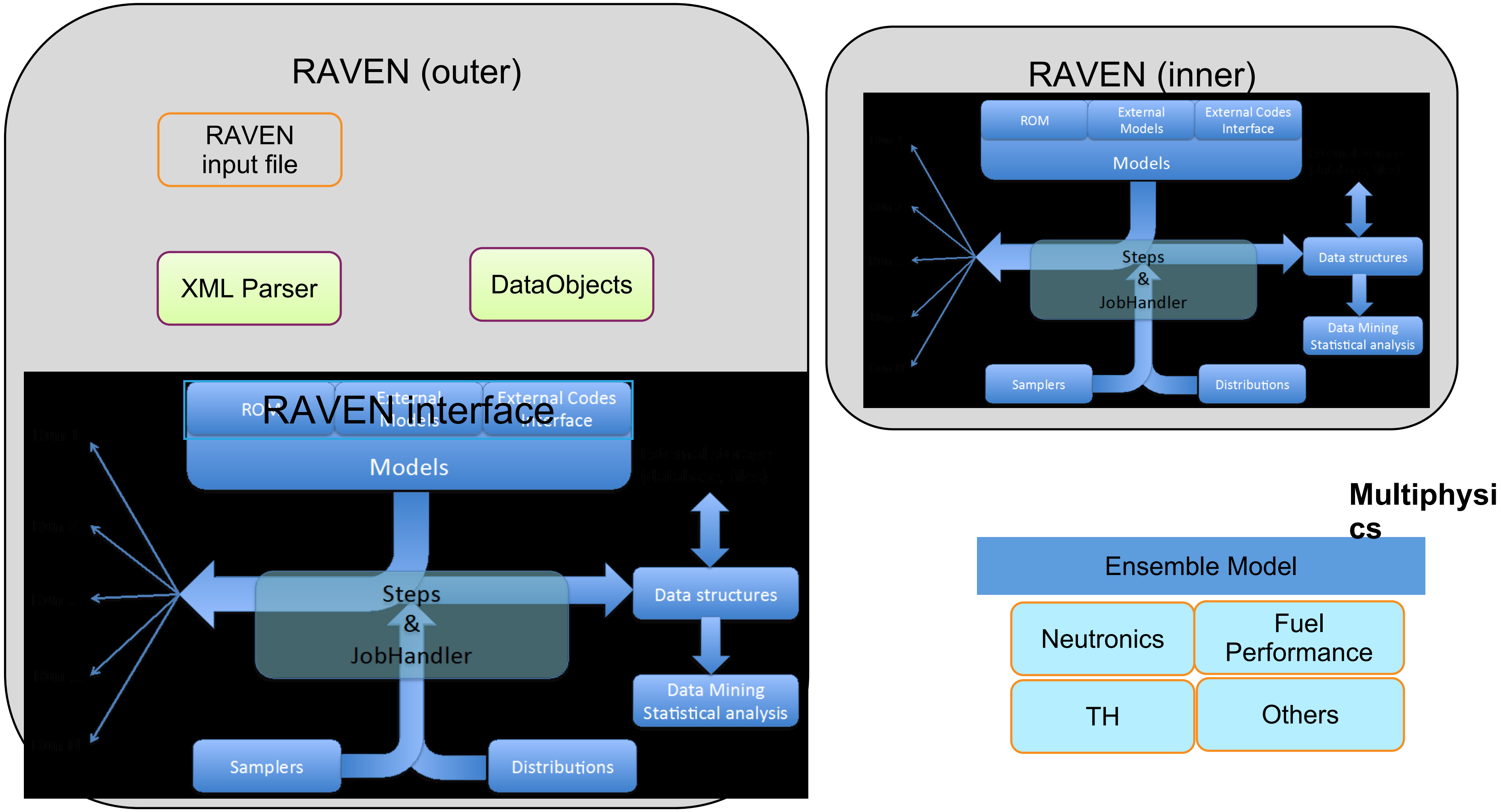
PHISICS

BISON



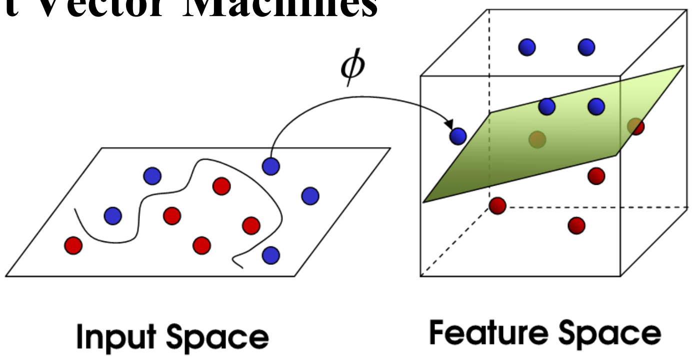
FPoli-AAP → RAVEN

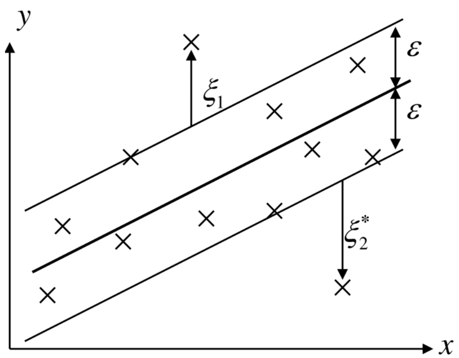
RAVEN driving multiple physics



Potential Surrogate models (i.e., ROMs)

Support Vector Machines





Given training data

$$(\mathbf{x}_i, y_i) \quad i = 1,\ldots,m$$

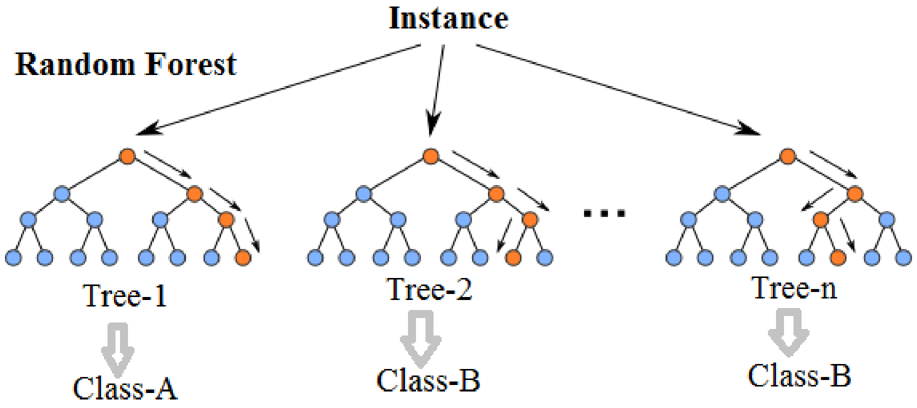
Minimize

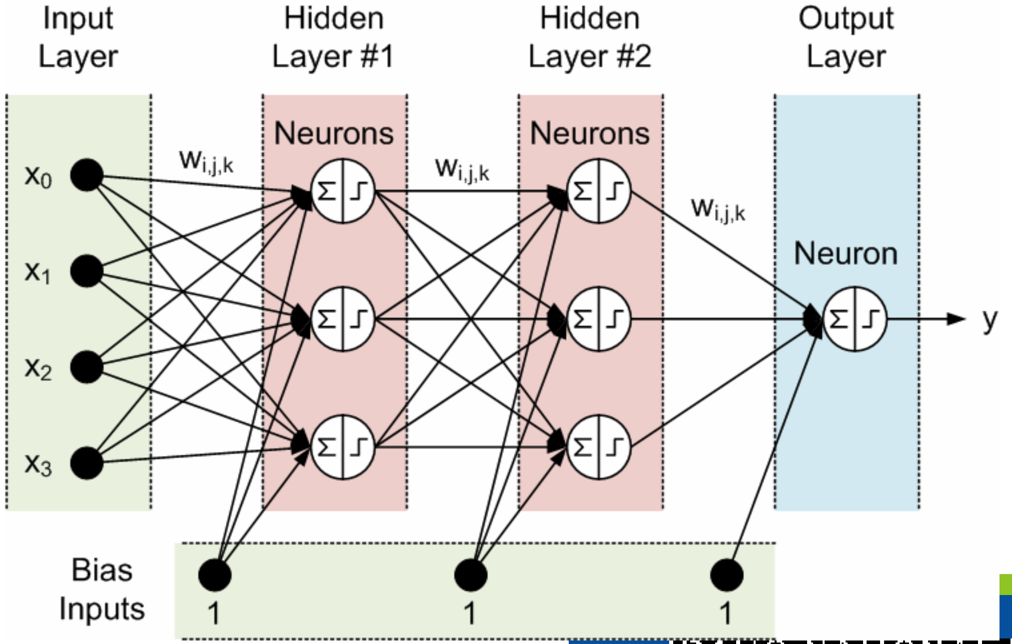
$$\frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m}(\xi_i + \xi_i^*)$$

Under constraints

$$\begin{cases} y_i - (\mathbf{w}\cdot\mathbf{x}_i) - b \le \varepsilon + \xi_i \\ (\mathbf{w}\cdot\mathbf{x}_i) + b - y_i \le \varepsilon + \xi_i^* \\ \xi_i, \xi_i^* \ge 0, i = 1,\ldots,m \end{cases}$$

Random Forest Simplified

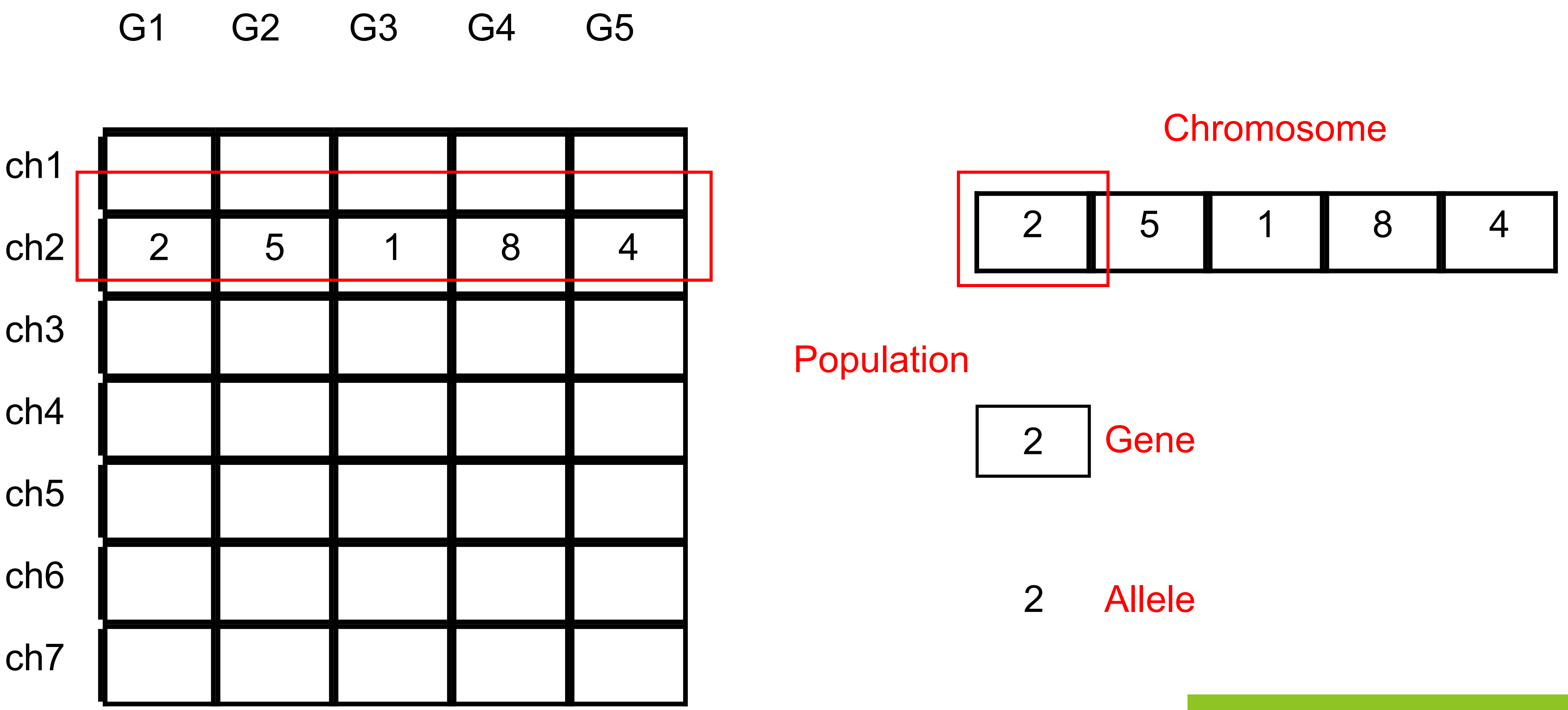




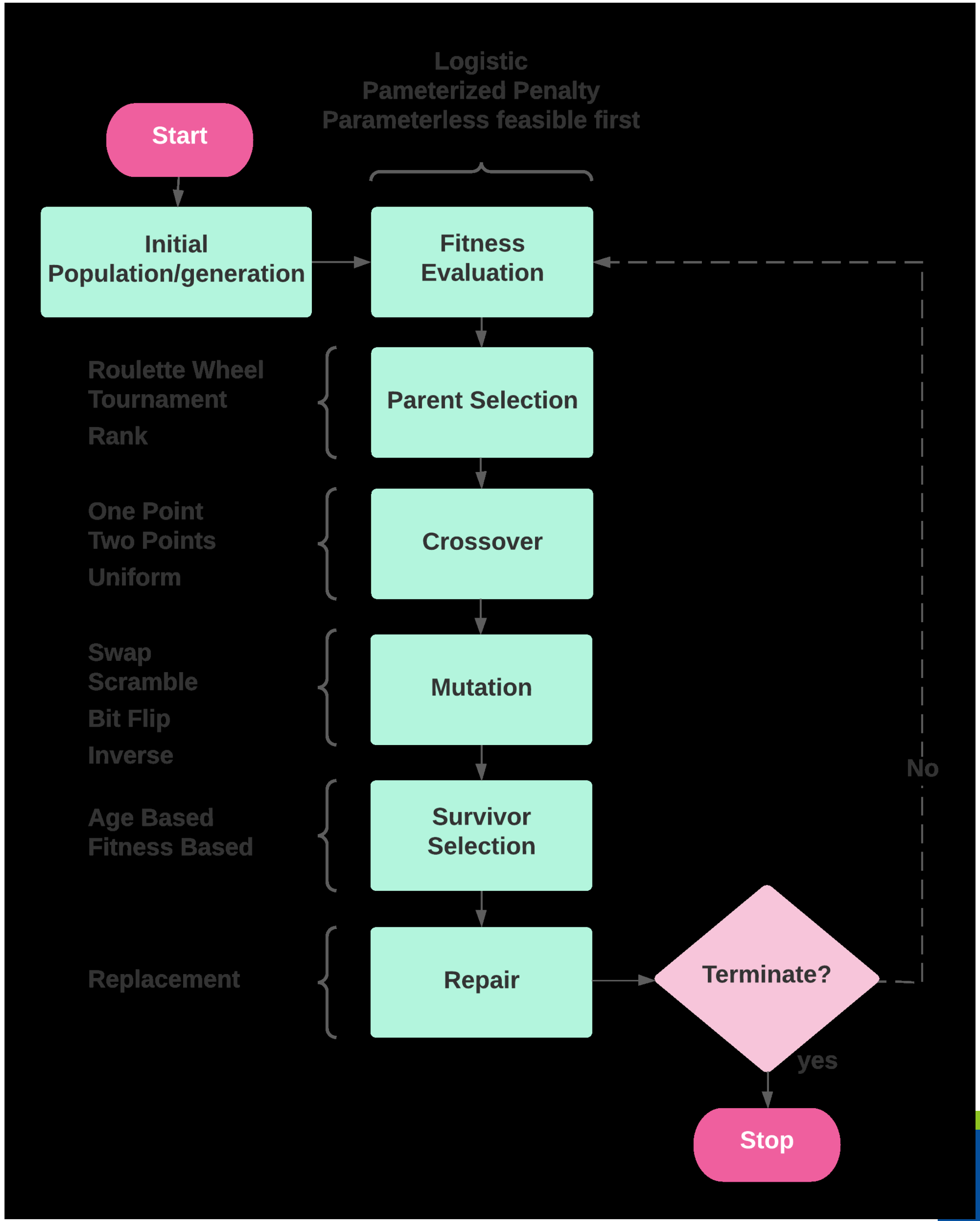
Optimization Algorithms

- Why Genetic Algorithms?
  - Metaheuristic algorithms stemming from biological evolution.
  - Preferred for non-differentiable, expensive to differentiate, or objective functions with no intrusive access (black-box).
  - Doesn’t get stuck in local minima, and hence works with non-convex problems.
  - Can handle both constrained and unconstrained problems.
  - Due to the encoding/decoding step it works with discrete, continuous, or mixed design spaces, with binary, integer, real, gray, or permutation encoding.

Nomenclature



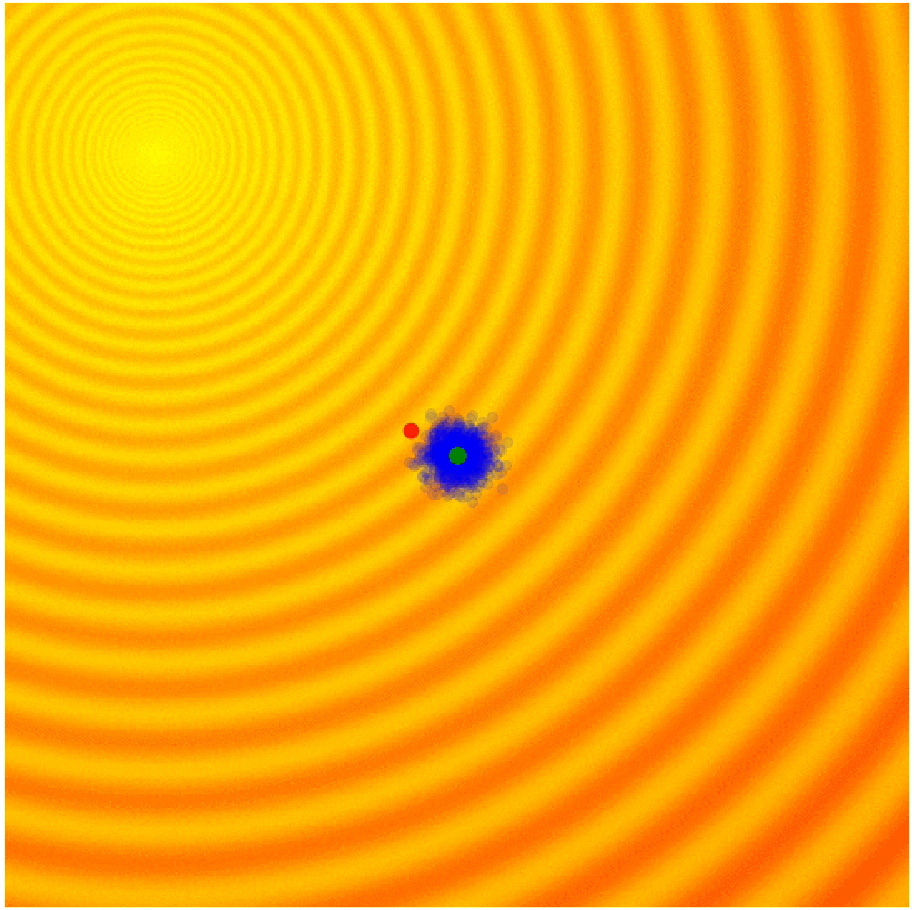
Flowchart



Logistic
Pameterized Penalty
Parameterless feasible first
Start
Initial Population/generation
Fitness Evaluation
Roulette Wheel
Tournament
Rank
Parent Selection
One Point
Two Points
Uniform
Crossover
Swap
Scramble
Bit Flip
Inverse
Mutation
Age Based
Fitness Based
Survivor Selection
Replacement
Repair
Terminate?
No
yes
Stop

Overview of GA

1. Encoding/decoding: Phenotype/Genotype variable representation (**binary**, integer, **permutation**, or real representation).
2. Create initial population
3. Fitness Evaluation
4. Parent selection
5. Crossover: creation of offsprings
6. Mutation: creation of mutated offsprings
7. Replacement/repair
8. Survivor selection
9. If Termination condition(s) is met terminate, else repeat Steps 3 through 7 (each iteration is a generation).



Source: A Visual Guide to Evolutionary Strategies. https://blog.otoro.net/2017/10/29/visual-evolution-strategies.

Evolutionary Operators for GA

Parent Selectors:

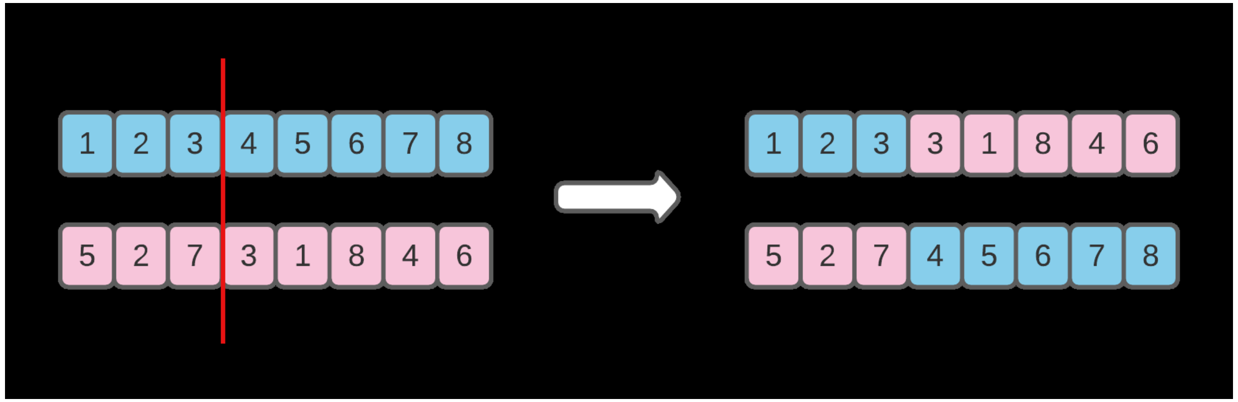
- Roulette Wheel
- Tournament Selection
- Rank Selection

Individual	Fitness
P1	5
P2	8.2
P3	1.4
P4	0.98
P5	2
P6	2.3

Evolutionary Operators for GA

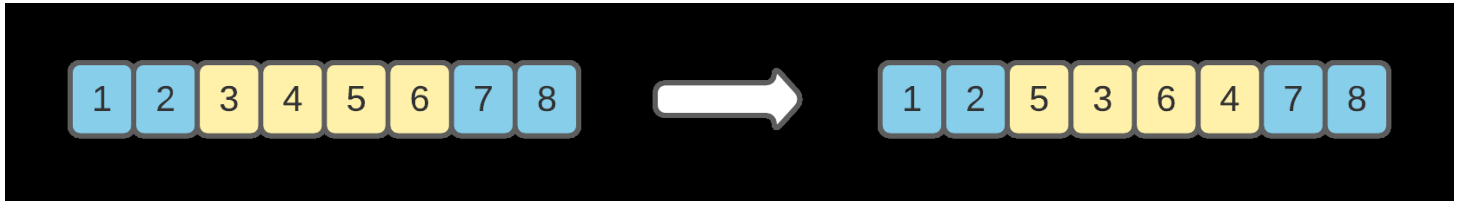
Cross Over:

- One Point
- Two points
- Uniform



Evolutionary Operators for GA

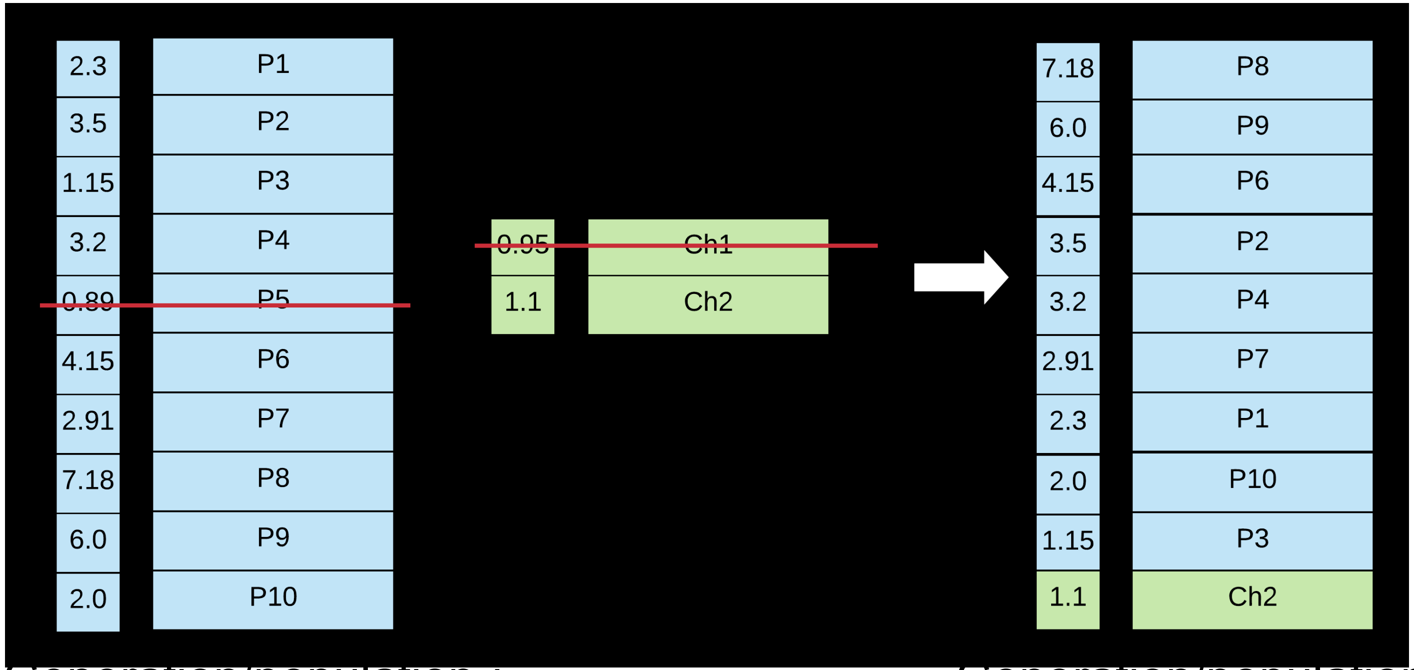
- Mutators:
  - Swap Mutation
  - Scramble Mutation
  - Bit Flip Mutation
  - Inversion Mutation



Evolutionary Operators for GA

Survivor Selection:

- Fitness Based
- Age Based

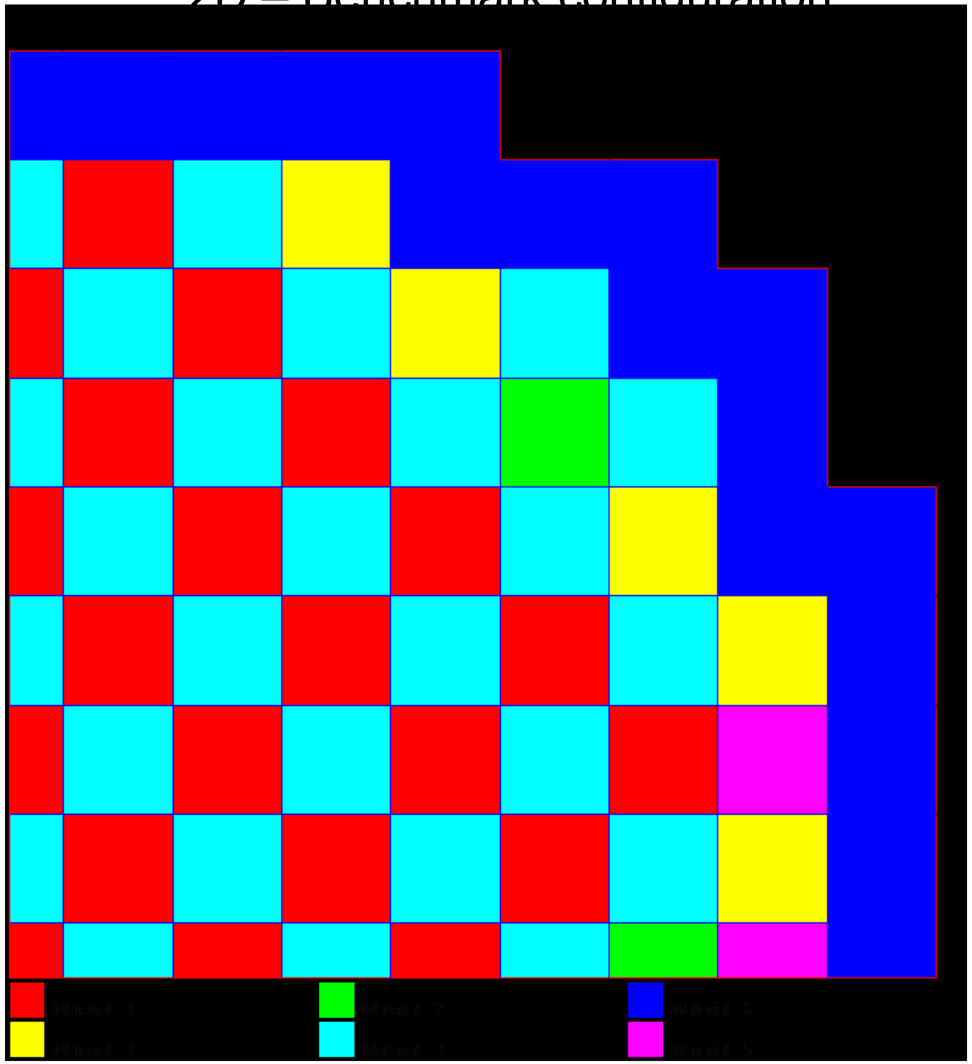


Generation/population *i* Generation/population *i+1*

Initial loading simplified problem

- Settings:
  - 1/4th of the core (PWR)
  - 56 variables (56 assembly locations to arrange)
  - 5 Materials (5 assembly types to “choose” from):
    - Material - 1: Enrichment 2.2% in U235, No burnable poisons
    - Material – 2: Enrichment 2.5% in U235, No burnable poisons
    - Material – 3: Enrichment 2.5% in U235, burnable poisons (8.e-06 #/(cm*barn))
    - Material – 4: Enrichment 3.5% in U235, No burnable poisons
    - Material – 5: Enrichment 3.5% in U235, burnable poisons (8.e-06 #/(cm*barn))
  - Objective:
    - Maximization of cycle length
    - The cycle length is determined based on a criticality search calculation (Soluble Boron Search): if SB <= 5 ppm, cycle ends

2D – Benchmark configuration



Initial results

Solution:

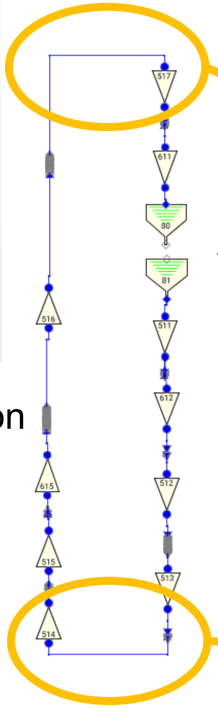
5	1	2	3	4	5	5	5	5	5	5	5
5	5	5	5	5	5	5	5	5	5	5	5
5	5	5	5	5	5	5	5	5	5	5	5
5	5	5	5	5	5	5	5	5	5	5	5
5	5	5	5	5	5	5	5				

Optimal Value:
598.9 days

Application 3 – TREAT Sodium Loop Cartridge Conceptual Design

Aaron Epiney, Mohammad Abdo, Cole Blakely, Bryce Kelly, Greg Core

- Estimate **loop pressure drop** (ALIP pump head) for both concepts.
- Bends and elbows modeled with **STARCCM+** to inform **RELAP5-3D** calculation (k-factors)



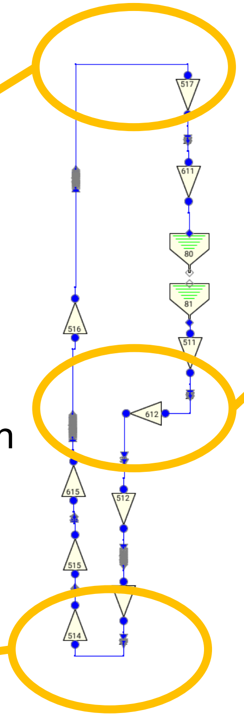
ALIP

Test section

Top elbow
Identical between concepts

Bottom turn
Different between concepts

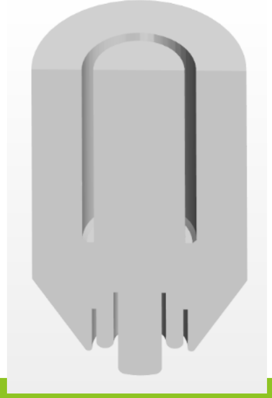
Mark 3



ALIP

Test section

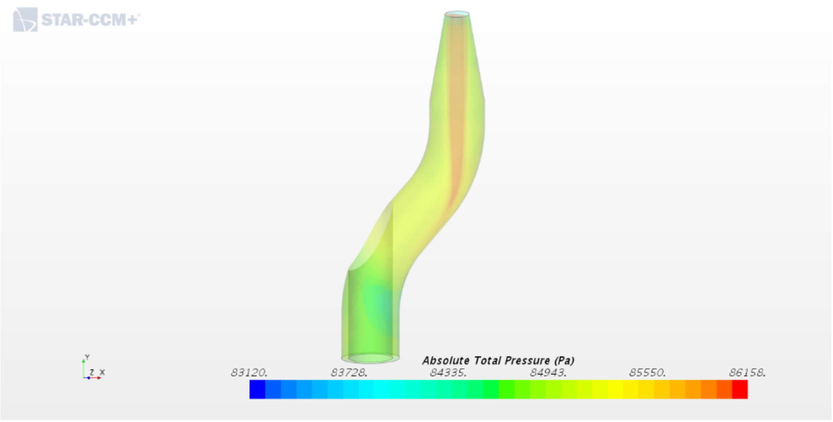
S-bend
Only in concept 4



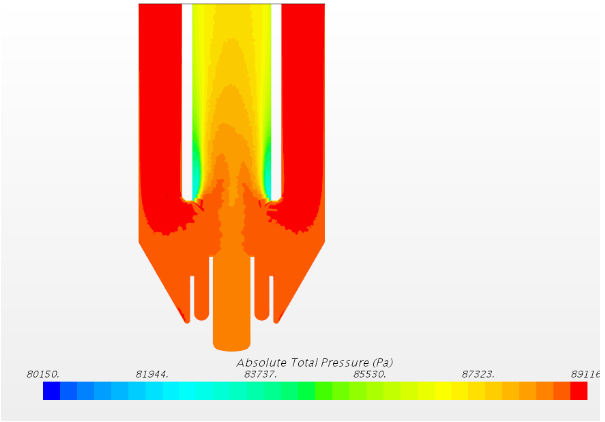
Concept 4

Experiment Performance (Pressure Drop)

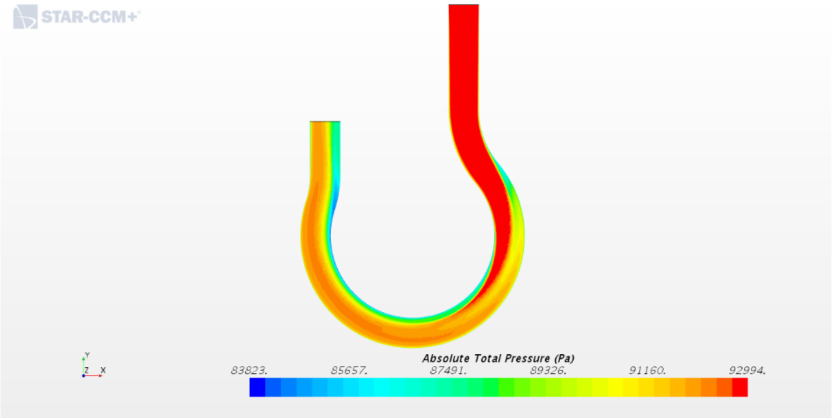
Loop Component Total Pressure Figures



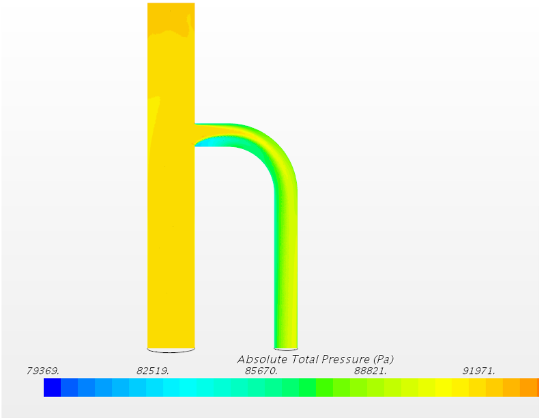
S-Bend



Core Catcher



Lower Bend



Upper Bend

Iteration	Pressure Drop
S-Bend	0.762 KPa (0.110 psia)
Flip	2.090 KPa (0.303 psia)
Lower Bend	2.360 KPa (0.342 psia)
Upper Bend	2.964 Kpa (0.430 psia)
Wire Wrap	27.596 KPa (4.002 psia)

Experiment Performance (Pressure Drop - BEPU)

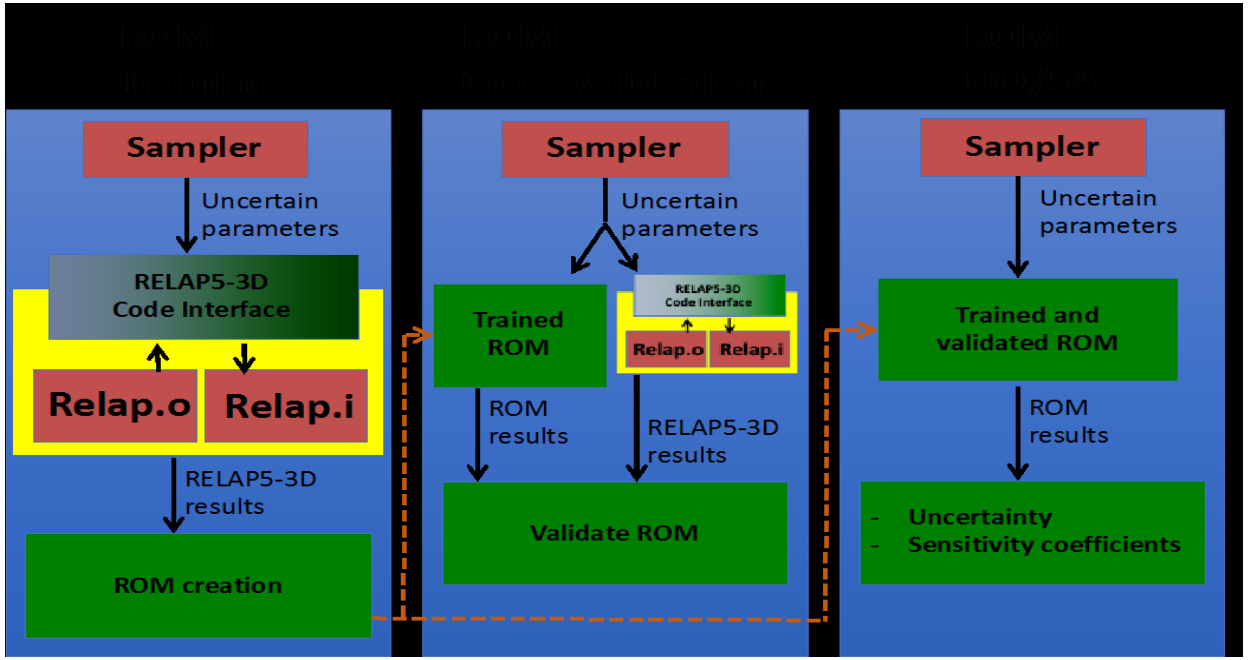
Uncertain parameters

Mark 3

Parameter	Accuracy	Nominal value	Name in plots
Top elbow k-factor	±10%	0.529076	PRT_kTop
Bottom turn k-factor	±10%	**1.12047**	PRT_kBottom
Test section friction	±10%	0.55	PRT_f
Mass flow rate	±1%	1.12047	PRT_mDot

Concept 4

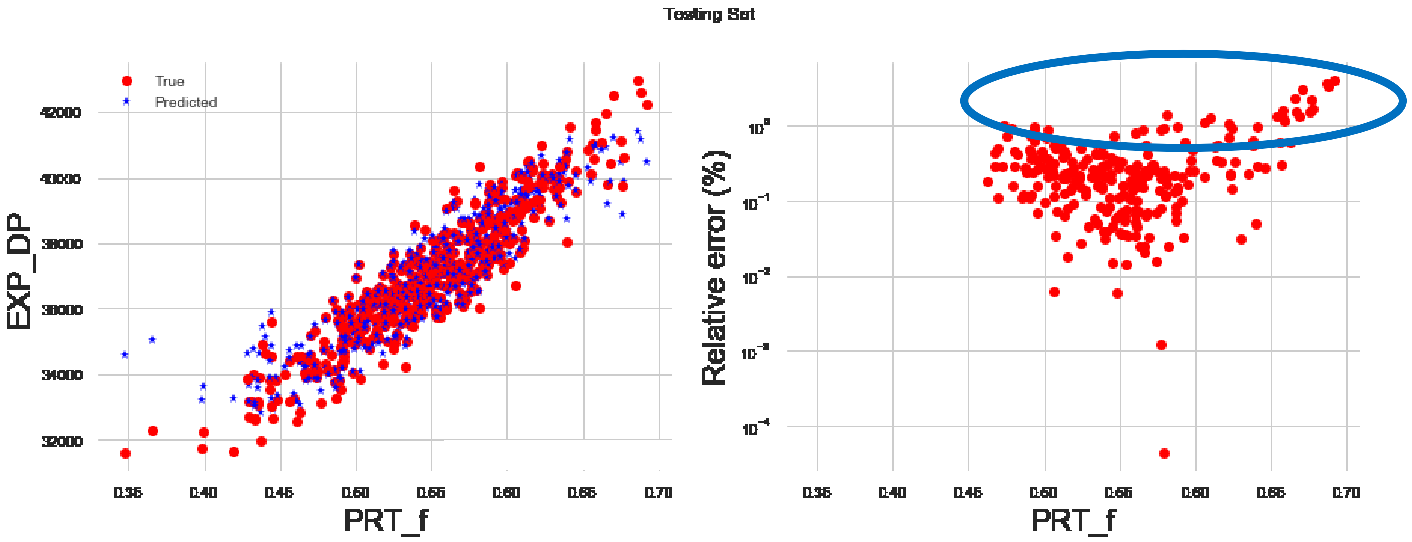
Parameter	Accuracy	Nominal value	Name in plots
Top elbow k-factor	±10%	0.529076	PRT_kTop
Bottom turn k-factor	±10%	**0.99210106**	PRT_kBottom
S-bend k-factor	±10%	**1.718622713**	PRT_kS
Test section friction	±10%	0.55	PRT_f
Mass flow rate	±1%	1.12047	PRT_mDot



- RAVEN model
  - **ROM needed**: For SA/UQ too many model evaluations needed to run RELAP5-3D
  - **HDMR** ROM used

(Pressure Drop BEPU Results)

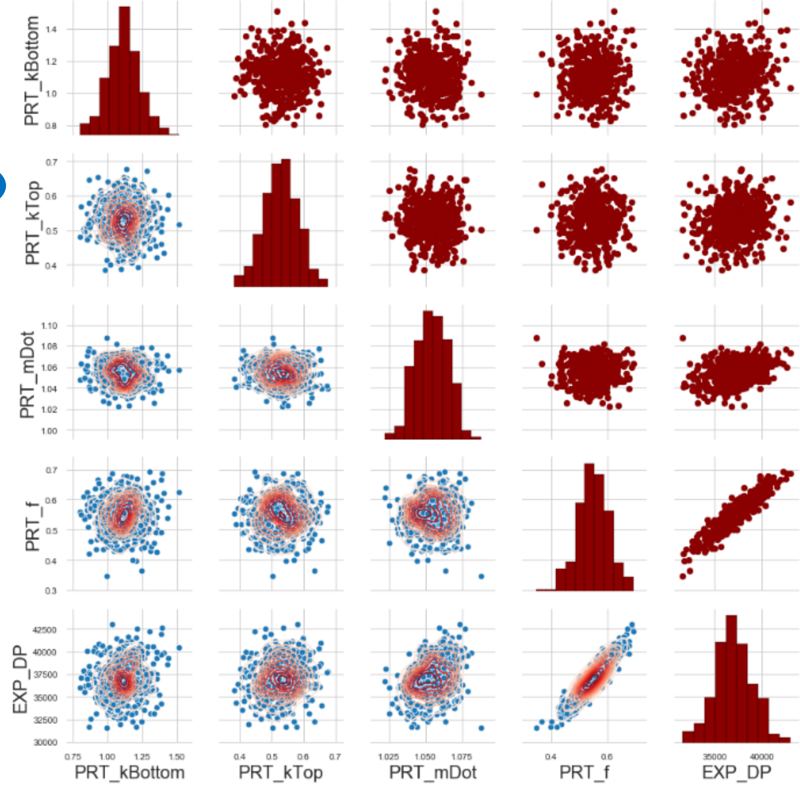
ROM validation



Mark 3

< 5% error
in ROM

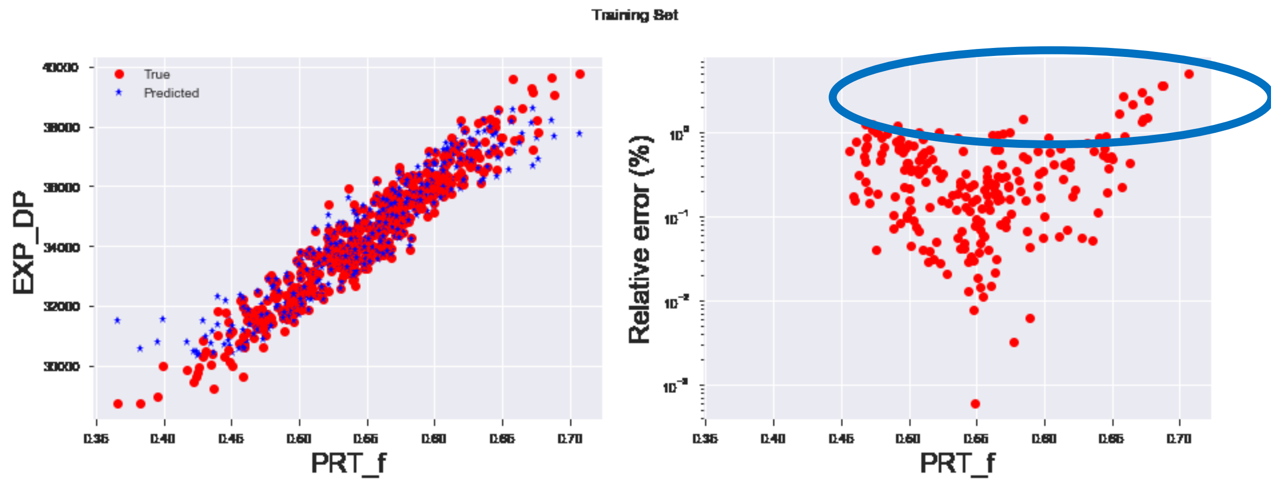
Data correlations



Mark 3

(Pressure Drop BEPU Results)

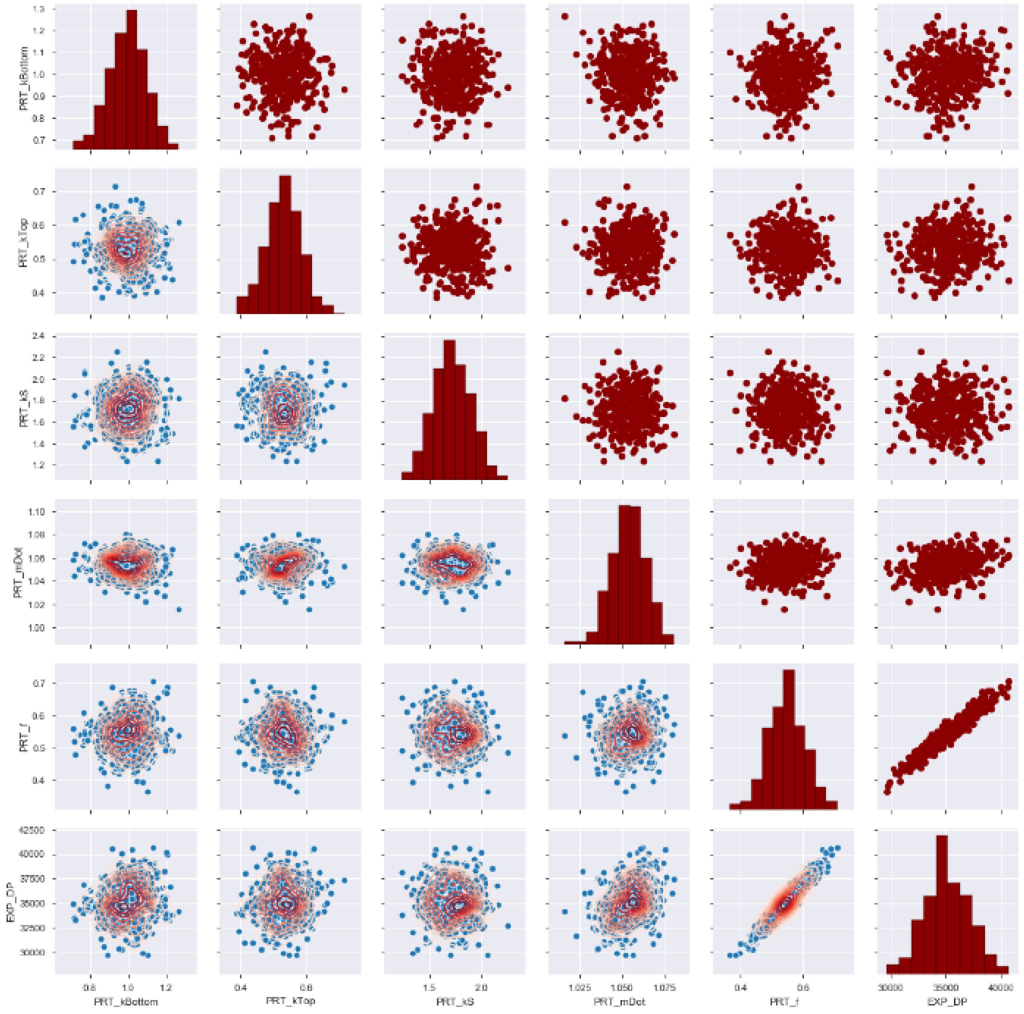
ROM validation



Concept 4

< 5% error
in ROM

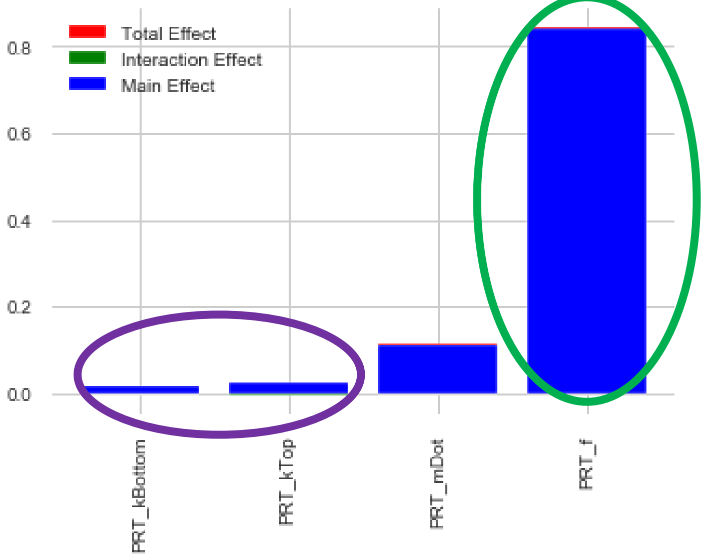
Data correlations



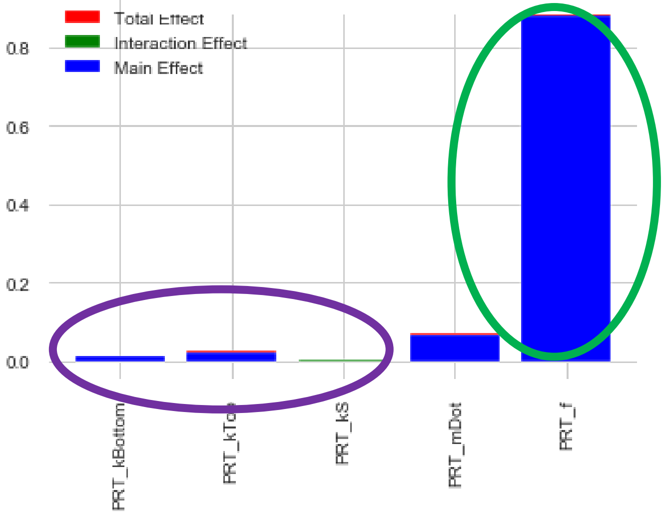
Concept 4

Pressure Drop BEPU Results

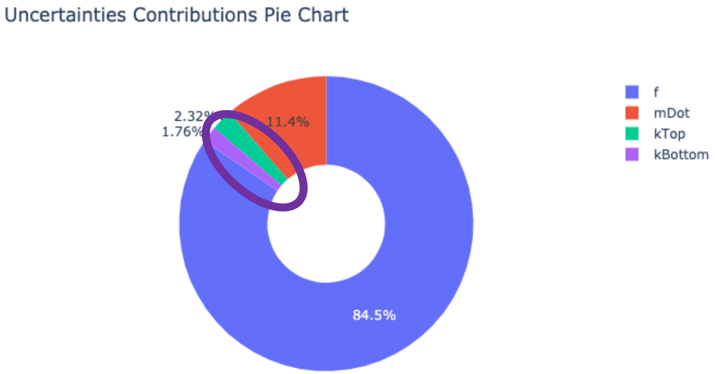
Mark 3



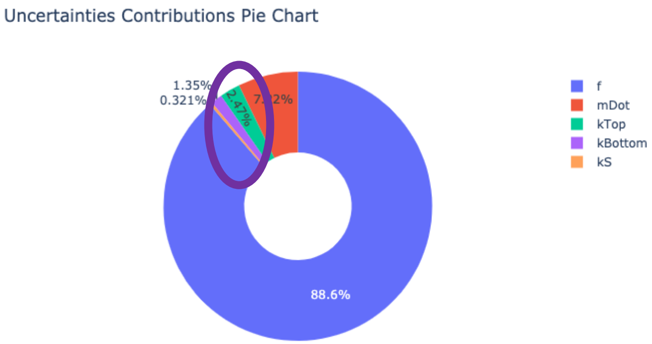
Concept 4



Friction in test section

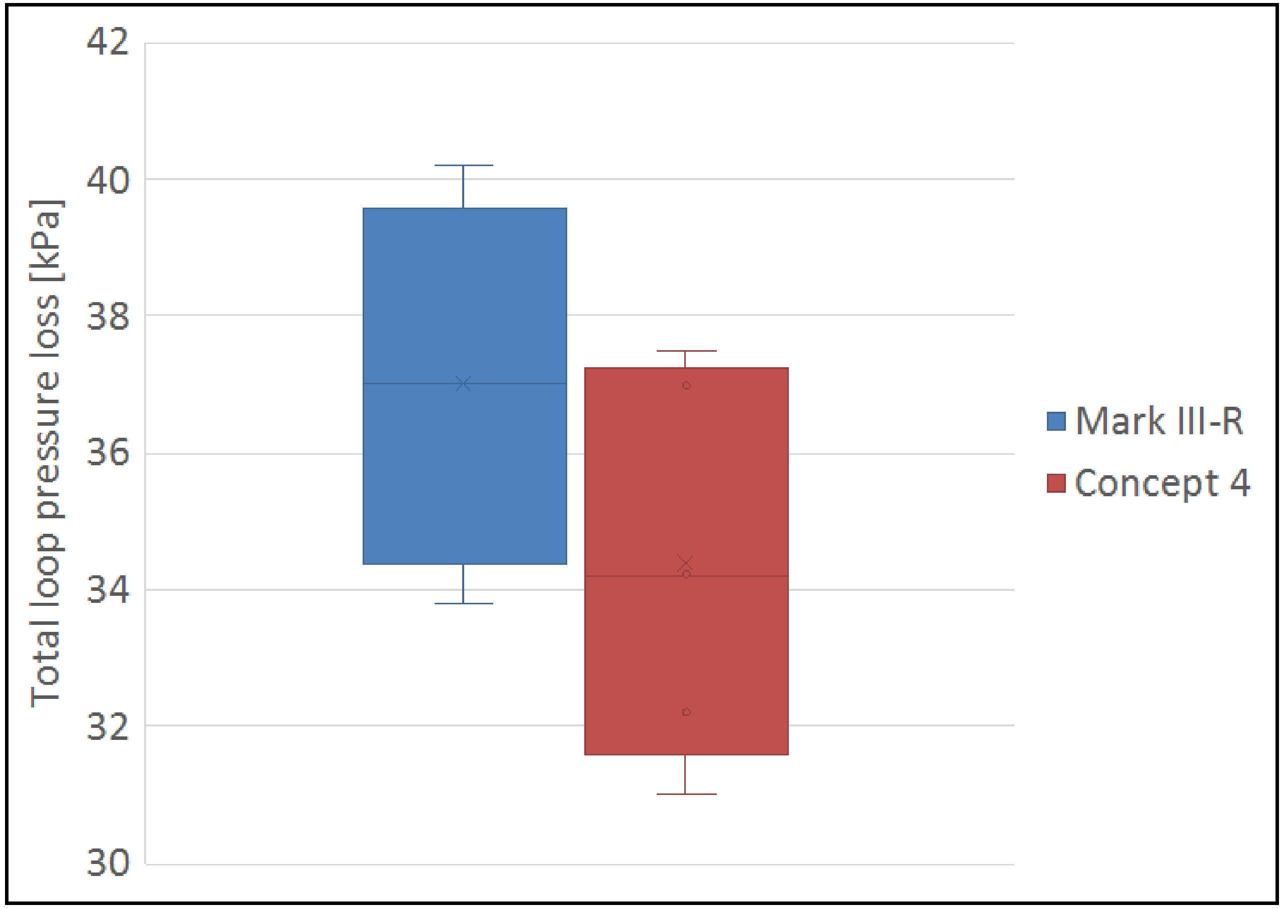


Uncertainty in bends



Pressure Drop Conclusions

- **Nominal value** loop pressure **3 kPa lower** for Concept 4
- Standard deviation for both concepts ~ 2 kPa
- **Test section friction dominates** total pressure loss
  - 85% in Mark 3
  - 89% in Concept 4
- UQ/SA
  - Uncertain values do not show second order effects
  - Sum of uncertainties from first order uncertainties match standard deviation.



Safety and Hazards (Maximum Wall Temperature)

ROM and Sensitivities

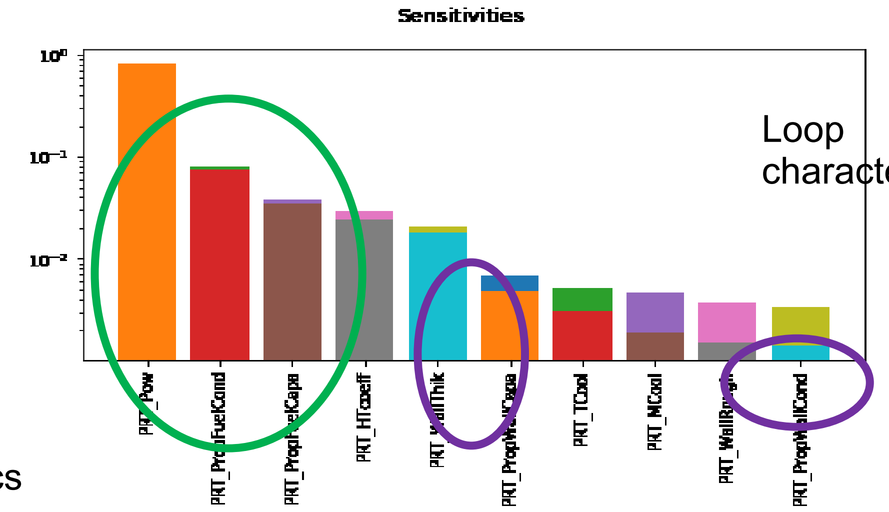
- High Dimensional Model Representation (HDMR):

- Sobol Indices:

Safety and Hazards (Maximum Wall Temperature BEPU)

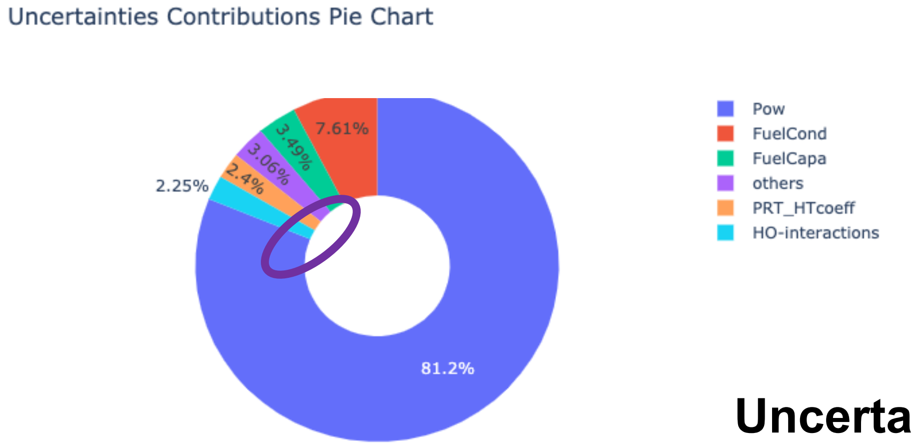
[redacted]

Sensitivities



Loop characteristics

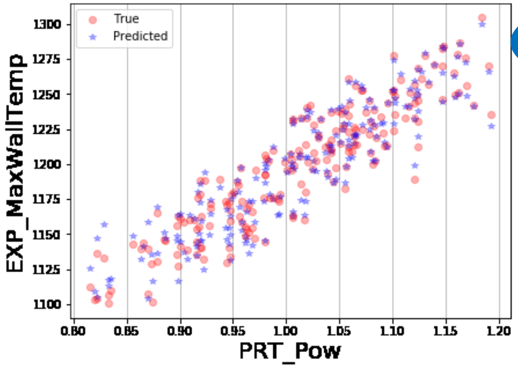
Experiment characteristics

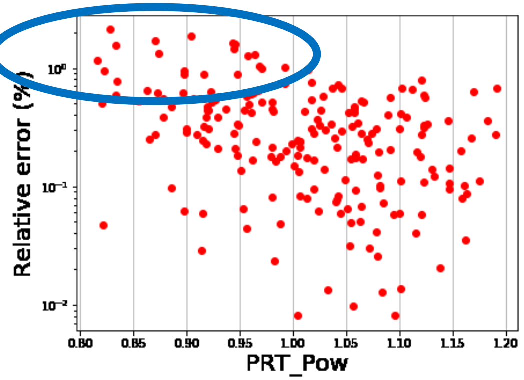


Uncertainties

ROM validation (testing set)

Max. 2% error in ROM





Safety and Hazards (Maximum Wall Temperature conclusions)

- **Safety**
  - Maximum Wall Temperature **bounded** by saturation and superheating **~1500K**
- **Sensitivity**
  - Wall temperature **most sensitive** to
    - Power
    - Fuel and cladding material properties

→ **Experiment** characteristics

  - Wall temperature **somewhat sensitive** to
    - Heat transfer coefficient

→ **Physics** model uncertainty

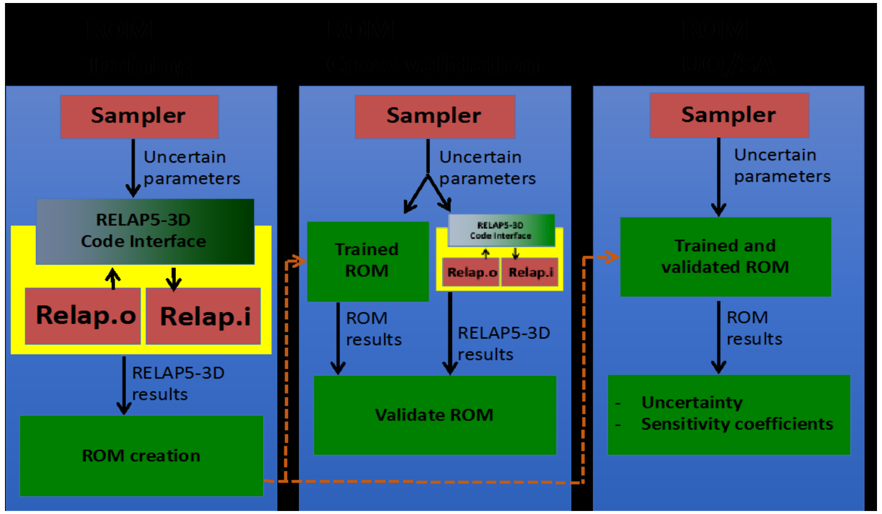
  - Wall temperature **least sensitive** to
    - Inlet temperature and mass flow
    - Wall thickness
    - Wall material properties

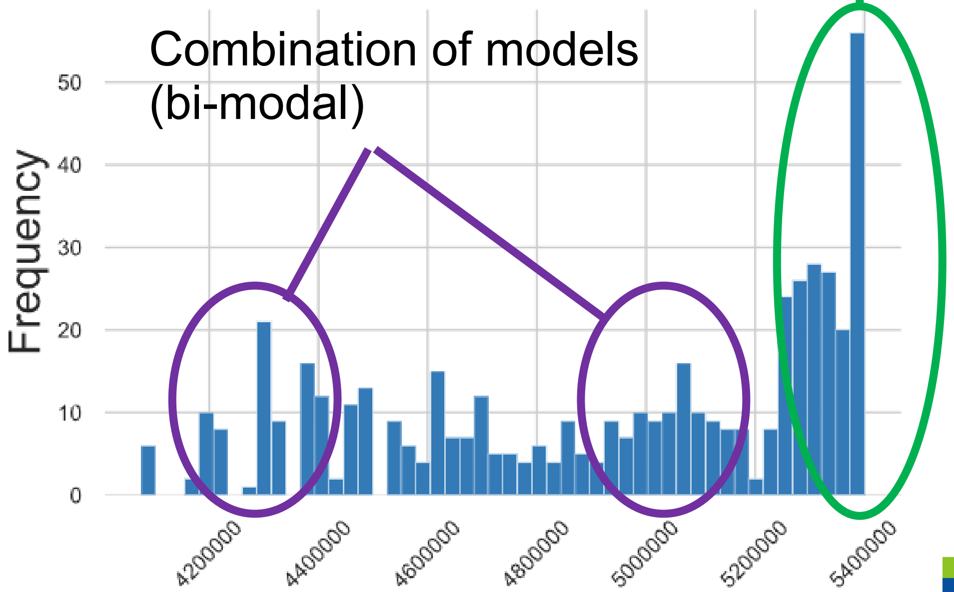
→ Experiment **boundary conditions**

→ **Loop** characteristics

- **Uncertainty**
  - **Mean** Maximum Wall Temperature ~ **1200K**
  - **Uncertainty** ~ 50K
  - ~ **93% of** uncertainty from **Experiment** characteristics ~ 46.5K
  - ~ **7% of** uncertainty from **Loop** characteristics,
    Boundary conditions, Physics models and second order effects ~ 3.5K

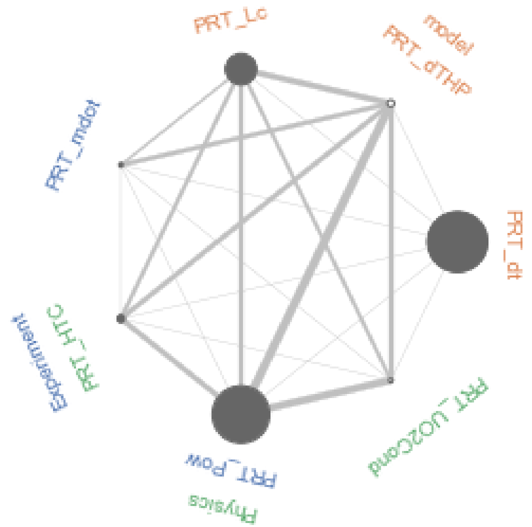
Safety and Hazards (Maximum Pressure)





- RAVEN model
  - **ROM needed**: For SA/UQ too many model evaluations needed to run RELAP5-3D
  - **HDMR** ROM used
  - Pressure Model difficult to fit
    - HDMR higher error
    - Other ROMs under investigation

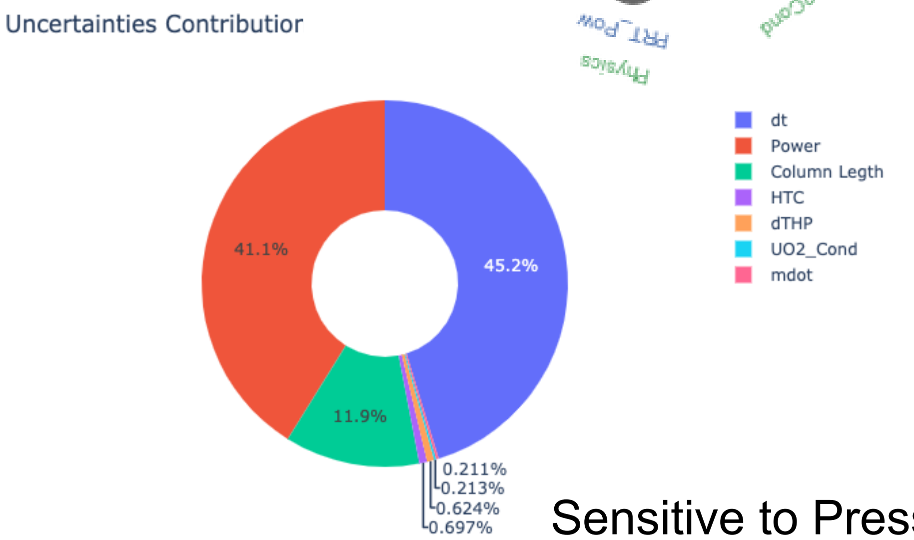
Safety and Hazards (Maximum Pressure)



- **Original model** (conservative)
  - Boiling / superheating occurs over the full length of the fuel

- Uncertain parameters

[redacted]

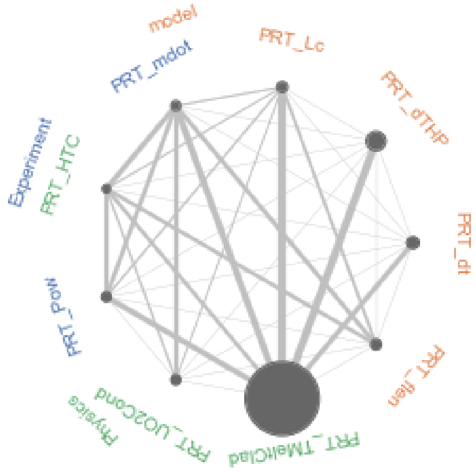


Sensitive to Pressure Model assumptions

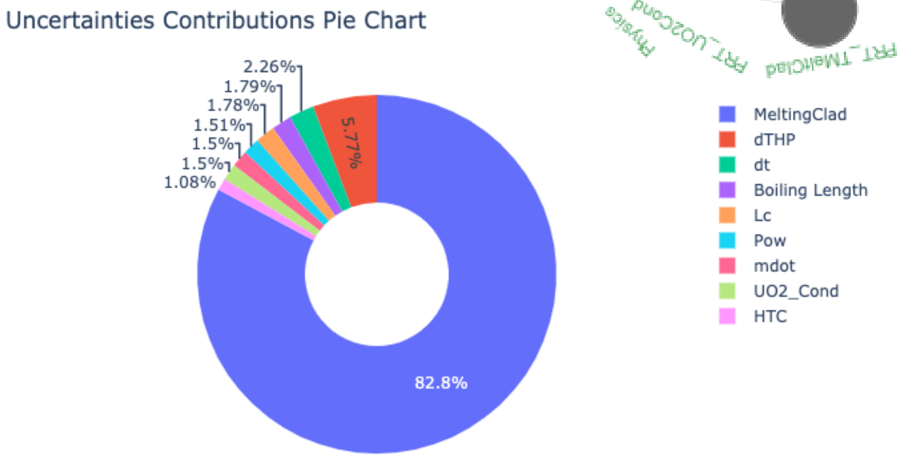
- Mean max pressure **12.9 MPa**, 95^{th} 15.9 Mpa, stdev 1.7 MPa (**13.2%**)
- Refine model assumptions to reduce uncertainty

Safety and Hazards (Maximum Pressure)

- **Informed refined model** (best estimate)
  - Boiling / superheating occurs only for the length of the fuel where $T_f > T_{sat}$.
  - Flashing at T_{melt} Clad outer
- Uncertain parameters



Parameter	Accuracy	PDF	Name in plots
Pressure pulse with	0.010 - 0.014 s	Uniform	PRT_dt
Time from onset of pulse to max power	0.15 - 0.19 s	Uniform	PRT_dTHP
Coolant column length	±10%	Normal	PRT_Lc
Boiling length of fuel	*□10%*	*Normal*	*PRT_flen*
Mass flow rate	±5%	Normal	PRT_mdot
Heat transfer coefficient	±25%	Normal	PRT_HTC
Power	±10%	Normal	PRT_Pow
Fuel conductivity	±7.5%	Normal	PRT_UO2Cond
Cladding melting temperature	*□50 K*	*Uniform*	*PRT_TMeltClad*



- Mean max pressure **4.9 MPa**, 95th 5.4 Mpa, stdev 0.4 Mpa (**8.1%**)

  Informed refinement of model reduced uncertainty

Safety and Hazards (Maximum Pressure - conclusions)

- Maximum pressure for sodium loop
  - The **Mean maximum pressure** for the Sodium loop is **4.9MPa**, with a **stdev of 0.41 Mpa**
  - **Conservative historic** SAS calculations and other literature show max **10MPa**
  - Historic data for the LO-7 **experiment** indicates a pressure peak of **3.77MPa**
  - For this analysis, Mark 3 and Concept 4 are identical

- SA/UQ
  - The informed **'best estimate' reduces uncertainty** in the predicted pressure
  - **Pressure model** substantially **refined** and debugged **through iterations with SA/UQ**. (Not all iterations shown here)

Thanks for attending
Questions?


INL
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