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NUCLEAR ENERGY AGENCY

OECD NEA NSC/WPRS/EGMUP

Benchmark on Artificial Intelligence and Machine Learning for Scientific Computing in Nuclear Engineering

Critical Heat Flux (CHF) Benchmark Exercise - Phase I Results

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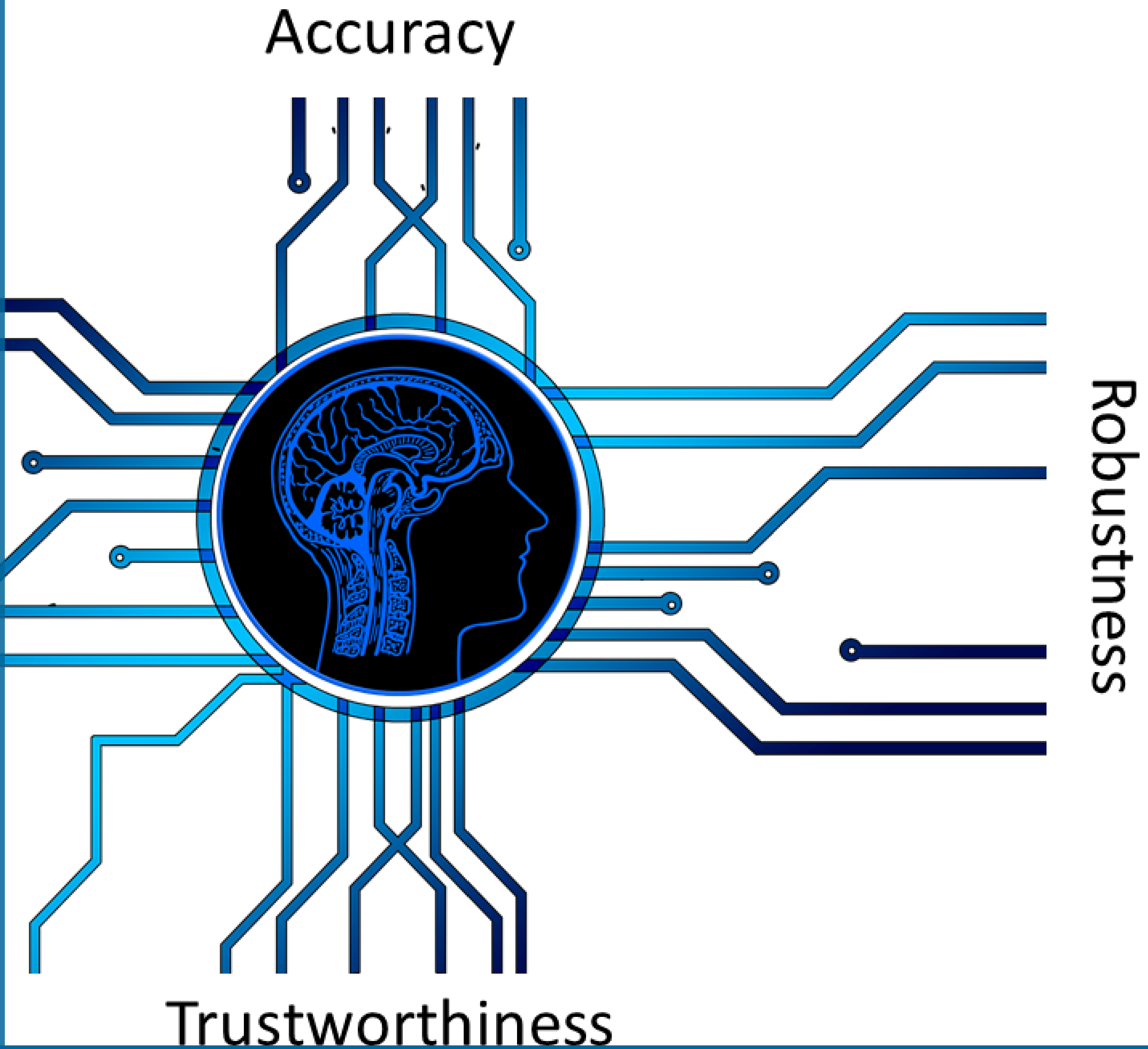
NEA Secretariat: O. Buss

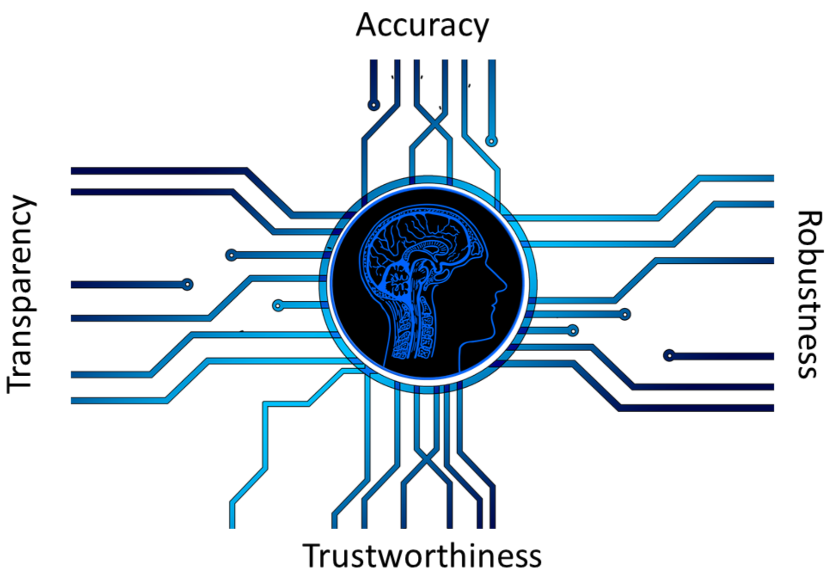


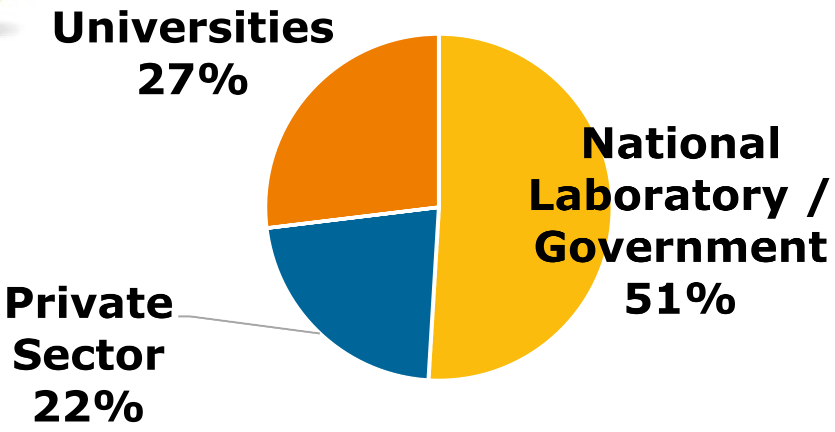
OECD NEA Task Force on AI&ML for Scientific Computing in Nuclear Engineering

Task Force Coordinators: X. Wu and G. Delipei, North Carolina State University (NCSU)

- **Targets:**
  - Build communities of practice to exchange know-how on AI and ML applications
  - Support the development and performance assessment of ML methods
  - Leverage the insights gained from the benchmarks to distill lessons learned and to **provide guidelines for future AI & ML applications** in scientific computing in nuclear engineering.
- **Developed first international AI/ML benchmark for Reactor Core Simulations: Critical Heat Flux (CHF) AI&ML Benchmark**
  - Leverage the NRC CHF database to train data-driven ML models ➔ Test improvement of CHF predictions
    - 47 submitted solutions from 30 institutions, Blind tests for interpolation and extrapolation performance
- **Future:** Benchmarks on **interpretation, classification, and prediction of time series data from research reactors**

NEW **November 2025: Start of benchmark based on PUR-1 data**

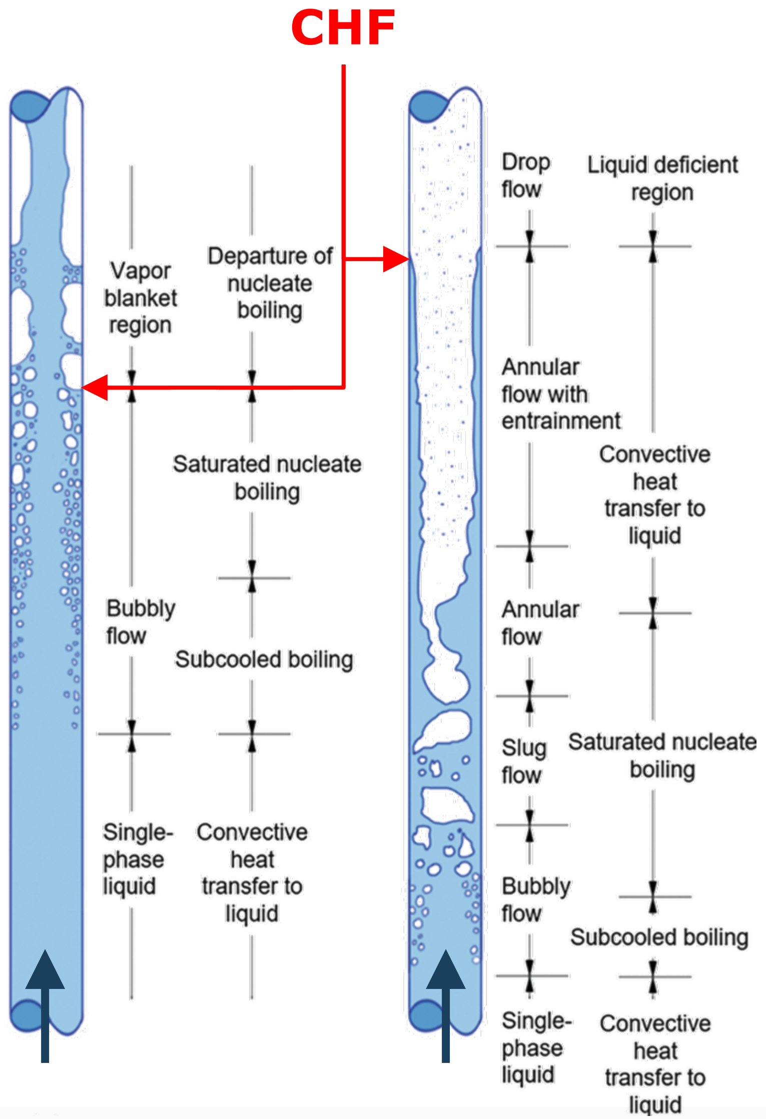




http://oe.cd/wprs-ai

Critical Heat Flux (CHF) in Convective Flow Boiling

- CHF defines a critical wall heat transfer transition
- Beyond CHF a significant increase in wall temperature is expected:
  - Accelerating wall oxidation
  - Potentially fuel rod failure
- Key safety and design criterion in nuclear reactor operation
  - Require costly test data
  - Predicted with (mostly) empirical models



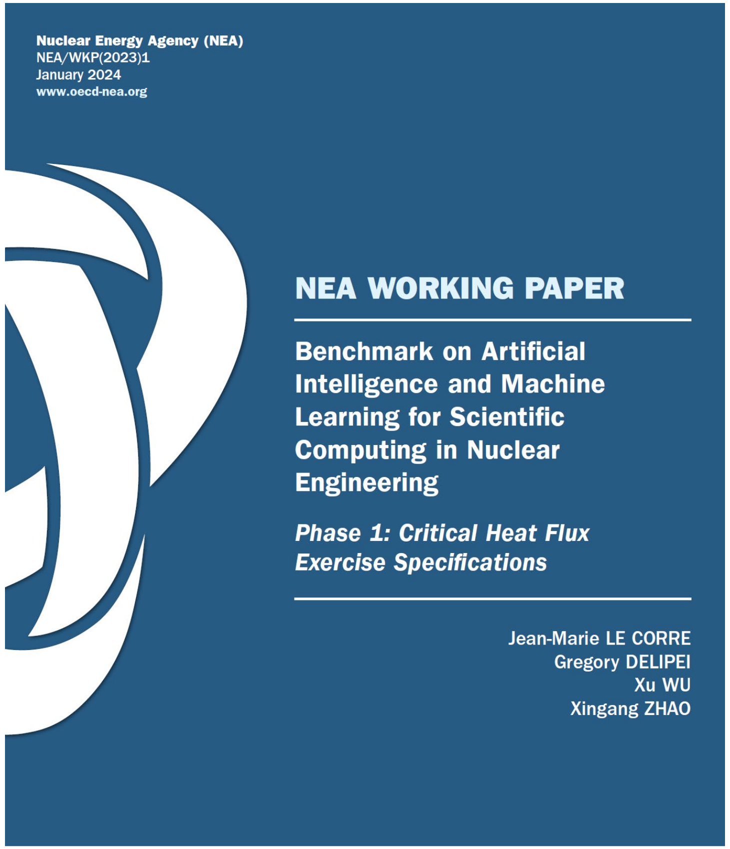
Liu, Y., Dinh, N. (2018). Flow Boiling in Tubes.
In: *Handbook of Thermal Science and Engineering*. Springer, Cham.

Critical Heat Flux Exercises

Coordinators: Dr. Jean-Marie Le Corre (Westinghouse Electric Sweden, benchmark lead), Dr. Xingang Zhao (UTK), Dr. Xu Wu and Dr. Gregory Delipei (NCSU)

- **Phase 1:**
  - **Regression & Feature Analysis**
  - Analyses
    - Statistical analysis and comparison to blind data
    - Extrapolation vs. interpolation performance
  - Schedule
    - Kickoff in November 2023
    - Submission dateline, August 2024
    - Preliminary results, November 2024

- **Phase 2:**
  - **Uncertainty Quantification**
  - Transfer learning: investigate if the ML models have predictive power for unseen geometries and conditions
  - Fuel bundle benchmark
  - To be started in 2025


Nuclear Energy Agency (NEA)
NEA/WKP(2023)1
January 2024
www.oecd-nea.org

NEA WORKING PAPER

Benchmark on Artificial Intelligence and Machine Learning for Scientific Computing in Nuclear Engineering

Phase 1: Critical Heat Flux Exercise Specifications

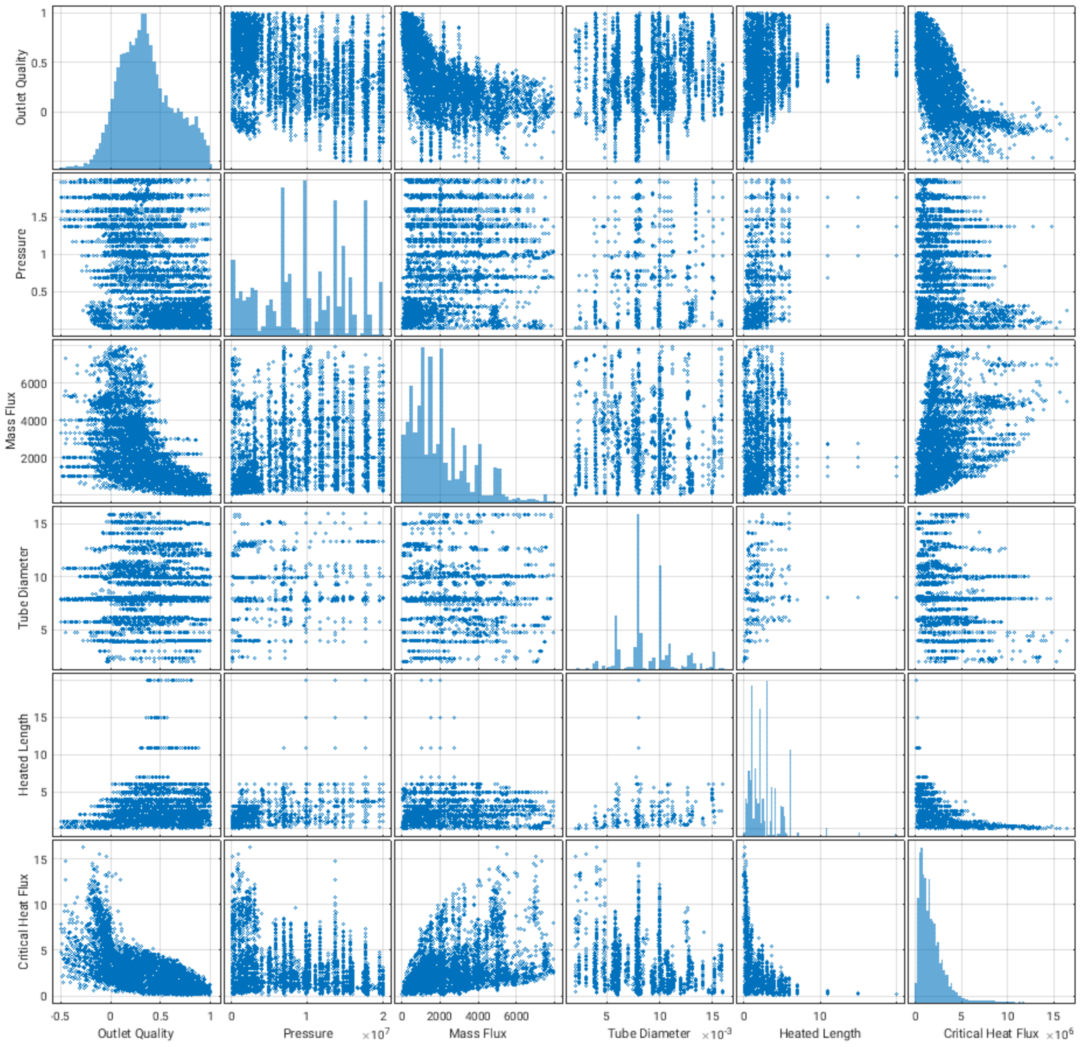
Jean-Marie LE CORRE
Gregory DELIPEI
Xu WU
Xingang ZHAO

Public Database – Overview

- Based on 2006 CHF lookup table data made available by US NRC
  https://www.nrc.gov/reading-rm/doc-collections/nuregs/knowledge/km0011/index.html

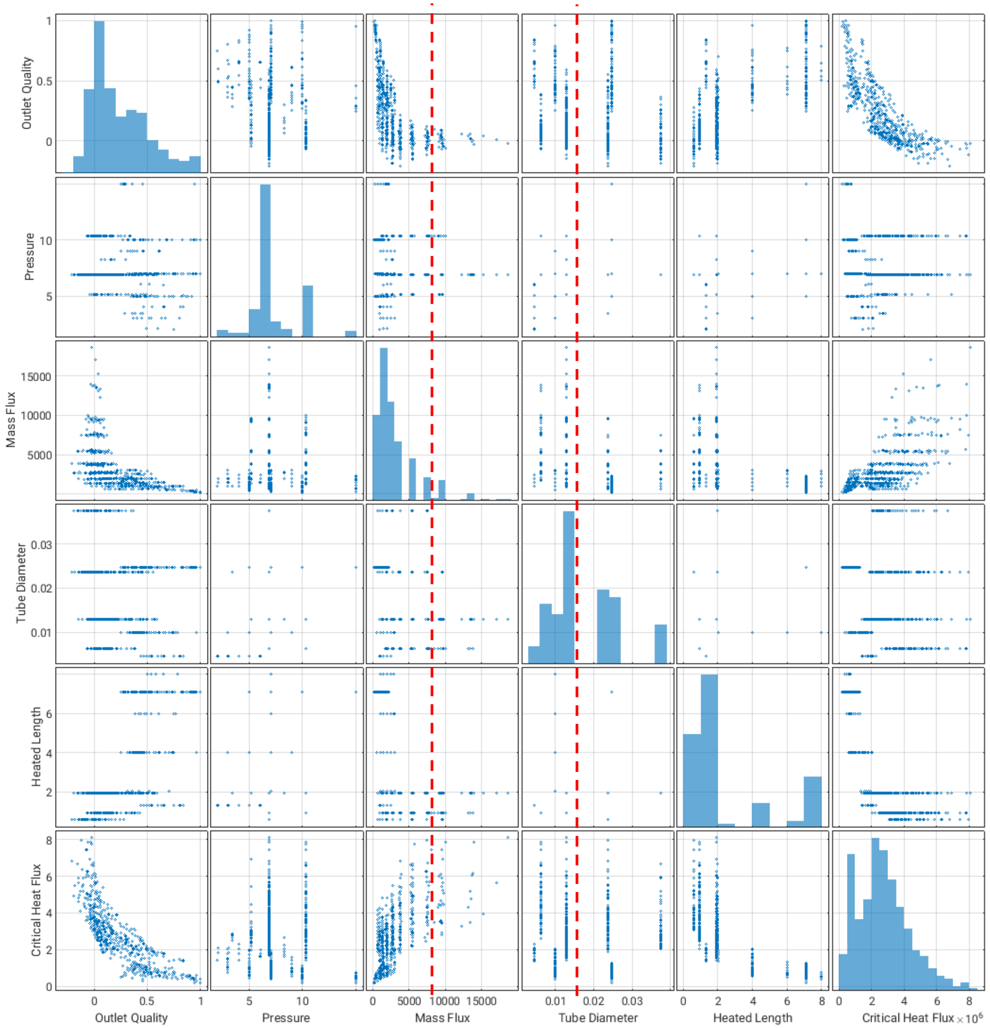
- Total of 24579 CHF data points
  - 59 sources, collected over 60 years
  - Vertical tubes, steady-state, uniformly heated
    → Outlet CHF only (0-D problem)

Variable	CHF [kW/m²]	P [kPa]	G [kg/m²/s]	X [-]	D [m]	L [m]
Min value	50	100	8.2	-0.497	0.002	0.05
Max value	16339.3	20000	7694	0.999	0.016	20



Blind Database – Overview

- 560 data points from 4 datasets
- About 250 data points outside NRC database range
  - D > 16 mm (219)
  - G > 8000 kg/m²/s (34)
- 1 interpolation and 2 extrapolation regions

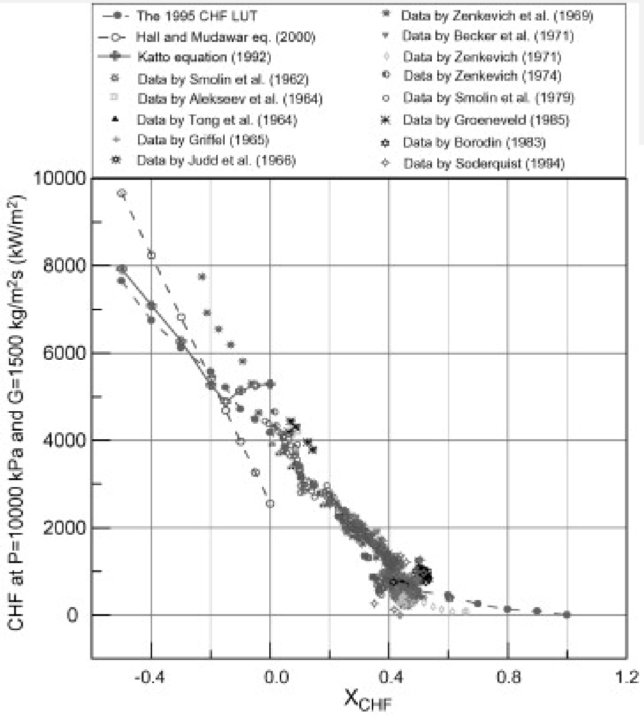


Variable	CHF [kW/m²]	*P* [kPa]	*G* [kg/m²/s]	*X* [-]	*D* [m]	*L* [m]
Min value	204	2040	179	-0.209	0.0046	0.61
Max value	8101.9	15000	18580	0.998	0.0375	8

Extrapolation

Slice Datasets – Overview

- Keep everything constant except one parameter



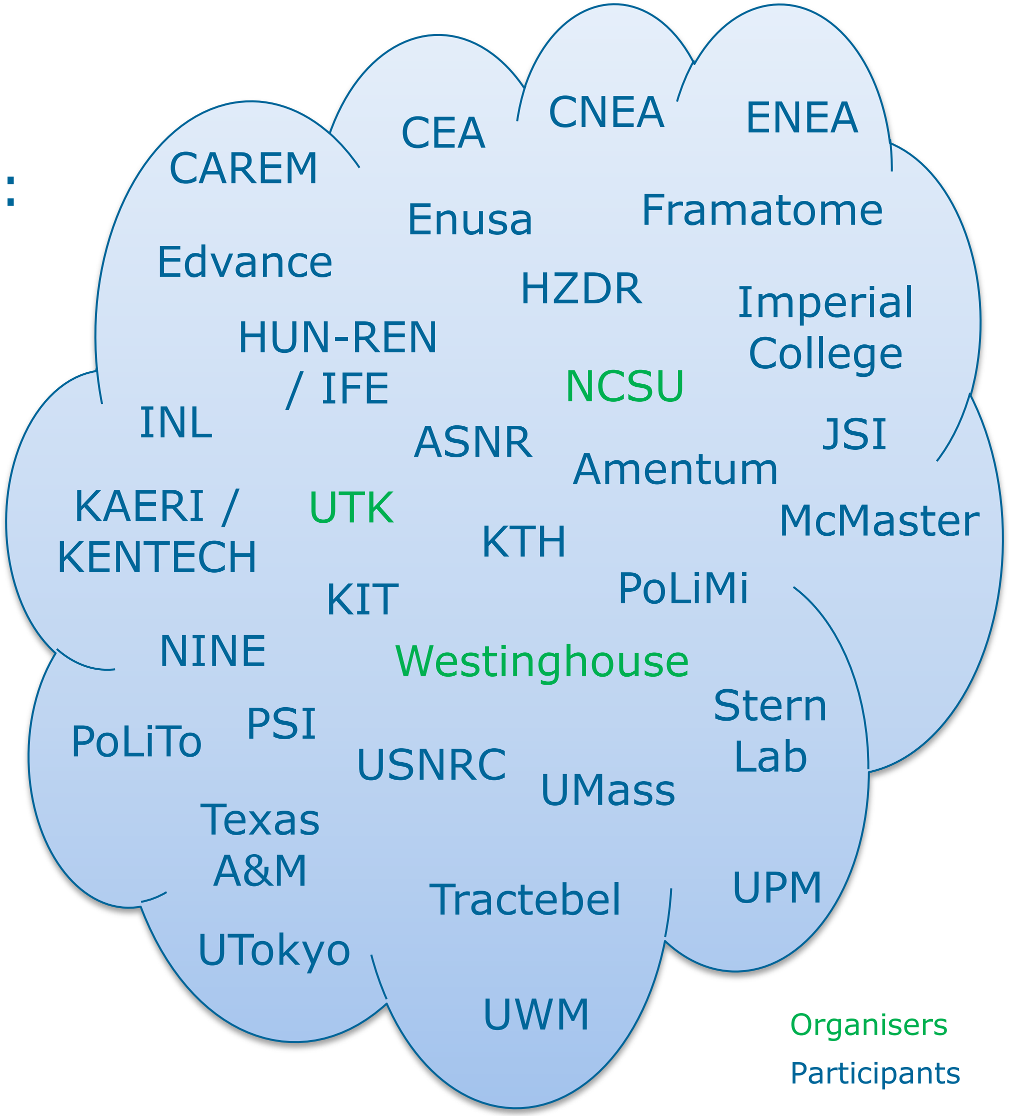
- Example of varying quality
- For each parameter (*D*, *L*, *P*, *G*, *X*)
  - Two regions are selected (10 datasets)
  - Arbitrary 15 equidistant values
- Allow to easily assess:
  - Correct physical behavior
  - Overfitting

Slice #	D [mm]	L [m]	P [kPa]	G [kg/m^2/s]	X [-]	Data file
1	**0 - 16**	6.000	14701	998.5	0.391	`Slice_01.csv`
2	**0 - 16**	6.000	9807	1003.3	0.529	`Slice_02.csv`
3	8.01	**0 - 20**	9806	1000.0	0.587	`Slice_03.csv`
4	8.11	**0 - 20**	2009	752.2	0.756	`Slice_04.csv`
5	8.00	0.998	**0 - 20000**	2006.0	0.140	`Slice_05.csv`
6	13.40	3.658	**0 - 20000**	20040.2	0.378	`Slice_06.csv`
7	8.00	1.570	12750	**0 - 8000**	0.144	`Slice_07.csv`
8	10.00	4.966	16000	**0 - 8000**	0.343	`Slice_08.csv`
9	8.14	1.943	9831	1519.5	**-0.5 - 1.0**	`Slice_09.csv`
10	8.00	0.997	17650	2002.7	**-0.5 - 1.0**	`Slice_10.csv`

Phase 1 Results Submission – Overview

- 48 models submitted from 31 institutions
- Various ML algorithms used, broadly categorized as:
  - Neural network based (30)
  - Tree based (17)
  - Gaussian Process (1)

  + 2 Reference models (from benchmark specifications)

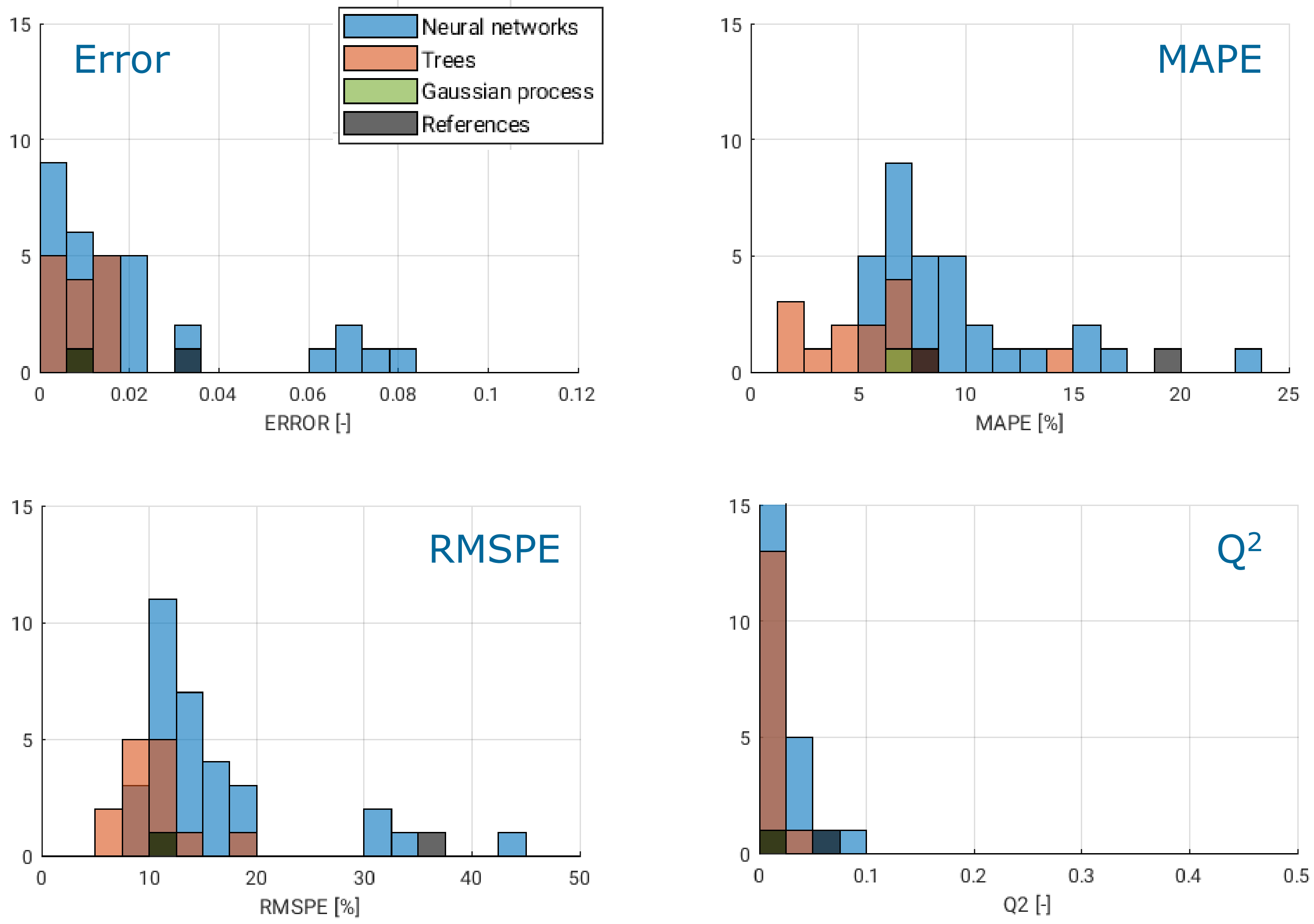


Dimensionality Analysis

- Optional task but highly recommended
- Not considered by most participants
- Most models: $CHF = f(D, P, G, X, L)$
- Limited use of non-dimensional parameters
- Limited use of data driven methods
- Did not provide conclusive results

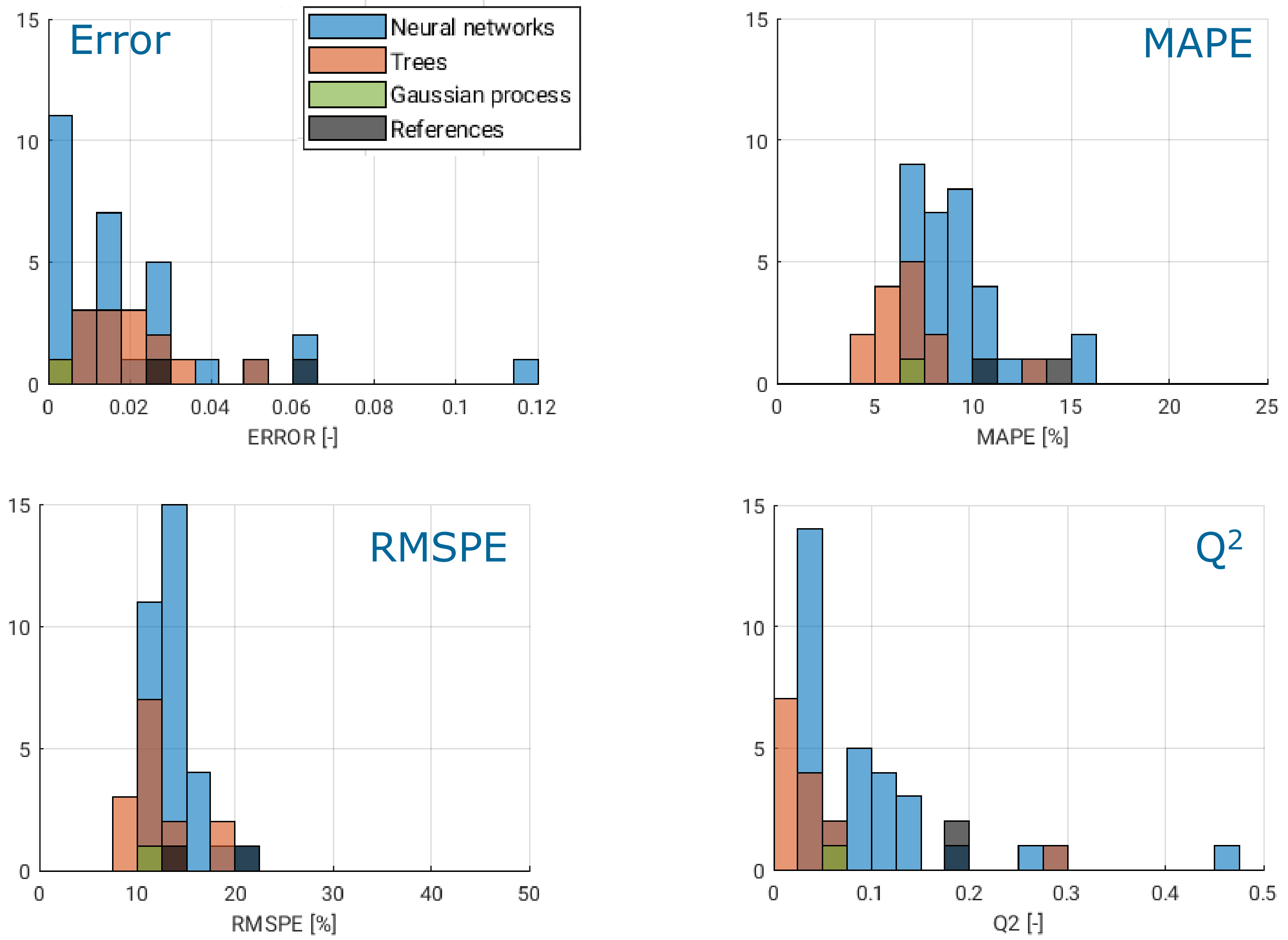
Public Database – Summary of Models Performance

- Color-coded P/M CHF performance comparison
- Up to 3 to 5 times lower metrics as compared to reference CHF LUT
- Tree-based models generally seems to perform better



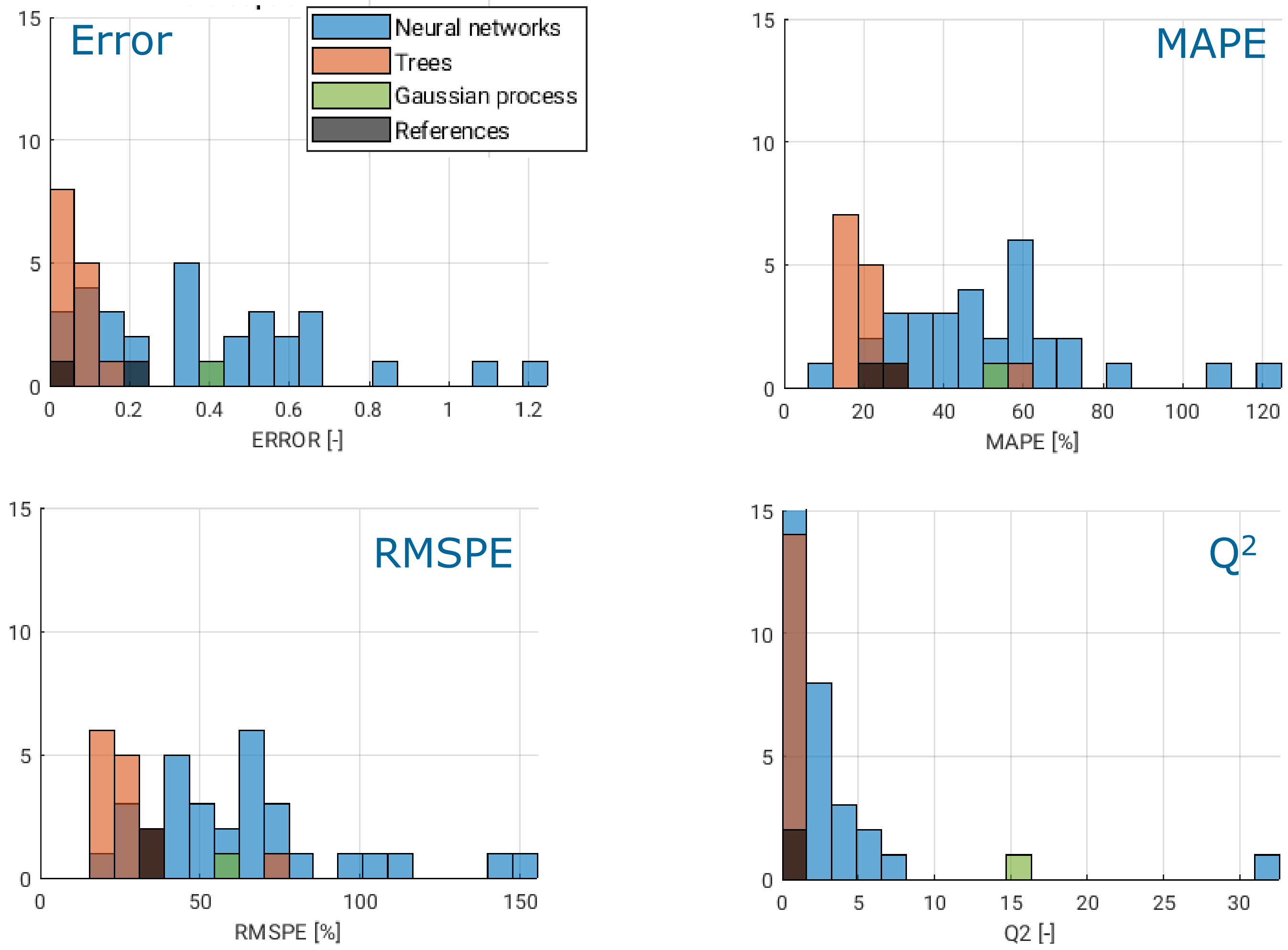
Blind Database – Summary of Models Performance (1)

- Interpolation region
  - Up to 2 to 3 times lower metrics as compared to LUT



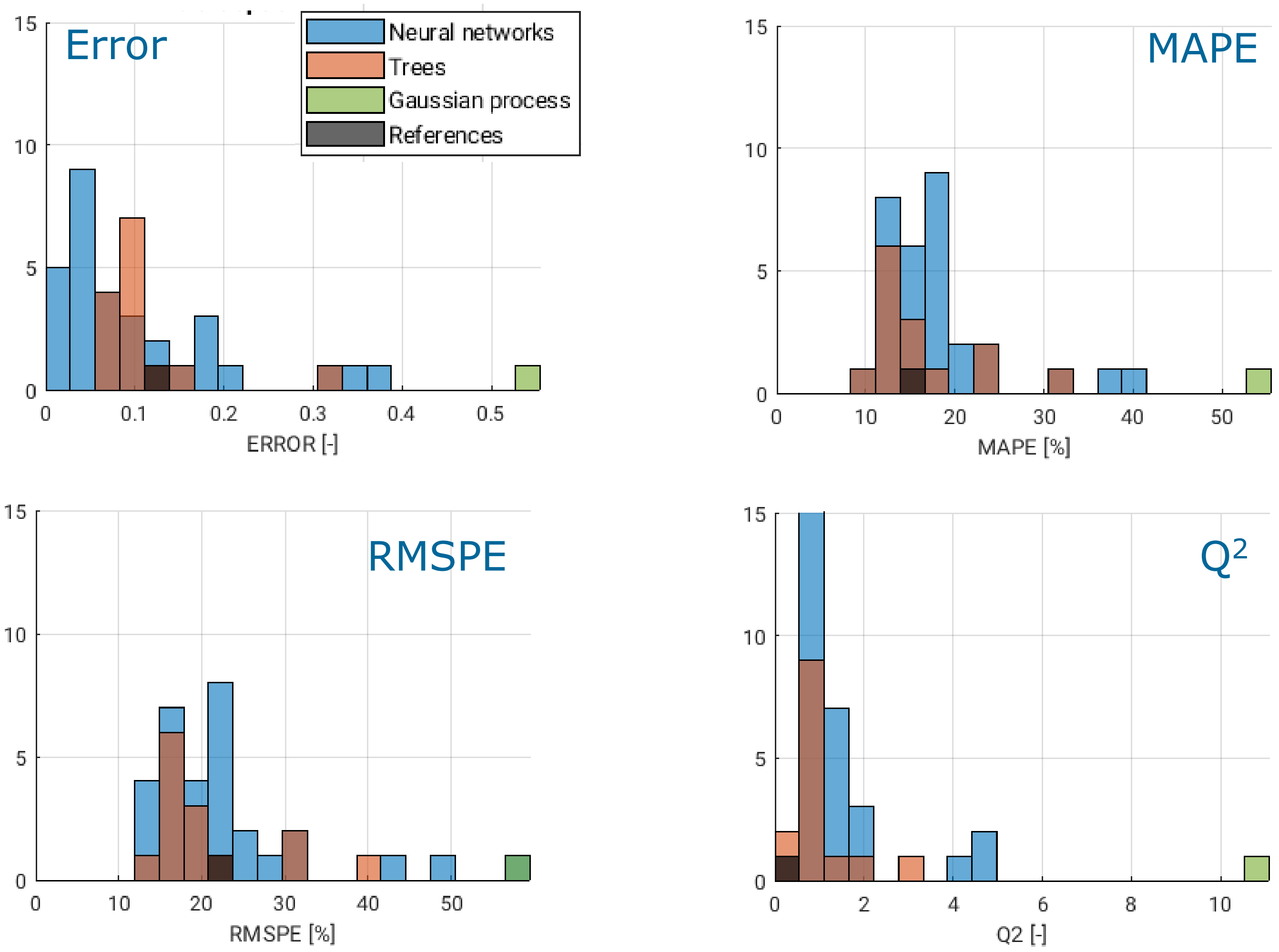
Blind Database – Summary of Models Performance (2)

- Extrapolation region #1
  - D > 16 mm
  - Up to 2 times lower metrics as compared to reference CHF LUT



Blind Database – Summary of Models Performance (3)

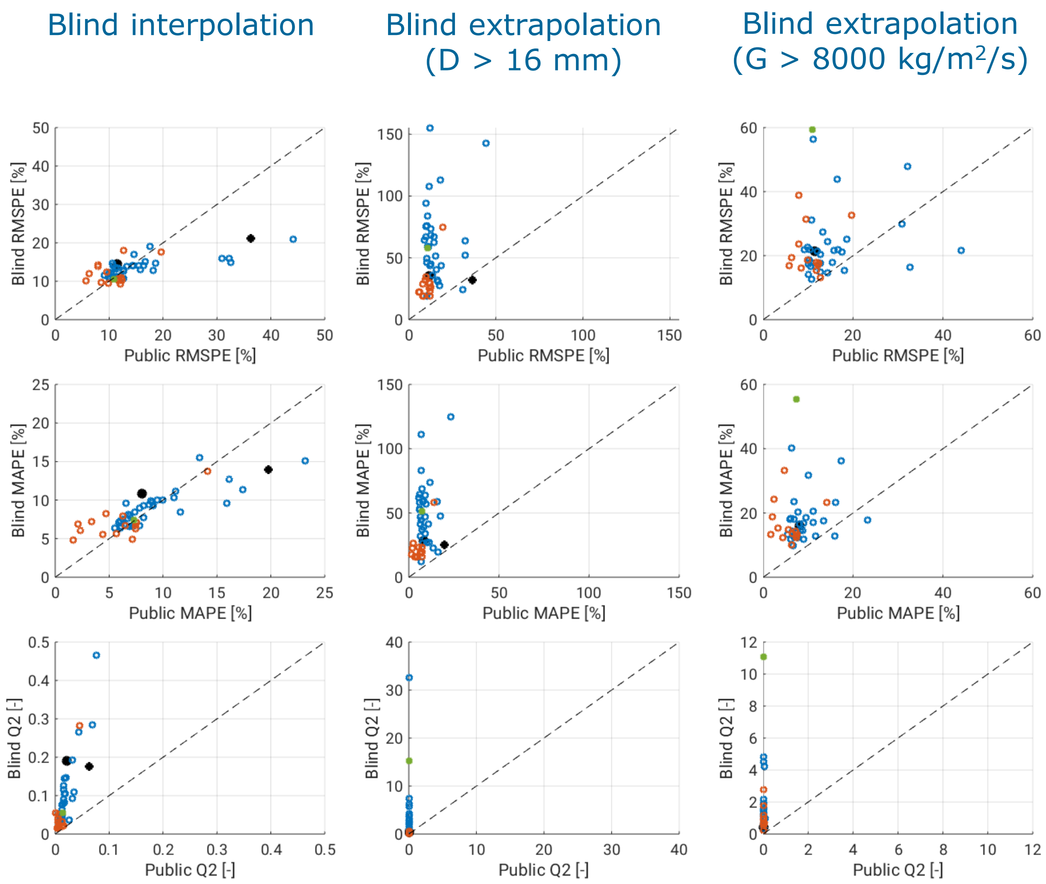
- Extrapolation region #2
  - G > 8000 kg/m²/s
  - No possible comparison with reference CHF LUT



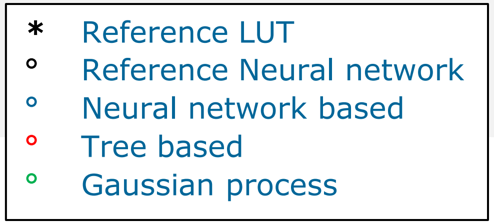
Statistical Metrics – Blind vs Public Databases

* Reference LUT
o Reference Neural network
o Neural network based
o Tree based
o Gaussian process

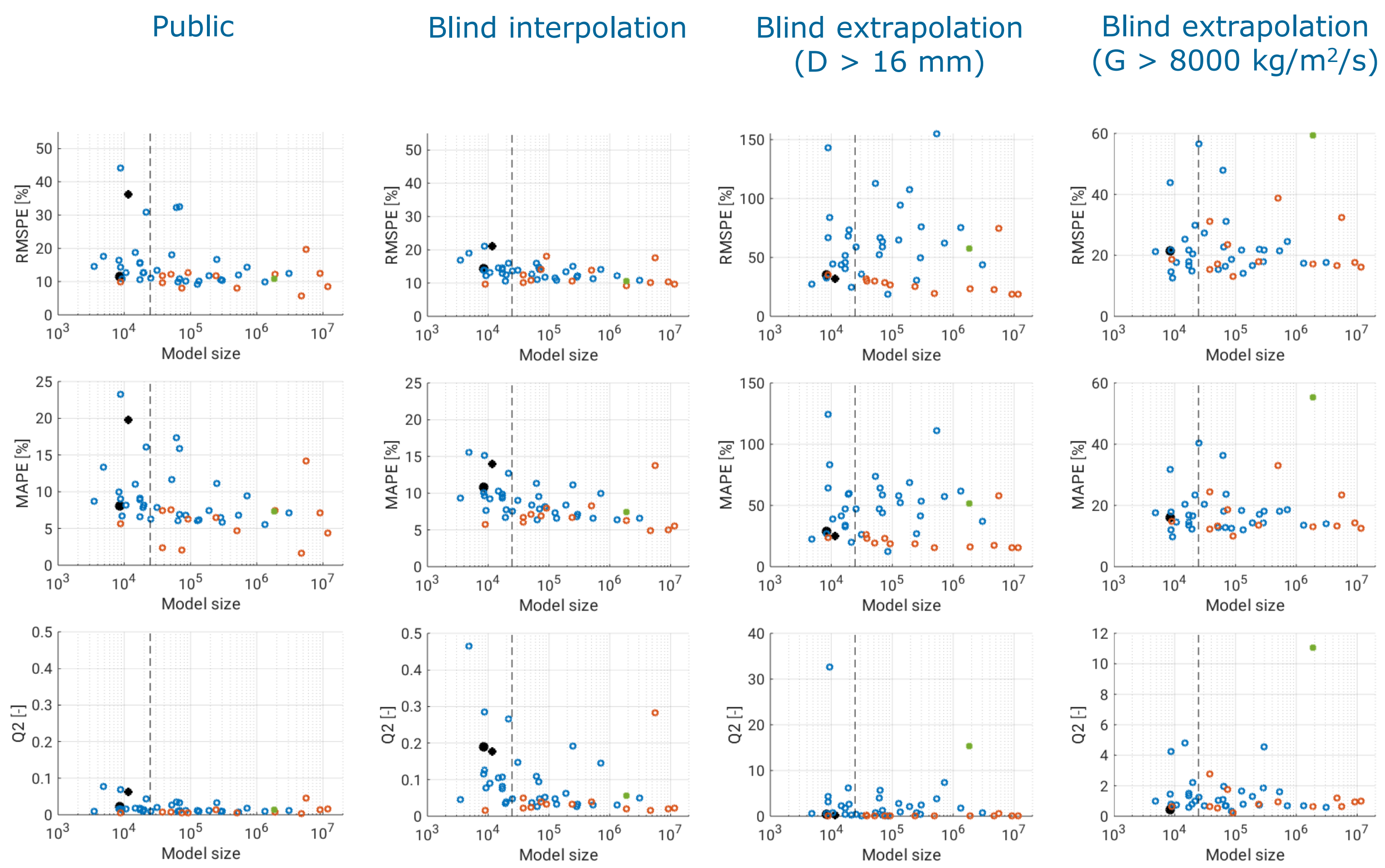
- ***How are the models performing when applied to the blind database, as compared to the public database?***
- Blind interpolation
  - Good behavior
  - General lower discrepancies with tree-based models
  - Improvements for models with large discrepancies
  - Degradation in Q^2 error (due to ≠ range of data)
- Extrapolation
  - Expected significant degradation
  - Higher degradation when extrapolating to large *D* (NN)
  - Tree-based models seems to extrapolate better



Statistical Metrics vs Model Size



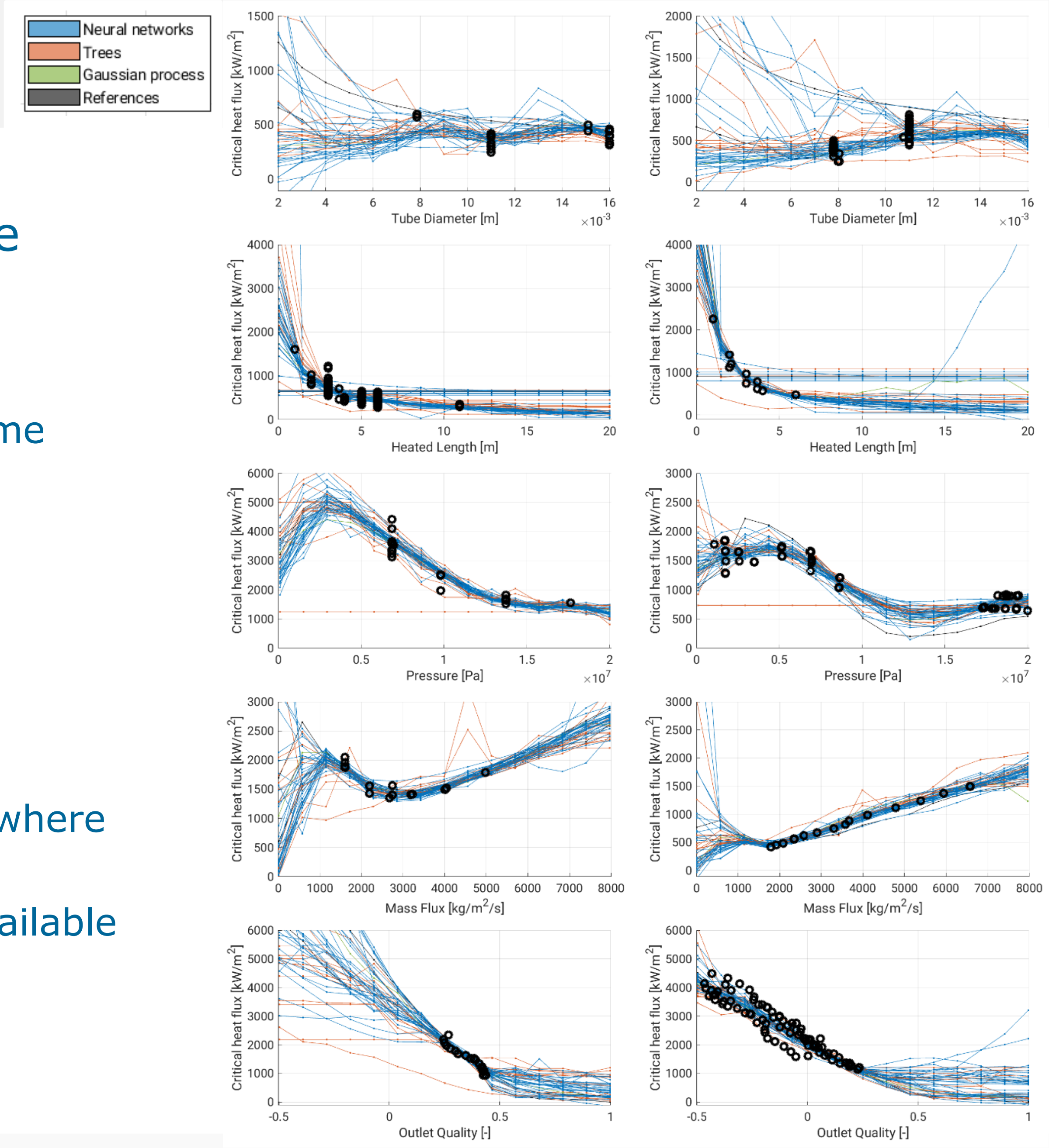
- ***How are the models performing with respect to their size?***
  - Note that most model sizes are larger than the training database (24579)…
  - … but regularization can help
- Public & blind interpolation
  - Performance increases with model size
  - However, smaller models with good performance may be of higher interest
- Blind extrapolation
  - Expected significant degradation
  - Tree-based models seems to extrapolate better, including for large size



Slice Datasets Results

- All submitted results plotted for each slice
  - Along with corresponding exprimental points (**o**)
  - Some models are independant of *L*
  - Strange constant results (with *L*, *P* and *G*) for some models → see Gitlab issue board

- Trends
  - No obvious over-fitting for most models
  - Larger variability wih *D*
  - Mostly consistent behavior with *G* and *X* (and *L*) where data is available
  - Large (epistemic) variability where data is not available (incl. within data range)



Initial Plans for Phase 2

Coordinators: Dr. Jean-Marie Le Corre (Westinghouse Electric Sweden, benchmark lead), Dr. Xingang Zhao (UTK), Dr. Xu Wu and Dr. Gregory Delipei (NCSU)

- **Phase 2:**
  - Benchmark specifications to be issued by end of 2025
  - New participants are welcome to join
  - Several CHF databases to be provided in specifications
    - Annulus
    - Tube with non-uniform axial power
    - Rod bundle (later)
    - Potentially: additional blind datasets
  - Three main tasks
    - Advanced uncertainty quantification
    - Transfer learning to more complex geometries
    - Model interpretability and explainability

Thank you for your attention

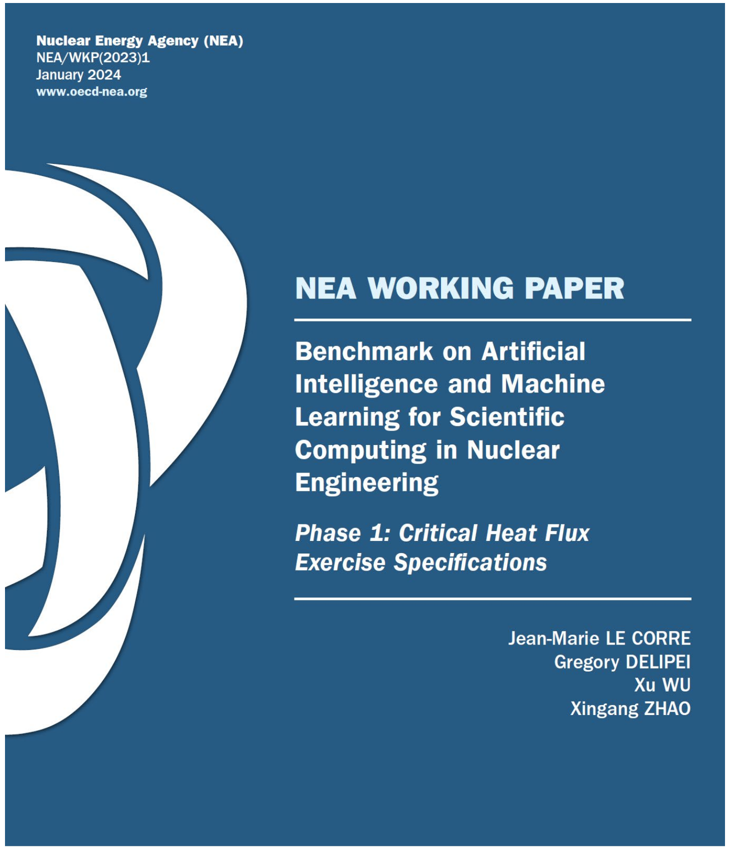
Please contact wprs@oecd-nea.org if you have any questions or comments regarding this presentation.

Backup slides

Critical Heat Flux Exercises (2)

Coordinators: Dr. Jean-Marie Le Corre (Westinghouse Electric Sweden, benchmark lead), Dr. Xingang Zhao (UTK), Dr. Xu Wu and Dr. Gregory Delipei (NCSU)

- **Phase 1:**
  - Benchmark specifications issued in January 2024
  - Three databases provided in specifications
    - Public database (24579 points)
    - Blind database (560 points)
    - Slice datasets (10*16 points)
  - Three main tasks
    - Dimensionality analysis
    - Selection and training of regression models
    - Blind and slice applications
  - Benchmark results documentation
    - WPRS benchmark meeting (July 2025)
    - NEA working paper (2025) – on-going
    - NURETH-21 paper & presentation (Sept. 2025)
    - Journal paper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NEA WORKING PAPER

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Phase 1: Critical Heat Flux Exercise Specifications

Jean-Marie LE CORRE
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List of Submitted Models

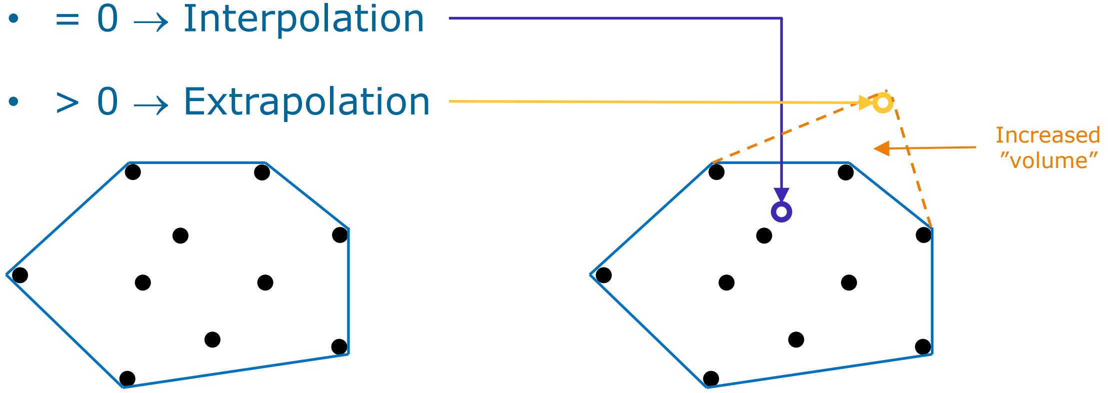
Reference models	(2)
Neural network based	(32)
Tree based	(15)
Gaussian Process	(1)

Geometrical parameters		**Saturated fluid properties**		
D	Diameter	k_l	Liquid thermal conductivity	
L	Length	Lo	Laplace length	$\left(\sigma/9.8\cdot(\rho_f-\rho_g)\right)^{0.5}$
S	Heated surface	σ	Surface tension	
		ρ_f	Liquid density	
Fluid parameters		ρ_g	Vapor density	
P	Pressure	μ_f	Liquid viscosity	
G	Mass flux	μ_g	Vapor viscosity	
X	Equilibrium outlet quality			
H_{out}	Outlet enthalpy	**Non-dimensional numbers**		
T_{in}	Inlet temperature	D^*	Diameter	$D/8$ mm
CHF	Critical Heat Flux	Re_f	Liquid Reynolds number	$G\cdot D/\mu_f$
		Re_g	Vapor Reynolds number	$G\cdot D/\mu_g$
Acronyms		We	Weber number	$G^2\cdot D/(\sigma\cdot\rho_f)$
MAPE	Mean Absolute Percentage Error	N_{rho}	Density ratio	ρ_f/ρ_g
PCs	Principal components	Ah	Ahmad number	$We^{1.333}\cdot Re_f^{-0.133}\cdot Re_g^{-0.2}$
RMSPE	Root Mean Square Percentage Error	Bo	Boiling number	$CHF/(G\cdot h_{fg})$
STD	Standard deviation			

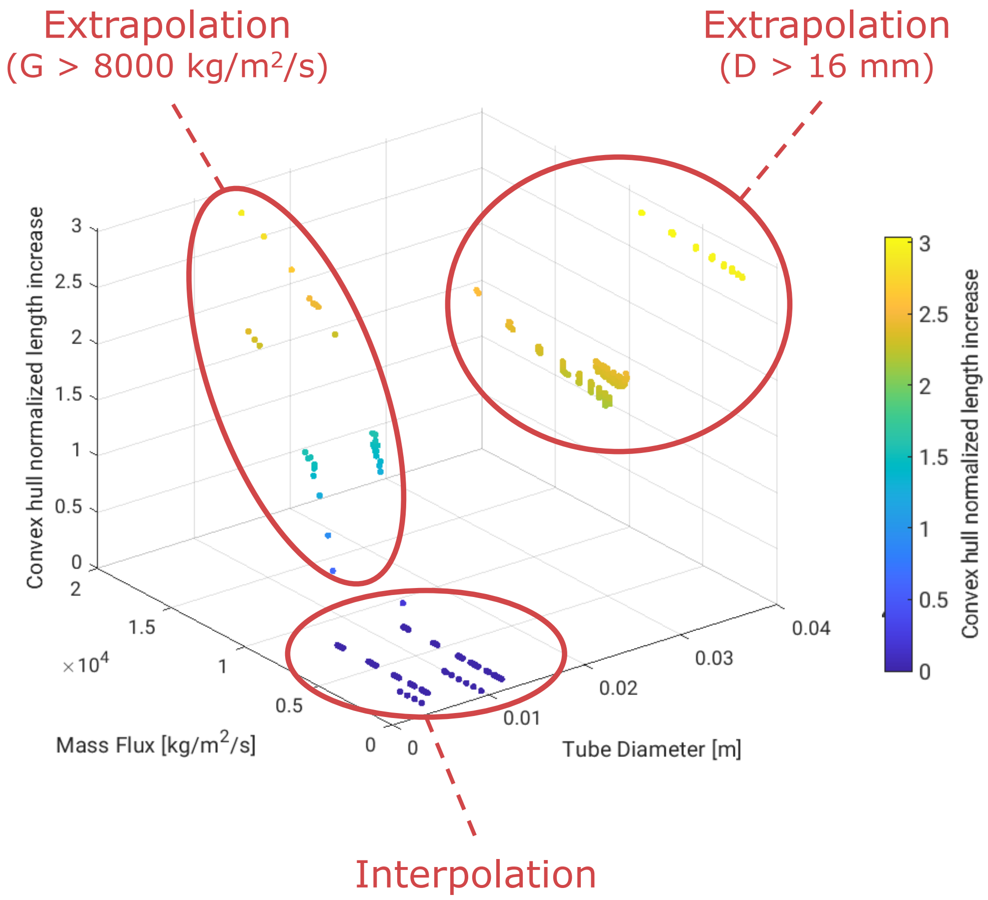
		ID	Algorithm	Inputs	Output
CHF look up table	1	LUT	Look up table	D, P, G, X	CHF
Westinghouse / Uppsala University	2	NN	Neural network	D, L, P, G, X	CHF
CAREM-CNEA	3	CAREM	Neural network	D, L, P, G, X	CHF
CEA Saclay	4	CEA	Residual neural network	D, L, P, G, X	CHF
Comisión Nacional de Energía Atómica	5	CNEA1	Neural network *2	D^*, G, X, Re_f, We, k_l, N_{rho}	CHF
	6	CNEA2	XGBoost	D^*, G, X, Re_f, We, k_l, Lo	$CHF/\sigma^{0.5}$
Edvance	7	EDVANCE	Neural network	D, P, G, X, H_{out}, S	CHF
ENEA	8	ENEA	Neural network	D, L, P, G, X	CHF
Enusa	9	ENUSA	Neural network	D, L, P, G, X	CHF
Framatome	10	FRAMATOME1	Bayesian additive regression trees	6 PCs	log(CHF)
	11	FRAMATOME2	Neural network	6 PCs	CHF
	12	FRAMATOME3	Neural network	6 PCs	CHF
HUN-REN Center for Energy Research / Institute for Energy Technology (IFE)	13	HUNREN&IFE1	Neural network	D, L, P, G, X	CHF
	14	HUNREN&IFE2	XGBoost	D, L, P, G, X	CHF
Helmholtz-Zentrum Dresden-Rossendorf	15	HZDR1	XGBoost	D, L, P, G, Tin	CHF
	16	HZDR2	XGBoost	D, L, P, G, X	CHF
Imperial College London	17	IMPERIAL	Deep gaussian process	D, L, P, G, X	CHF
Idaho National Laboratory	18	INL1	Random forest (1 tree)	D, L, P, G, X	CHF
	19	INL2	Random forest (2 trees)	D, L, P, G, X	CHF
	20	INL3	Kolmogorov–Arnold network	D, L, P, G, X	CHF
Autorité de sûreté nucléaire et de radioprotection	21	ASNR	XGBoost	D, L, P, G, X	CHF
Amentum	22	AMENTUM1	Neural network	D, L, P, G, X	CHF
	23	AMENTUM2	Neural network	D, L, P, G, X	CHF
	24	AMENTUM3	Neural network	D, L, P, G, X	CHF
Jozef Stefan Institute	25	JSI1	CatBoost	D, L, P, G, X	CHF
	26	JSI2	Gradient boosting	D, L, P, G, X	CHF
	27	JSI3	XGBoost	D, L, P, G, X	CHF
Korea Atomic Energy Research Institute / Korea Institute of Energy Technology	28	KAERI1	Dense neural network	D, L, P, G, X	CHF
	29	KAERI2	XGBoost	L/D, ρ_f/ρ_g, $We^{0.5}$, X	Bo
Karlsruhe Institute of Technology	30	KIT	Neural network	$\ln(\rho_f/\rho_g)$, ln(L/D), X, ln(Ah)	ln(Bo)
Royal Insitute of Technology	31	KTH1	Ennsemble neural network	D, L, P, G, X	CHF
	32	KTH2	Ensemble physics-informed NN	D, L, P, G, X	CHF
McMaster University	33	MCMASTER1	Neural network (standard)	D, P, G, X	CHF
	34	MCMASTER2	Neural network (normalized)	D, P, G, X	CHF
North Carolina State University	35	NCSU	Extremely randomized forest	D, L, P, G, X	CHF
NINE	36	NINE1	CatBoost	D, L/D, P, G, X	CHF
	37	NINE2	Neural network	D, L/D, P, G, X	CHF
US Nuclear Regulatory Commission	38	NRC	Neural network	D, L, P, G, X	CHF
Politecnico di Milano	39	POLIMI1	Convolutional neural network	D, L, P, G, X	CHF
	40	POLIMI2	Convolutional neural network	D, L, P, G, X	CHF
Politecnico di Torino	41	POLITO	Neural network ensemble	D, L, P, G, X	CHF
Paul Scherrer Institut	42	PSI	Neural network	D, L, L/D, P, G, X	CHF
Stern Laboratories	43	STERN	Neural network	D, L, P, G, X	CHF
Texas A&M University	44	TAMU	Neural network	D, L, P, G, X	CHF
Tractebel	45	TRACTEBEL1	Neural network	D, L, P, G, X	CHF
	46	TRACTEBEL2	Residual neural network	D, L, P, G, X	CHF
University of Massachusetts Lowell	47	UMASS	Bayesian neural network	D, L, P, G, X	CHF
Universidad Politecnica de Madrid	48	UPM	Random forest	D, L, P, G, X	CHF
The University of Tokyo	49	UTOKYO	Transformer	D, L, P, G, X	CHF
University of Wisconsin - Madison	50	UWM	Neural network	D, L, P, G, X	CHF

Blind Database – Interpolation vs Extrapolation Regions

- Convex hull approach
  - Smallest convex enveloppe enclosing database
  - Convex hull (5-D) ”volume” increase for each blind data
    - = 0 → Interpolation
    - > 0 → Extrapolation



- Applied to entire blind database
  - Identify ”true” interpolated points
  - Quantify level of extrapolation for remaining points ($L = V^{\frac{1}{5}}$)



Dimensionality Analysis (1)

- Optional task but highly recommended
- Not considered by most participants, except (to some extent):
  - CNEA
  - FRAMATOME
  - KIT
  - EDVANCE
  - KAERI
- Most models: $CHF = f(D, P, G, X, L)$
- Use of non-dimensional parameters (CNEA, KAERI, KIT) + *L*/*D* (NINE, PSI)
  - CNEA: trial & error ("limited success")
  - KAERI & KIT: fluid-to-fluid scaling considerations
- Not data driven, except
  - EDVANCE: Feature ranking & engineering
  - FRAMATOME: PCA

Dimensionality Analysis (2)

- Use of logarithms (KIT)
  - Provide more normal distribution of parameters
  - Improve model performance
- Heated length (*L*)
  - Clear correlation (but no causation!) in database
  - Used by all models, except CNEA & MCMASTER (but not replaced by other ”non-local” parameter)
  - Attempt to address this issue with PINN (KTH)

Model Optimization and Training

- Hyperparameter optimization
- Training strategies
- Documented in upcoming CHF bechmark Phase I results report

Conclusions for Phase 1

- ML/AI CHF benchmark has **48** submissions from **31** institutions (+ 2 reference models)
- Post-process of phase 1 on-going
- Preliminary conclusions
    - Up to factor 2 or 3 reduction in statistical metrics (as compared to LUT)
    - Limited success from dimensionality analysis
    - Tree-based algorithms seems to perform better
    - No obvious over-fitting
    - Good blind performance within interpolation range
    - Some models can reasonably extrapolate

Publications related to Phase 1

- List of benchmark related publications
  - Please inform benchmark coordinators about publications (wprs@oecd-nea.org)
  - https://git.oecd-nea.org/science/wprs/egmup-task-force-on-ai-and-machine-learning/phase1-chf-exercises/-/blob/main/publications/README.md
- NURETH-21 special sessions
  - 1 summary paper submitted by organisers
  - Many others from participants + related activivites based on US NRC database
- NEA working paper (2025)
  - Document generic results
  - All detailed results (per model) in appendices
- Journal publications
  - 1 summary paper in a selected journal
  - Other individual publications

Initial Plans for Phase 2 (2)

- Advanced uncertainty quantification
  - Field still under development
  - Example for deep NN: dropout-based, ensemble-based and Bayesian NN-based
  - Associate specific epistemic & aleatory uncertainties to each prediction
  - Demonstration using unseen CHF data
- Transfer learning to other geometries
  - Transfer of knowledge from one database to the other to improve performance
  - Example: Tube database → Annulus database → Rod bundle database
- Model interpretability vs explainability
  - Interpretability: Better understand how predictions are generated – *Model transparency*
  - Explainability: Discover meaning between inputs and outputs – *Understand behavior*

Initial Plans for Phase 2 (3)

- Fuel bundle benchmark
  - BFBT, PSBT and EPRI (11077 data points) CHF databases
  - Preliminary step: Generate local TH parameters (on-going in collaboration with UWM)
  - Combine all previously acquired knowledge from Phases 1 and 2
  - Assessment for reactor safety analysis (?)