EUROfusion

ENR-08 Theory

Development of machine learning methods and integration of surrogate model predictor schemes for plasma-exhaust and PWI in fusion

2021 Report, S. Wiesen

Nov 26th 2021

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Content

- Overview
- HPC resources
- ACH support
- Reporting / Dissemination of work
- Summaries of Subprojects SP1-4

Rationale of ENR

Enable and facilitate optimized and improved modelling that allows a more flexible integration of physics models in the light of extrapolations towards future fusion devices.

Demonstrate the applicability of Machine-Learning (ML) and Artificial Neural Network (ANN) methods in fusion with a special focus on plasma-exhaust (scrape-off layer and pedestal region) and PWI.

This ENR project elaborates on the conceptual basis for an improved model predictor scheme involving new methods and computational technologies based on **ML/ANN for exploitation in fusion device design studies.**

Include **uncertainty quantification (UQ)** to enable an efficient selection of the numerical data, i.e. its cardinality, on which the training must be based and **how reduced models are efficiently and quantifiably calibrated**

This ER project aims at expanding and disseminating new expertise & knowledge in the field of ML/ANN into the fusion community.

Manning

Name	RU	kEUR/y @50%	Year 1	Year 2	Year 3	Total kEUR	Role inside ER Project	background
Wiesen, Sven	FZJ		6	6	6		PI, Senior Scientist	Comp. Plasmaphysics
Dasbach, Stefan (PhD, SW)	FZJ		12	12	8		Physicist, ML/Data Scientist	Comp. Neuroscience
Reiser, Dirk	FZJ		3	3	3		Senior Scientist	Comp. Plasma Physics
Brenzke, Martin (PostDoc)	FZJ		4	6	6		Physicist, ML/Data Scientist	ML, Plasma Physics
TOTAL FZJ		44,125	91,93	99,28	84,57	275,78		
Menkovski, Vlado	DIFFER/TuE		2	2	2		Senior Scientist	ML Medical,Physics,Biology
Poels, Yoeri (PhD, VM)	DIFFER/TuE		10	10	10		Machine Learning	ML scientist
v.d. Plassche, Karel L. (PostDoc)	DIFFER		2	2	2		Integrated Modeling / ML	Integr. Modelling Plasma
Ho, Aaron (PostDoc)	DIFFER/TuE		2	2	2		Physicist, ML/Data Scientist	Data Science
Westerhof, Egbert	DIFFER		2	2	2		Senior Scientist	Comp. Plasmaphysics
TOTAL DIFFER		55,5	83,25	83,25	83,25	249,75		
Gillgren, Andreas (PhD, PS)	VR/Chalmers		6	6	6		Physicist , ML/Data Scientist	ML Plasmaphysics
TOTAL VR		49,125	24,56	24,56	24,56	73,69		
Jaervinen, Aaro	VTT, Aalto		6	3	6		Senior Scientist	Comp. Plasma Physics, ACH
Groth, Mathias	VTT, Aalto		6	0	0		Senior Scientist	Comp. Plasma Physics
Kit, Adam (Master/PhD, MG, AJ)	VTT, Helsinki		6	12	12		Physicist, Data Science	Data Science
TOTAL VTT		46,875	70,31	58,59	70,31	199,22		
Total all RU kEUR			270,05	265,69	262,70	798,44		

Supervisors of PhDs: [SW] S. Wiesen (FZJ), [VM] V: Menkovski (TU Eindhoven), [PS] P. Strand (Chalmers U/VR), [MG] M. Groth (Aalto U/VTT)

Sub-projects

SP1 Development of a surrogate model for power & particle exhaust
(S. Dasbach)

SP2 Development/improvement of ML/ANN methods for training based on experimental data for pedestal physics
(A. Jaervinen)

SP3 Model discovery for erosion yields through ML methods
(D. Reiser)

SP4 Towards time-dependent surrogate models for exhaust
(E. Westerhof)

Start of ENR: May 1st, 2021
Status End of 2021: all SPs on track, no modifciations in 2022 required

HPC resources

Marconi cycle 6 call for March 2022 – February 2023

→ ENR-08 specific HPC project proposal submitted: ***EXML***

21.000 node-hs on conventional (A3) nodes
for data generation, parallelised (MPI & OpenMP)

150.000 node-hs on GPU based (C1) nodes
mainly PyTorch/TensorFlow/CUDA

Data Storage & Access:

Ideally: ENR work and data storage on GitHUB, licensing issues,
(relevant when disseminating ENR results into the community)

Currently we use Sciebo Cloud for internal data exchange

Collaboration with ACH-05

- ENR-08 plans to collaborate with the ACH-05 that is focused on Data Management as well as aspects of AI & VVUQ

- ENR-08 generates large database of simulation data, as well as databases of experimental data preprocessed to be suitable for ML and ANN algorithms

- It is expected that the ACH-05 is very well suited to provide support in developing professional data management workflows for the ENR-08 work

- As the ENR-08 work has been initiated in 2021, it is now the time to plan discussions with the ACH-05 team to find the appropriate data management solutions

Reporting / Dissemination of work

- Regular Progress meetings with all ENR contrinbutors/SPs

  Progress #1 September 24th 2021

  Progress #2 December 3rd 2021

  Progress #3 Spring 2022 - with external attendees & interested parties
- SP regular meetings:

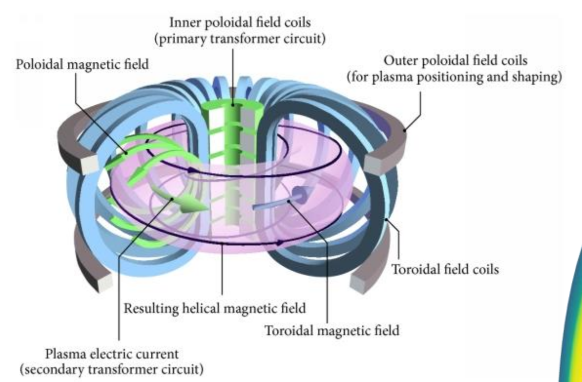
  SP1 weekly, SP2 biweekly, SP3 on site, SP4 monthly
- Communication through Slack (e.g. SP2)
- Wiki page – updated, annual report
- Publications:

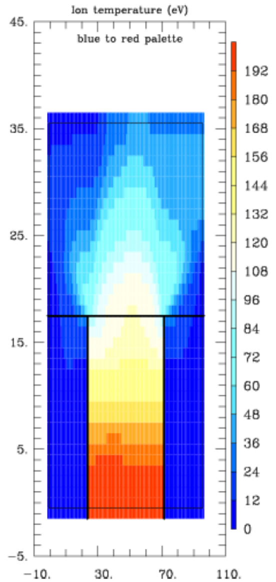
  PPCF, PSI2022 (2 contributions, NME), EPS2022(tbd)
- Theses: BSc’s, MSc’s, 4 PhDs

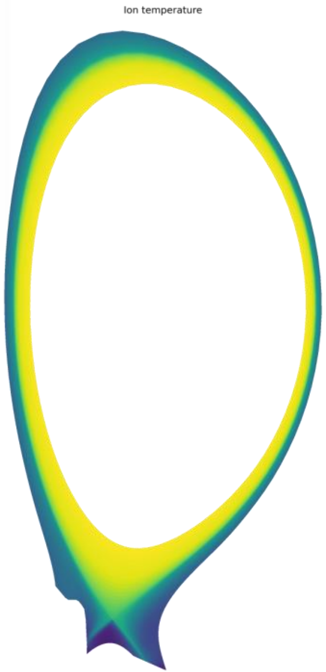
SP1 Development of a surrogate model for power & particle exhaust

SP1: Towards fast SOL models

- Simulation of the SOL is possible with SOLPS-ITER code
- Combine data from various machines (AUG, JET, ITER, DEMO)
- A single **simulation can take weeks or months** on a single CPU, depending on chosen settings
- System codes or plasma control **need faster** prediction (s – ms)
- Compromise between fidelity and performance / speed of code







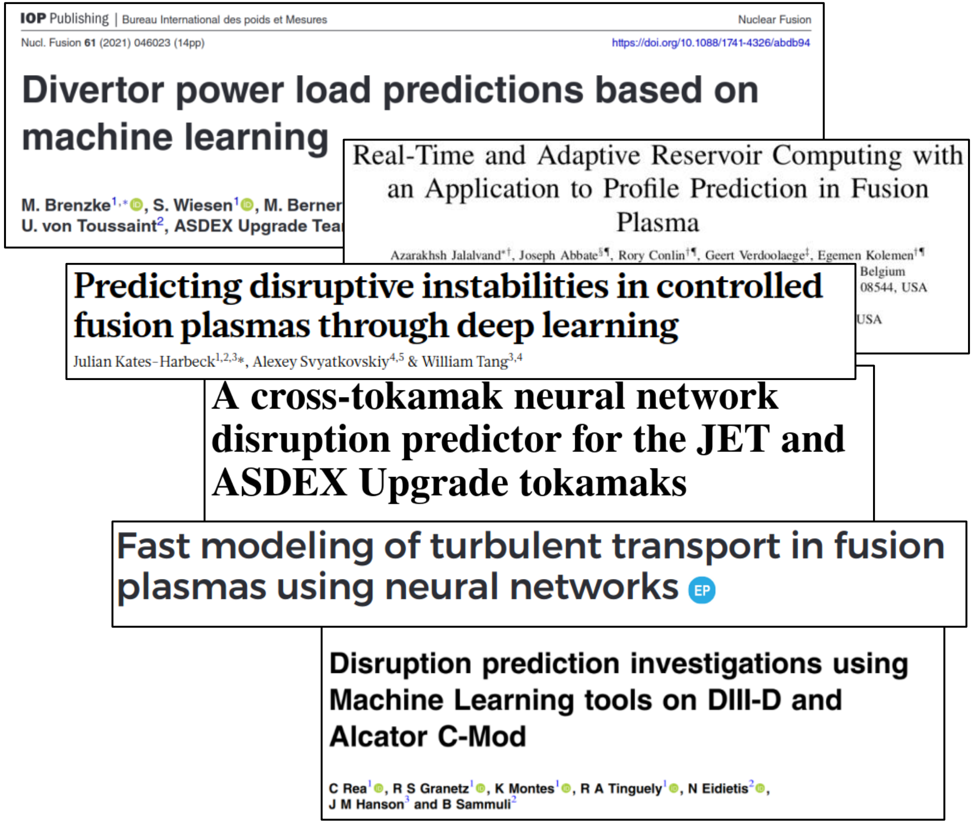
SP1: SOLPS based surrogate models

- Use Machine Learning (ML) and Neural Networks (NN) for fast predictions

- Train a surrogate model on SOLPS-ITER simulations

- Why not experimental data?
  - Restricted to existing experiments: No experimental results for ITER exists
  - In experiments you have less freedom in choosing parameters
  - Can't control everything (hidden parameters)
  - Can only predict was is measured in experiment

- **Goal through this ENR:** Show a proof-of-concept and estimate requirements


IOP Publishing | Bureau International des poids et Mesures Nuclear Fusion
Nucl. Fusion 61 (2021) 046023 (14pp) https://doi.org/10.1088/1741-4326/abdb94

Divertor power load predictions based on machine learning

M. Brenzke[1,*], S. Wiesen[1], M. Berner
U. von Toussaint[2], ASDEX Upgrade Tea

Real-Time and Adaptive Reservoir Computing with an Application to Profile Prediction in Fusion Plasma

Azarakhsh Jalalvand[*†], Joseph Abbate[§¶], Rory Conlin[†¶], Geert Verdoolaege[‡], Egemen Kolemen[†¶]
Belgium
08544, USA
USA

Predicting disruptive instabilities in controlled fusion plasmas through deep learning

Julian Kates-Harbeck[1,2,3*], Alexey Svyatkovskiy[4,5] & William Tang[3,4]

A cross-tokamak neural network disruption predictor for the JET and ASDEX Upgrade tokamaks

Fast modeling of turbulent transport in fusion plasmas using neural networks EP

Disruption prediction investigations using Machine Learning tools on DIII-D and Alcator C-Mod

C Rea[1], R S Granetz[1], K Montes[1], R A Tinguely[1], N Eidietis[2],
J M Hanson[3] and B Sammuli[2]

Setting up the case

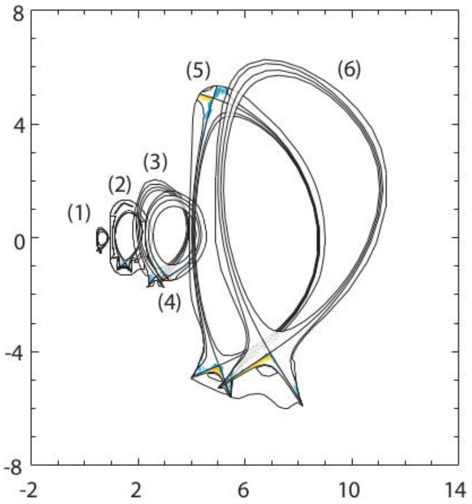
Consider relevant parameters can be varied in the code

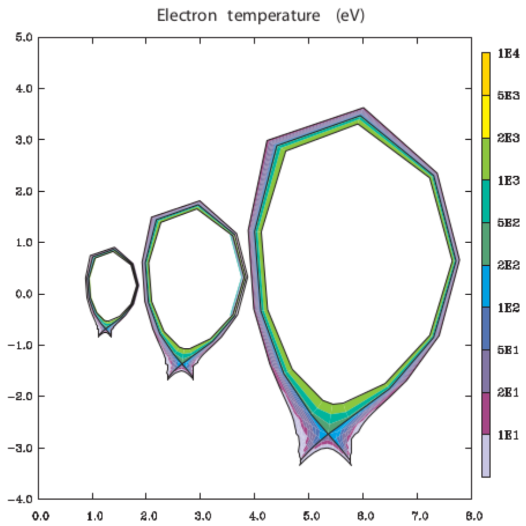
- Relevant tokamak parameters
  - Machine size
  - Plasma current
  - Toroidal B-Field
  - Plasma shape
  - Divertor shape
  - Heating power
  - Gas-puff strength
  - Impurity seeding rate
  - Pumping speed

Physical model
  - Transport coefficients
  - Boundary conditions
  - Kinetic or fluid neutrals

Numerical parameters
  - Grid resolution
  - Convergence metric

E.g. inclusion of Size Scaling





Using geometries of existing machines

+ SOLPS cases exist -> easy to do
+ Surrogate output matches existing experiments

- Can't change parameters independently
- Unclear which parameters to choose as surrogate input
- Difficult to infer what effect contributes to specific results
- How simulations compare, question of validation,…

Conformal scaling of one geometry

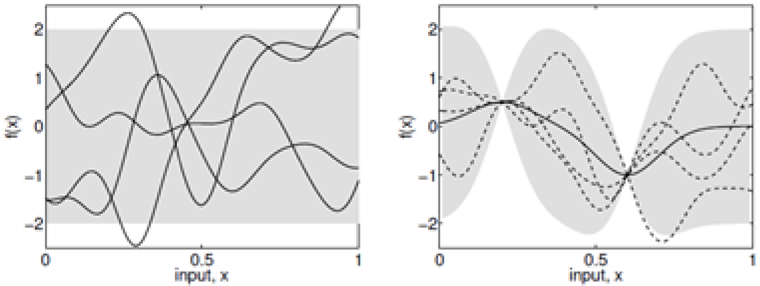
- More work to implement
- Surrogate output valid for imaginary experiments
- Makes some assumption on scenario (eg. use baseline at fixed q_{95} and w/ similar flux exp.)

+ Parameters can be changed independently
+ Same parameters can be used as surrogate input
+ Effect contribution to specific results is clear

Training of ML models

- Try out several candidate models
- Hyperparameter optimization of the most promising ones

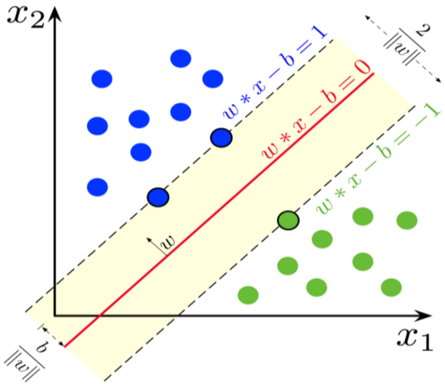
Gaussian process regression



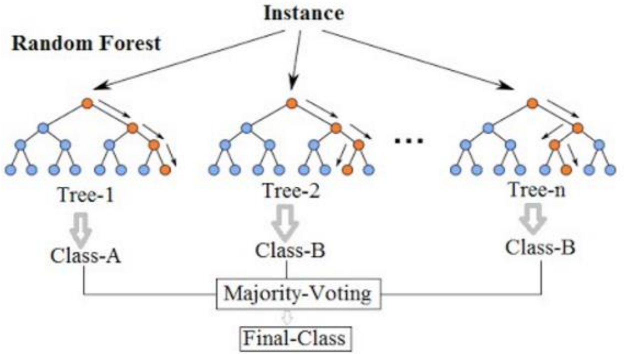
(a), prior (b), posterior

C. E. Rasmussen & C. K. I. Williams, Gaussian Processes for Machine Learning, the MIT Press, 2006

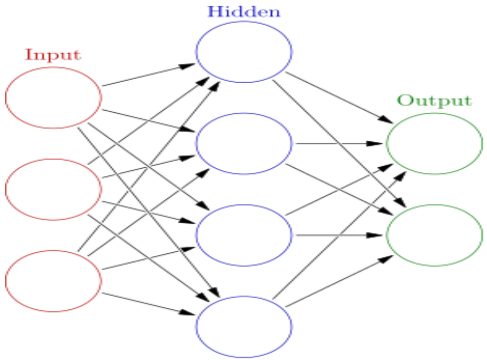
Support-vector machine



Random Forests



Neural Networks



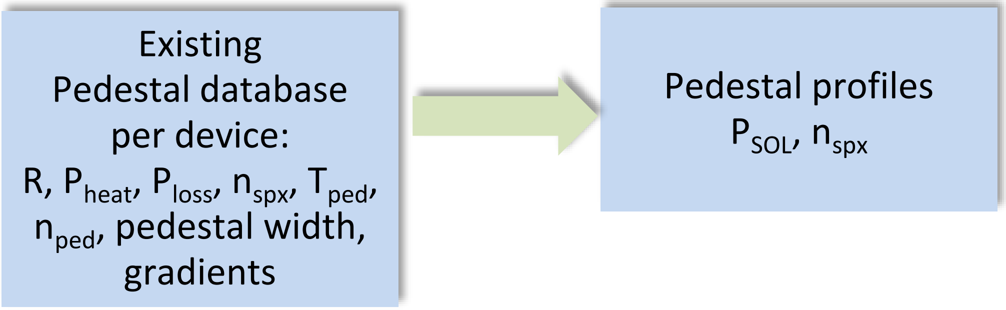
SP1 Current Status

- Setup SOLPS-ITER on Jureca-DC ✅
- Get accustomed with the software code ✅
- Setting up the simulation case
- Run many simulations
- Train Machine Learning model on the simulation data
- Improve Machine Learning models (incorporation of higher fidelity data, uncertainty quantification, ...)

SP2 Development/improvement of ML/ANN methods for training based on experimental data for pedestal physics

SP2 - Workflow

Development/improvement of ML/ANN methods for training based on experimental data for pedestal physics

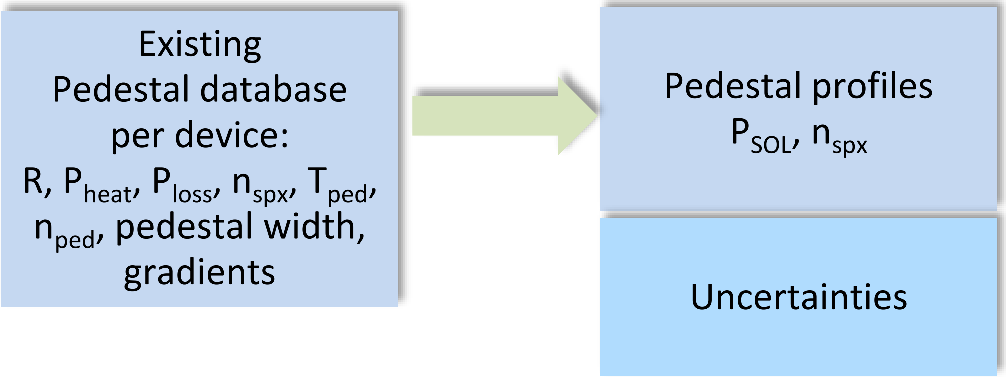


SP2.1 Assessment of the status of existing pedestal databases

- No sufficiently predictive model for the pedestal that allows for example connection of the SOL to pedestal top
- Leveraging on existing data (e.g. EUROfusion pedestal database) as much as possible and will document the status of the pedestal databases.
- Generalised pedestal-SOL coupling requires a hierarchy of fidelity: e.g. full profiles or reduced information (e.g. P_{SOL} & $n_{e,sep}$)

SP2 - Workflow

Development/improvement of ML/ANN methods for training based on experimental data for pedestal physics



SP2.2 Development of methods for UQ for the databases

- The pedestal surrogate model should deal with varying levels of uncertainty in the data derived from various sources
- Uncertainties of different kinds (systematic, random, diagnostics, human) including inherited profile shifts
- Should be generalized and a method is to be developed that codes the uncertainties into the surrogate model (WP2.3)

SP2 - Workflow

Development/improvement of ML/ANN methods for training based on experimental data for pedestal physics

Existing Pedestal database per device:
R, P_{heat}, P_{loss}, n_{spx}, T_{ped}, n_{ped}, pedestal width, gradients

Generalized physics parameters
ρ^*, ν^*, f_{GW}, f_{rad}

→

Pedestal profiles
P_{SOL}, n_{spx}

Uncertainties

→

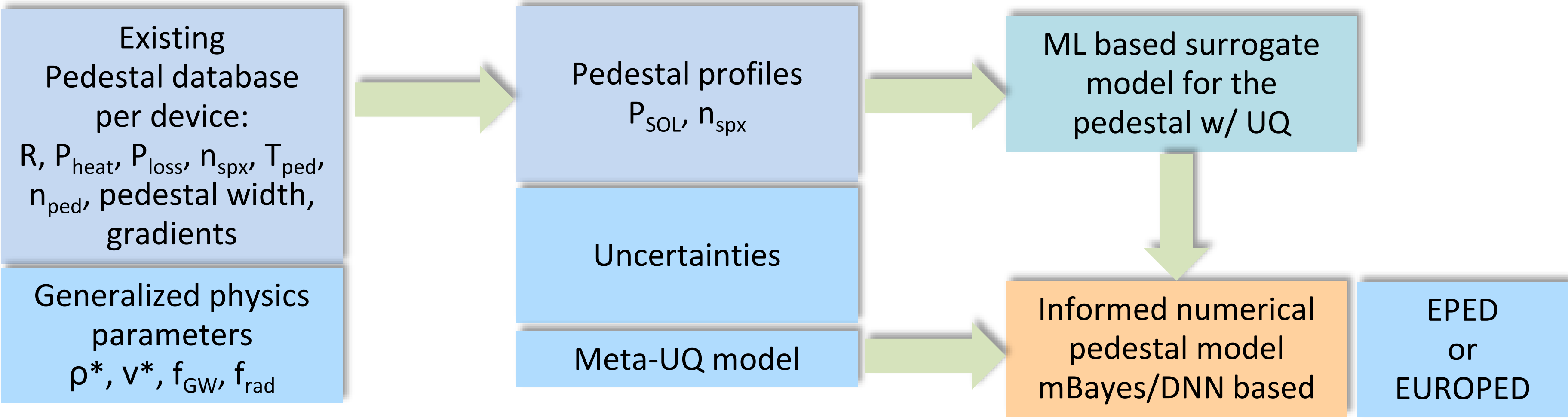
ML based surrogate model for the pedestal w/ UQ

SP2.3 Development of methods to train surrogate model for individual machine and multi-machine database

- The main goal of this subtask is how to deal with system size and machine dependent phase transitions in pedestal physics (towards low ρ^*, low ν^*, high f_{GW}, high f_{rad}, etc).
- Employ IMAS IDS
- Previous work exists on the development of ANN surrogate models for JET pedestal prediction (A. Gillgren et al); this shall be extended to process general uncertainties and multi-machine training.

SP2 - Workflow

Development/improvement of ML/ANN methods for training based on experimental data for pedestal physics

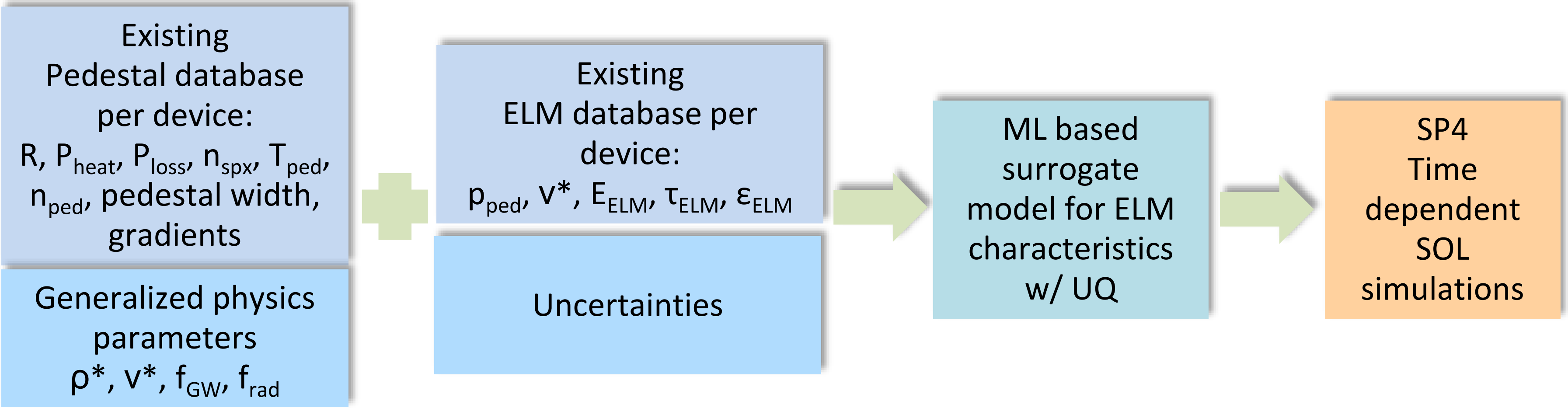


SP2.4 Towards improved numerical pedestal models through inverse UQ and generative models using experimental data

- Develop the foundations to bridge the gap between (partially incomplete) numerical pedestal models and observed experimental data → informed numerical model (e.g. “enhanced EPED”) → exploit Bayesian calibration
- Two approaches: A) a (modular) Bayesian / inverse-UQ approach to describe code-vs-expt discrepancies
  B) a deep generative model approach based on deep-learning NNs that may predict, based on a previously trained model, “unseen”, i.e. not observed, experimental data.

SP2 - Workflow

Development/improvement of ML/ANN methods for training based on experimental data for pedestal physics



SP2.5 Models for ELM characteristics → meta-model for ELMs and SOL perturbations → input for SP4

- Assess the status of the existing ELM database for the devices
- Prepare the data and uncertainties in the ELM database to be used for ML surrogate model development
- Training of the ML model for ELM characteristics / SOL perturbations

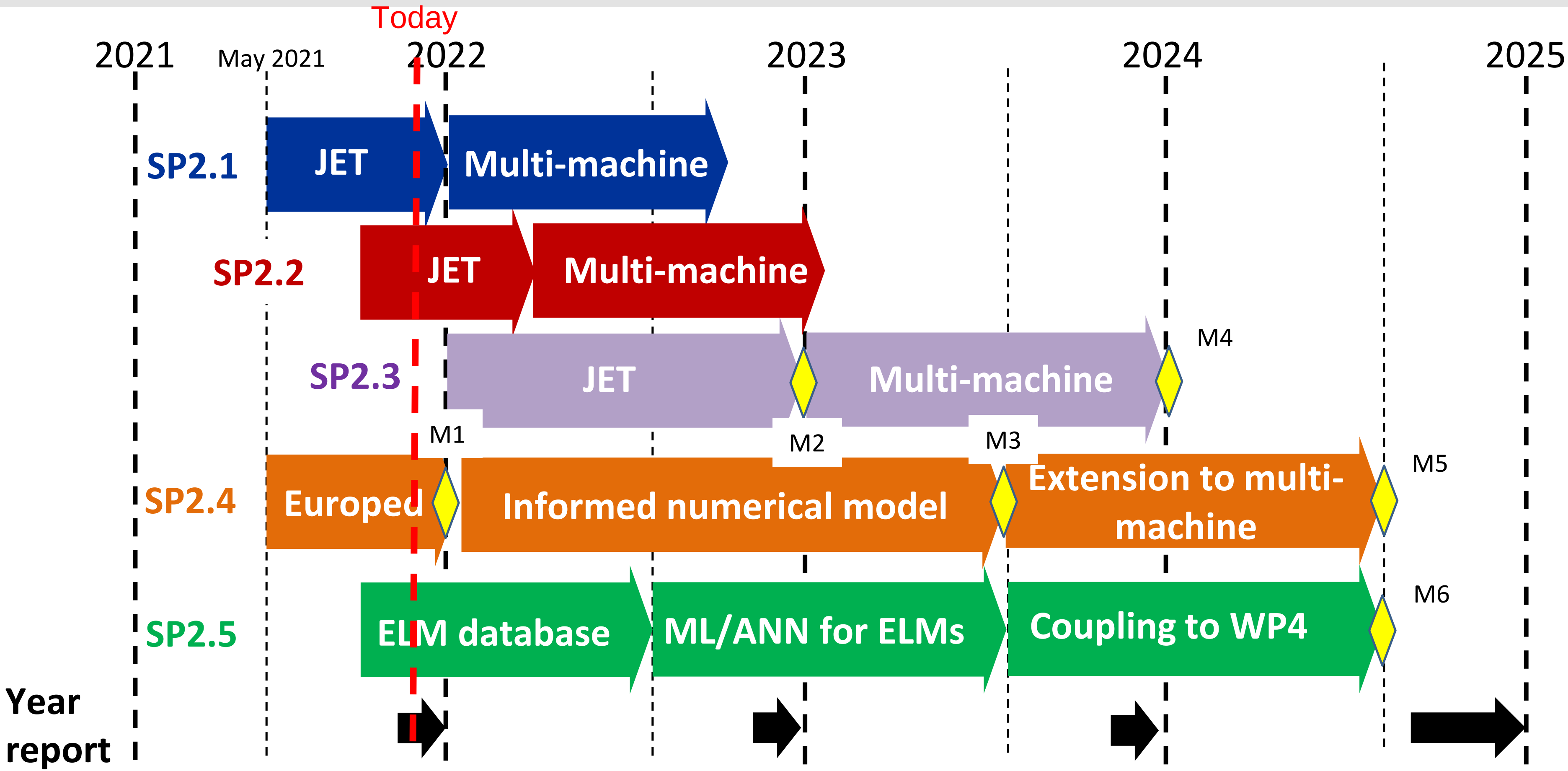
SP2 Current Status

- Progress since the progress meeting #1 (Sep 2021)

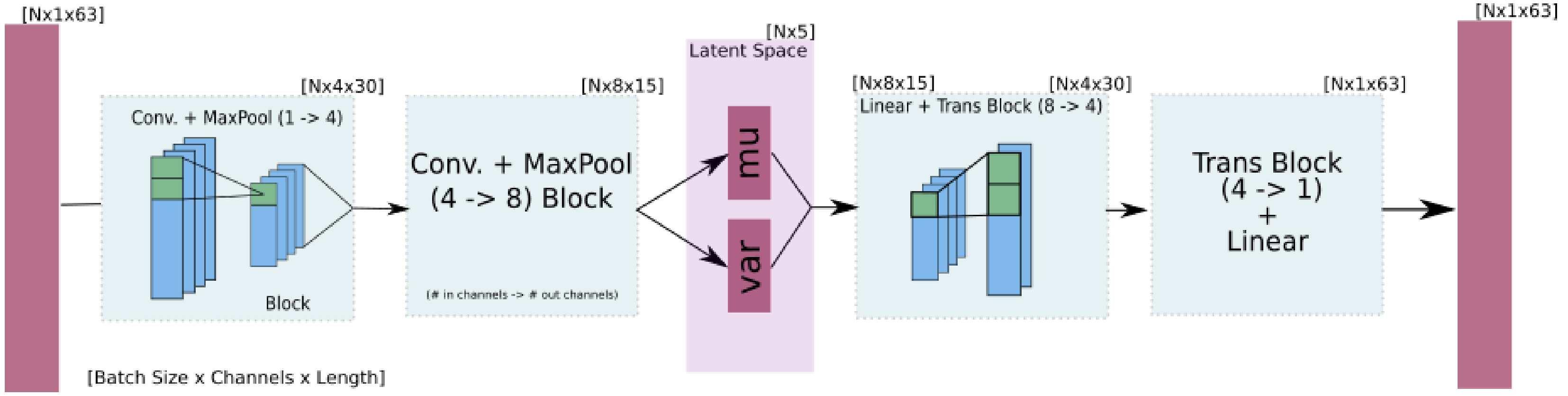
  - A. Kit has prepared a manuscript on the investigations of using tree and neural network based machine learning algorithms to develop predictors for $n_{e,\,PED}$ → to be uploaded to the pinboard by the end of the year
  - A. Gillgren has prepared a new version of his manuscript based on internal EUROfusion review
  - A. Kit has started to work with the full pedestal profile data in addition to the tabular EUROfusion database
    - Variation Autoencoder with convolutional layers able to generate density profiles near experimental observations (figures below) → PSI 2022 abstract
  - A. Gillgren gave a summary of the AUG pedestal database → Currently the number of entries is too low for extensive ML applications and discussions with the AUG team needed to figure out paths forward
  - A. Panera & A. Ho have started to work with the EPED/EUROPED database → Expecting EPED/EUROPED emulator by the end of the year (Panera's BSc thesis)
  - Work with the ELM database started by extracting plasma energy time traces for the entries in the EUROfusion JET pedestal database for further review. Also JET data access requested for Y. Poels.

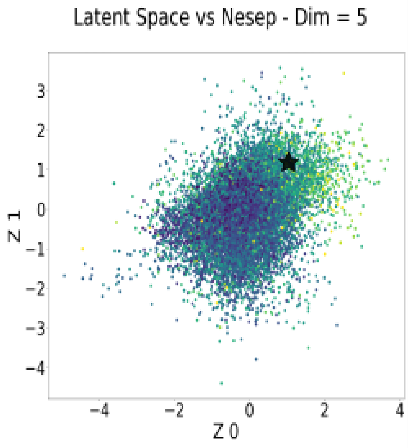
- Overall, SP2 is mostly on track with the planned execution. Identification of multi-machine coding parameters has not been started yet, as so far the work has focused on JET, but it is reasonable to expect this work to start in Spring 2022

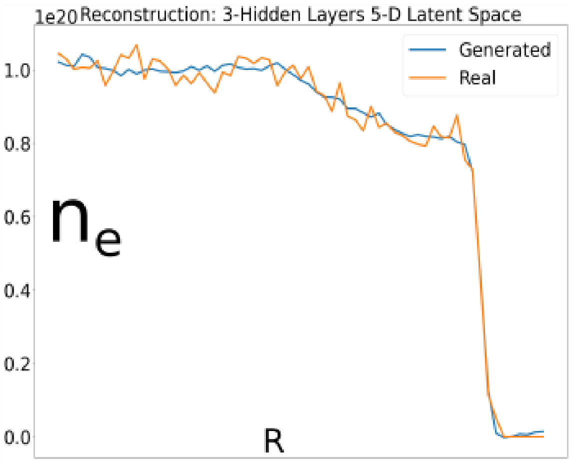
SP2 Gantt Chart



SP2 Current Status







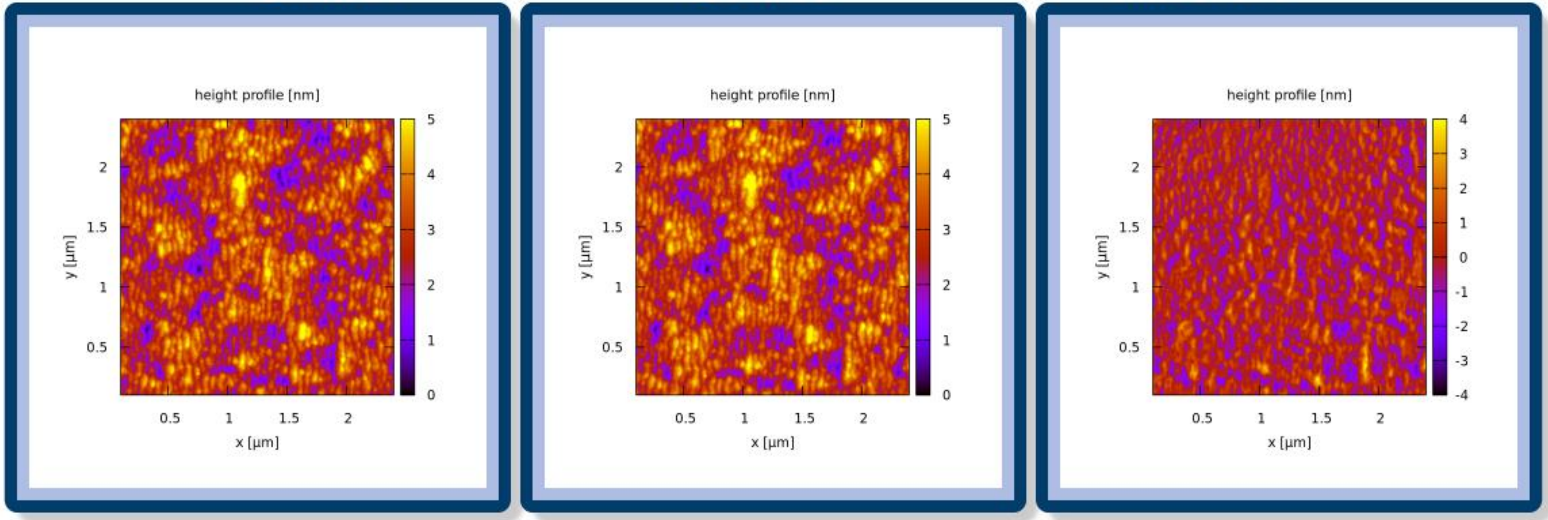
SP3 Model discovery for erosion yields through ML methods

Surface structures, Experimental Data

Data from HZDR campaign Si-Ar$^+$

Extensive AFM data sets are available

profile 1 **profile 2** **difference**



Problem: Displacement between irradiation phases.
An automatic numerical correction is needed!

Data driven model discovery

Regression

- At least 2 detailed profiles $\mathbf{h}^t$ and $\mathbf{h}^{t+\Delta t}$ are required
- N equations for M parameters (overdetermined system)
- The regression Model $\mathbf{f}$ must be sufficient
- Pseudoinverse $\mathbf{f}^+$ is needed
- Actually Least Squares approach

$$\boldsymbol{\alpha}^+ = \mathbf{f}^+ \cdot \frac{\mathbf{h}^{t+\Delta t} - \mathbf{h}^t}{\Delta t}$$

Profile data from experiment or microscopic simulations serve as input

Data driven model discovery

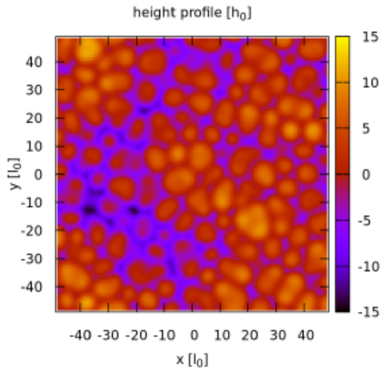
Possible Regression Models

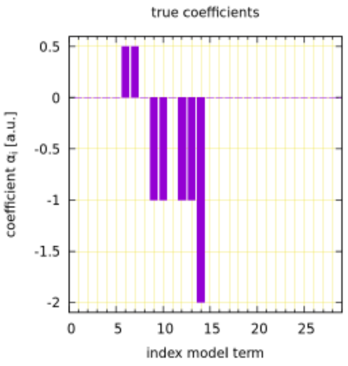
Example: Regression Model containing 30 different terms: Many of them might be zero!

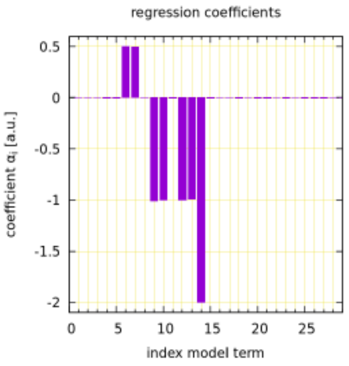
$$
\begin{aligned}
\sum_{k=1}^{M} \alpha_k f_k \quad = \quad & \alpha_1 + \alpha_2 h + \alpha_3 h^2 + \alpha_4 \partial_x h + \alpha_5 \partial_y h + \alpha_6 (\partial_x h)^2 + \alpha_7 (\partial_y h)^2 + \alpha_8 (\partial_x h)(\partial_y h) \\
& + \alpha_9 \partial_{xx} h + \alpha_{10} \partial_{yy} h + \alpha_{11} \partial_{xy} h + \alpha_{12} \partial_{xxxx} h + \alpha_{13} \partial_{yyyy} h + \alpha_{14} \partial_{xxyy} h \\
& + \alpha_{15} (\partial_{xx} h + \partial_{yy} h) [(\partial_x h)^2 + (\partial_y h)^2] + \alpha_{16} (\partial_x h)^3 + \alpha_{17} (\partial_y h)^3 + \alpha_{18} \partial_{xxx} h \\
& + \alpha_{19} \partial_{xxy} h + \alpha_{20} \partial_{xyy} h + \alpha_{21} \partial_{yyy} h + \alpha_{22} (\partial_x h)(\partial_{xx} h) + \alpha_{23} (\partial_x h)(\partial_{yy} h) \\
& + \alpha_{24} (\partial_y h)(\partial_{xx} h) + \alpha_{25} (\partial_y h)(\partial_{yy} h) + \alpha_{26} \partial_{xx} (\partial_x h)^2 + \alpha_{27} \partial_{xx} (\partial_y h)^2 \\
& + \alpha_{28} \partial_{yy} (\partial_x h)^2 + \alpha_{29} \partial_{yy} (\partial_y h)^2 + \alpha_{30} \overline{h}
\end{aligned}
$$

Error analysis with synthetic data

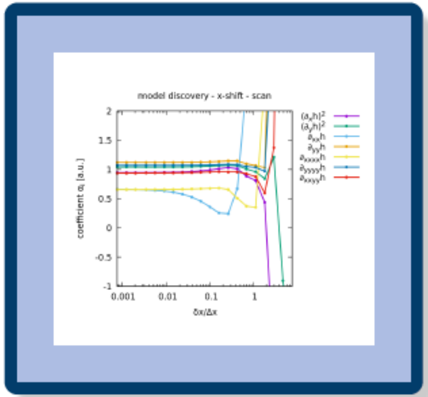
Regression parameters varying with shift in x-direction:

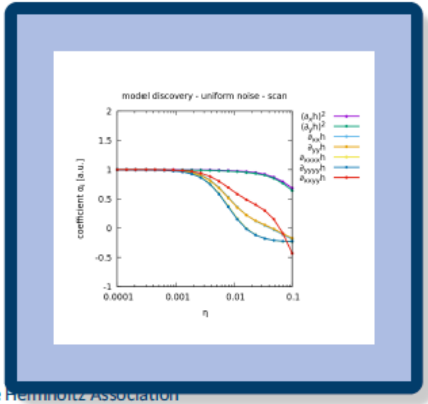






Error analysis with synthetic data





In general the straight forward application of Model Regression is very prone to small displacements and noise!

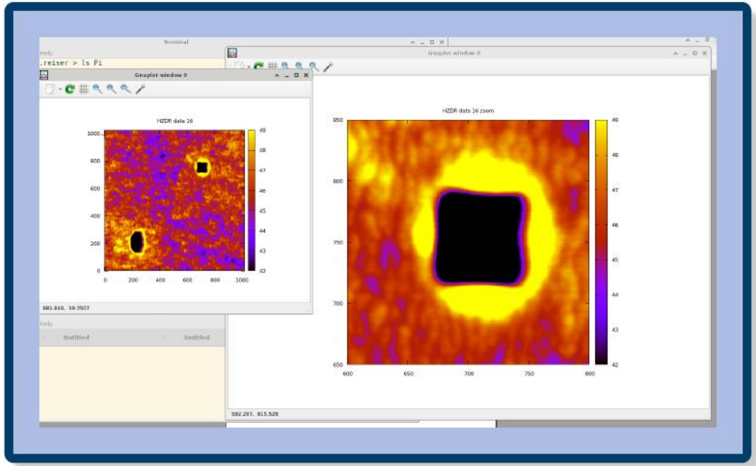
Difficult requirements to be met in experiments:

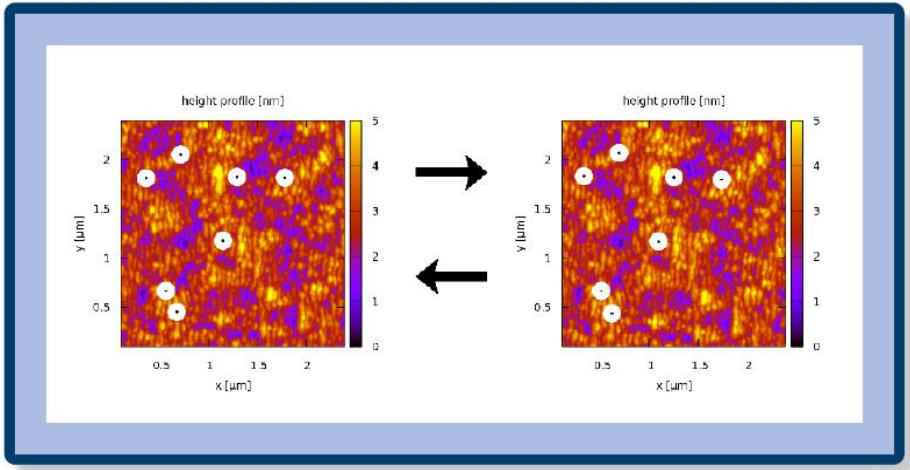
- **lateral displacements $\delta x \leq \Delta x$**
- **noise level $\leq$ 1%**

This is probably not feasible !?

How to cope with this?

Profile Corrections





Smoothing techniques
Markers in Experiments
Pattern Recognition
Single Snapshot Analysis
Other..

More „intelligent“ techniques

Scale Invariant Feature transform (SIFT)
- Rotation and scale-invariant feature detector
- Based of difference of Gaussians, local extrema (in space & scale) as keypoints
- Construct histograms of orientations
- Convolute sub-regions for keypoint descriptor

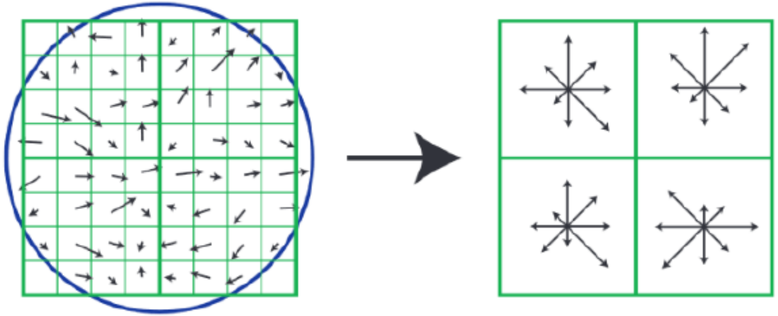


Image gradients

Keypoint descriptor

Image alignment
- SIFT keypoints with transformations
- Compute homography matrices from identified points

Original and transformed image

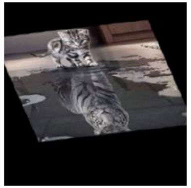
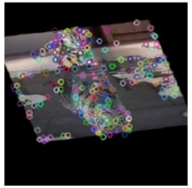


Image after alignment with SIFT keypoints

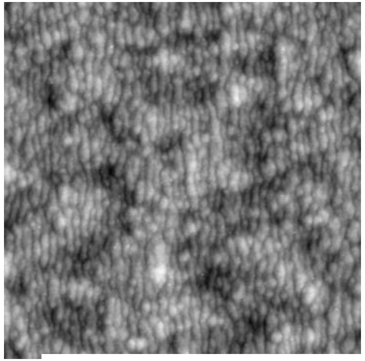
Exemplary image stolen from the internet, not meant for publication

Identified keypoints in each image

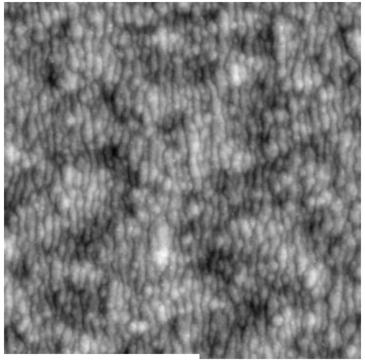


Height profiles need to be aligned to reconstruct model parameters → Image alignment via SIFT keypoints

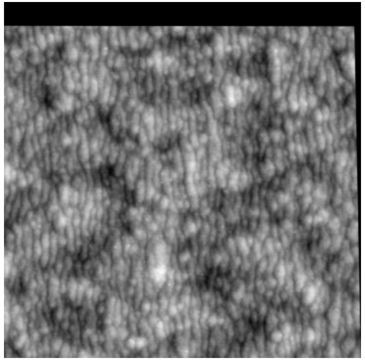
Profile 1



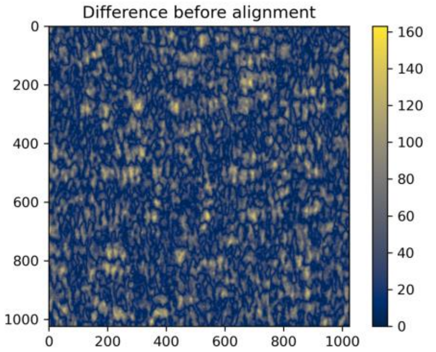
Profile 2



Profile 2 aligned with SIFT

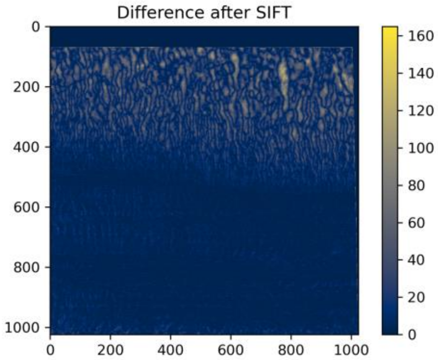


Shown is the absolute difference in arbitrary units



The difference between the profiles can be reduced over a large part of the image

Some improvement still necessary



NN approach

- For a neural network based approach a convolutional recurrent neural network has been set up (similar to the figure below)

- The model will be trained and tested within the coming year and further machine learning based approaches might be tested on the data produced

- The model will also be tested on experimental data where the convolutional approach should reduce the need for dedicated profile alignment steps

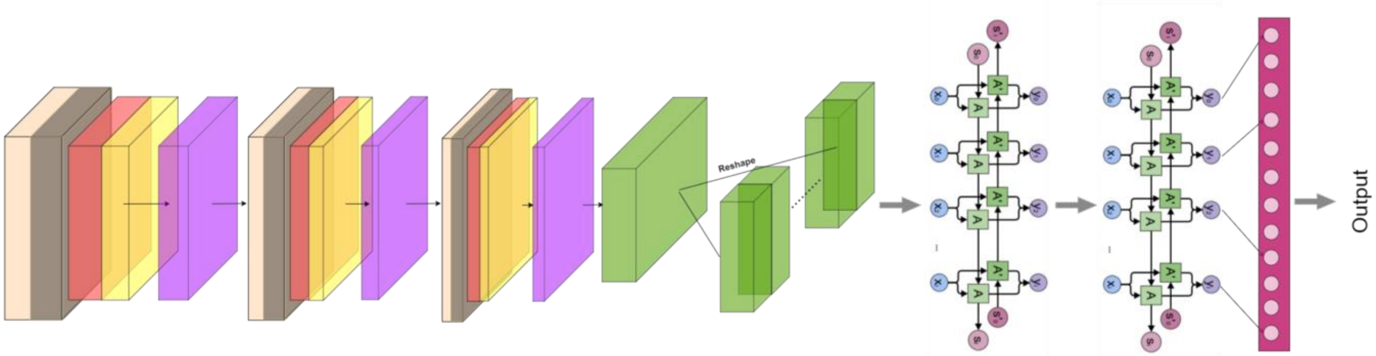


Image from: https://towardsdatascience.com/an-approach-towards-convolutional-recurrent-neural-networks-a2e6ce722b19

SP3 Current Status

Model discovery for PWI
Identify model parameters from plasma irradiated surface profiles (cf. [Reiser2019])

Current objectives:

- Data generation of simulated height profiles
- Alignment of surface profiles in preparation for experimental data
- Setup of a machine learning/neural network based approach to model discovery (cf. [Loew2021])

- The code for the data production of simulated surface profiles is in place but still needs to be applied on a large scale to produce sufficient data for the machine learning based approaches; currently applying for computing resources
- Image alignment via SIFT algorithm is under investigation
- The overall neural network architecture has been set up

[Reiser2019] D. Reiser, Phys. Rev. E 100, 033312 (2019)
[Loew2021] K. M. Loew and R. M. Bradley J. Phys.: Condens. Matter 33 025901 (2021)

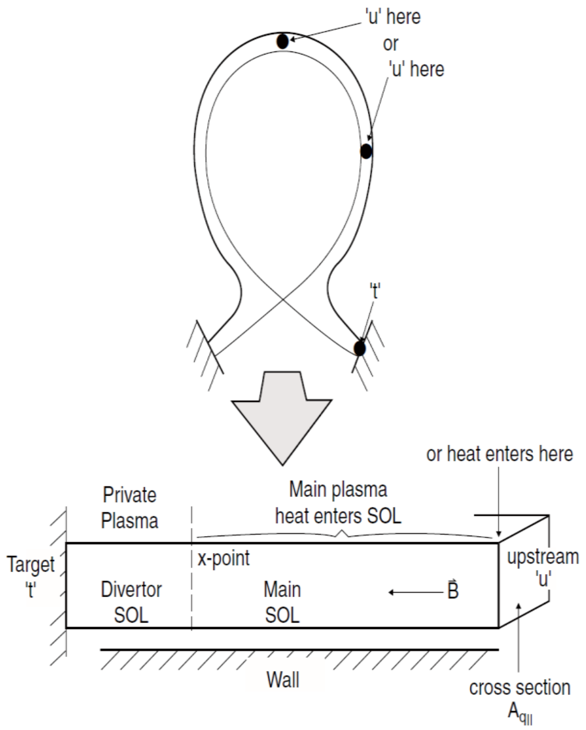
SP4 Towards time-dependent surrogate models for exhaust

SP4 objectives

Review and test application of time-dependent surrogate model techniques for the SOL

To keep things simple start from a 1D model

- DIV1D (plasma particle / momentum / energy balance & neutral particles)
- Dynamics: gas-puff, core fuelling, recycling, wall sources, ELMs, …
- Even simpler?: 2 Point Model – can be made dynamic by making inputs (n_X, q_X, …) or parameters (f_{power}, $f_{momentum}$, …) time dependent



Collaboration with ENR on Control (PI Matthijs van Berkel)
Multivariable feedback control of radiative loss-processes using multi-spectral imaging
WP5 Dynamic modelling for MIMO-control (Ben Dudson SD1D)

SP4 tasks

1) 1D divertor model development and data generation

- Extension of the DIV1D model
- Benchmark of DIV1D to SOLPS-ITER
- Selection of dynamic cases to be simulated
- Data generation

2) Review and test of time dependent surrogate model techniques

- Review of time dependent ML/ANN (recurrent NN, Sequence-to-Sequence, Neural ODE – Latent ODE model, …)
- Train network on selected data from Task 1
- Validation and performance

DIV1D model

Assumptions: equipartition Ti = Te; no radial losses

- Plasma Particle balance $$\frac{\partial n}{\partial t} = -B\frac{\partial}{\partial x}\left(\frac{\Gamma_n}{B}\right) + S_n, \qquad \Gamma_n = nv_{\parallel}$$
- Momentum Balance $$\frac{\partial nmv_{\parallel}}{\partial t} = -B\frac{\partial}{\partial x}\left(\frac{nmv_{\parallel}^2}{B}\right) - \frac{\partial}{\partial x}p + S_{\mathrm{mom}},$$
- Energy Balance $$\frac{\partial 3neT}{\partial t} = -B\frac{\partial}{\partial x}\left(\frac{q_{\parallel}}{B}\right) + v_{\parallel}\frac{\partial}{\partial x}p + Q, \qquad q_{\parallel} = 5neTv_{\parallel} - \kappa_{\parallel}\frac{\partial}{\partial x}T,$$
- Neutral Particle Balance $$\frac{\partial n_n}{\partial t} = \frac{\partial}{\partial x}D\frac{\partial}{\partial x}n_n - S_n,$$

DIV1D data generation

Most code parameters are fixed (including divertor leg length L)

Except for n_x, $q_{||,X}$ and Carbon concentration

We simulate series of density ramps (up and down) at different ramp rates, for different heat fluxes and a range of Carbon concentrations

Density ramps from 2.5 – 5.0 x 10^{19} m^{-3} and vice versa (2 options)

Duration of density ramps 2.5 ms to 250 ms (7 values)

Heat flux from 3 - 8 x 10^7 W/m^2 (6 values)

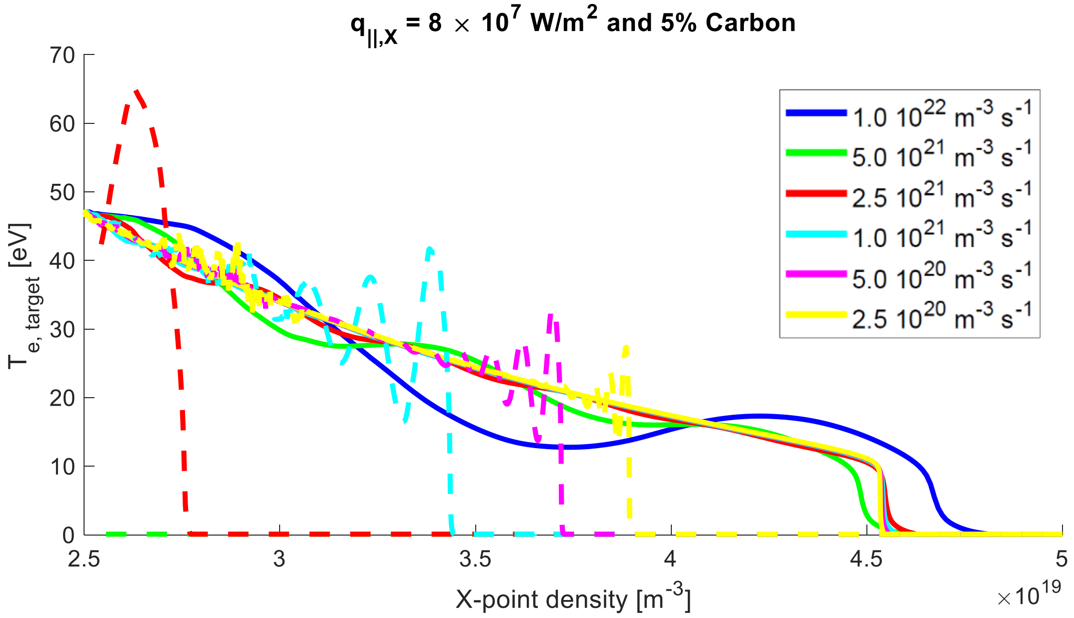
Carbon concentration 1 to 5 % (5 values)

Total of 420 cases. Full solution is stored every 10 μs

DIV1D results

Results of density ramp-ups (solid) and ramp-downs (dashed)

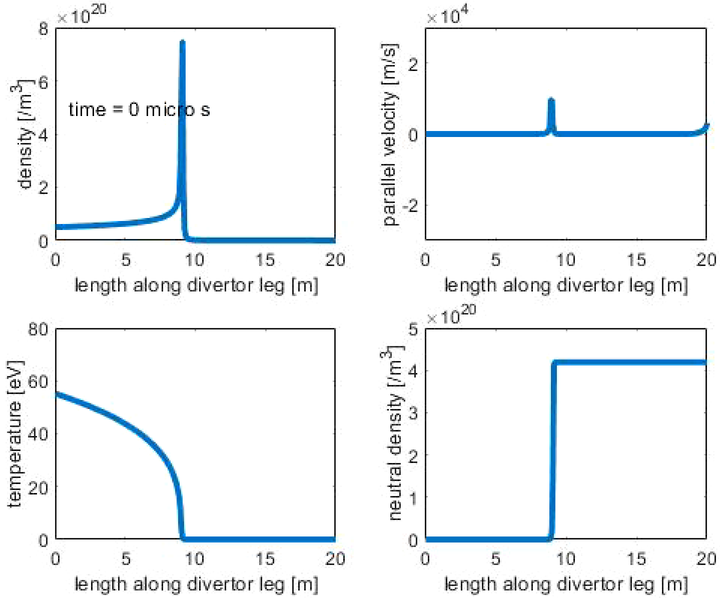
- The target temperature is shown as a function of the upstream density (i.e. time)
- Bifurcations are seen which are a consequence of impurity radion lossess



DIV1D results for ramp-down

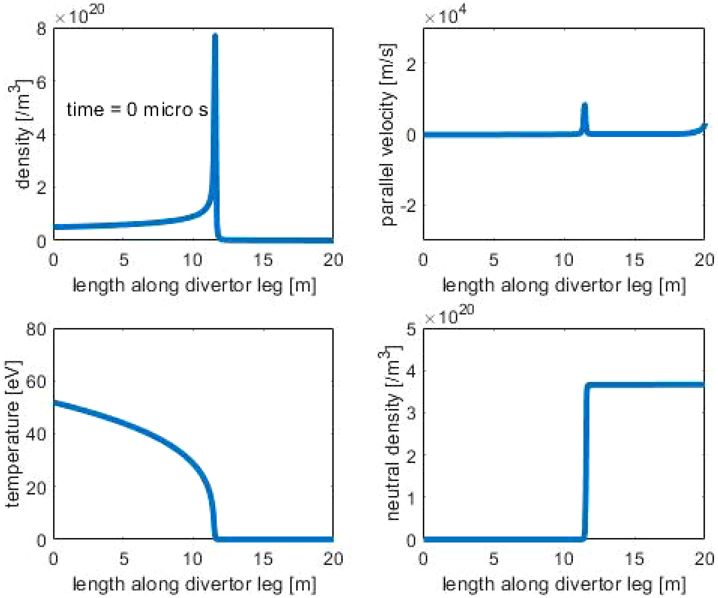
Conditions: $q_{||,X} = 8\ 10^7\ W/m^2$, 5% Carbon, ramp down speed = $-\ 10^{21}\ m^{-3}s^{-1}$

Note bifurcation @ 16 ms with transition from detached to attached solution



Conditions: $q_{||,X} = 5\ 10^7\ W/m^2$, 1% Carbon, ramp down speed = $-\ 10^{21}\ m^{-3}s^{-1}$

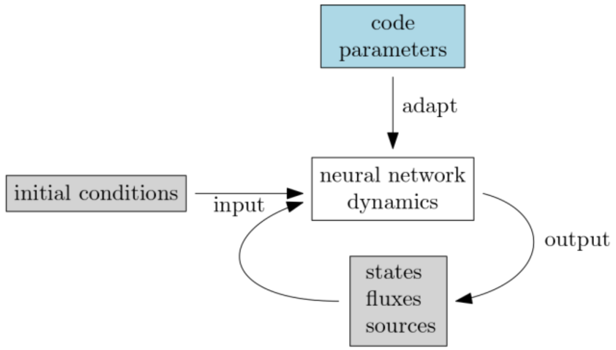
Smooth transition from fully detached to attached



ML – Preliminary approach

Use 4 DIV1D simulations and train a model to re-simulate these from the initial conditions & the parameters. The simulations used are as follows:

- Heat flux of 8 x 10^7 W/m^2
- Carbon concentration of 1%
- Density ramps from 2.5 – 5.0 x 10^{19} m^{-3}, over timescales {2.5ms, 5ms, 10ms, 25ms}
- Autoregressive model that evolves the profiles from time t to time $t + \Delta t$, where Δt = 0.025ms.
  - Do multiple forward passes to simulate over longer stretches of time.
- Build upon a model architecture used for simulating PDEs, Fourier Neural Operators[1].
- Train using batches of 250 steps randomly sampled from the 4 simulations.
- Evaluate by providing the initial state and the density ramp up: Predict the profiles evolving over time (For the 4 simulations, this involves simulating {250, 500, 1000, 2500} steps into the future).



[1] Zongyi Li et al. "Fourier Neural Operator for Parametric Partial Differential Equations." ICLR (2020).

ML – Preliminary approach: First results

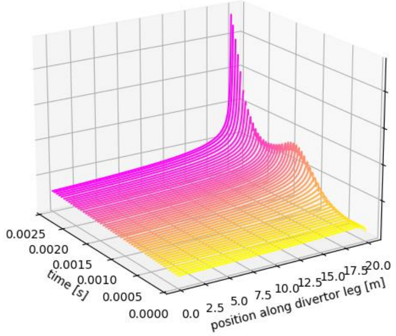
To visualize the results, we plot the profile evolving over time (using a subset of 50 lines/points in time, to keep the figure uncluttered).

Yellow = first timestep (the first yellow line, at *t=0*, is the input for the ML model), purple = last timestep.

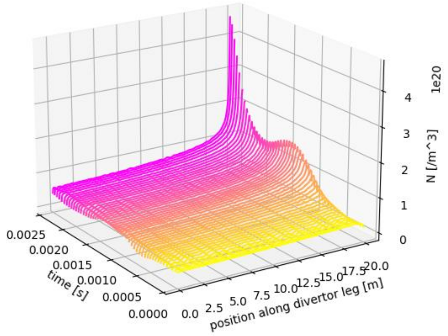
Caveats: (1) Little variation in the 4 simulations/parameters, (2) Some noise, especially near the X-point/target, (3) These simulation parameters are found in the training data (the model does not have to inter/extrapolate) — this is really a proof-of-concept.

Plasma particle density

DIV1D

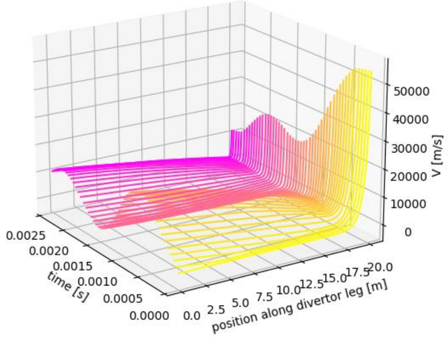


ML model

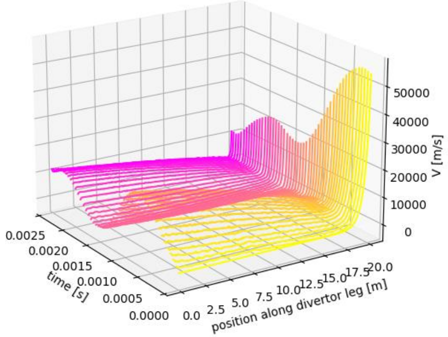


Plasma velocity

DIV1D



ML model



Backup

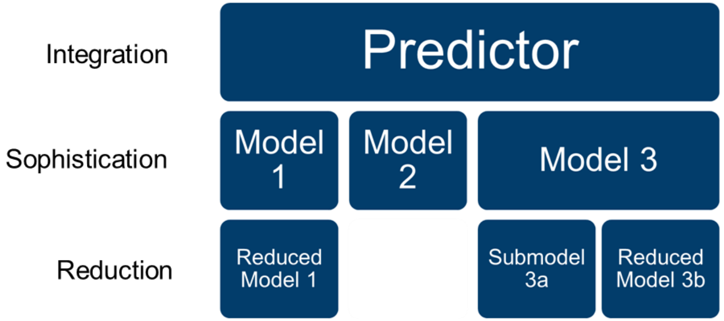
THE CASE FOR A CONCEPTUAL BASIS FOR AN ML BASED MODEL PREDICTOR SCHEME

- First principle exhaust plasma and edge **transport codes require long convergence times** due to their fluid-kinetic schemes (e.g. SOLPS-ITER, or worse, like purely (gyro-)kinetic approaches) – **a severe bottleneck**
- For **rapid design studies for future fusion devices** (e.g. DEMO, HELIAS) systems codes require **reduced physics models for plasma exhaust and PWI**
- The reduced models must be **calibrated against first principle plasma transport and PWI codes** and/or be informed through the use of massively parallelized transport code analysis
- Numerical **surrogate models must be fast** & should include an element of size scaling

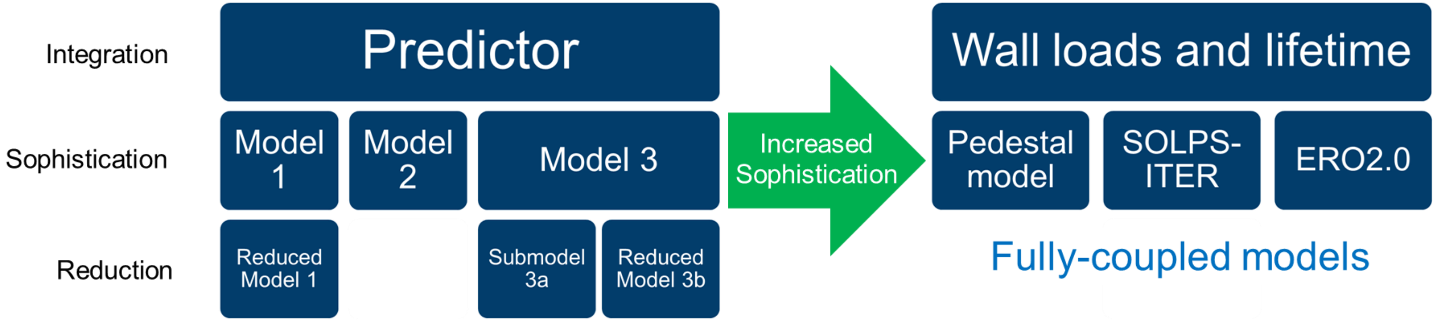
The integration of (fast) predicting models (e.g. for flight simulators) requires balancing numerical accuracy and physics content

- **A conceptual basis for a model predictor scheme is required** that includes new developments of methods and computational technologies for identifying reduced/surrogate models and the exploitation of these in fusion science **– focus on machine learning (ML) and artificial neural networks (ANN) methods**

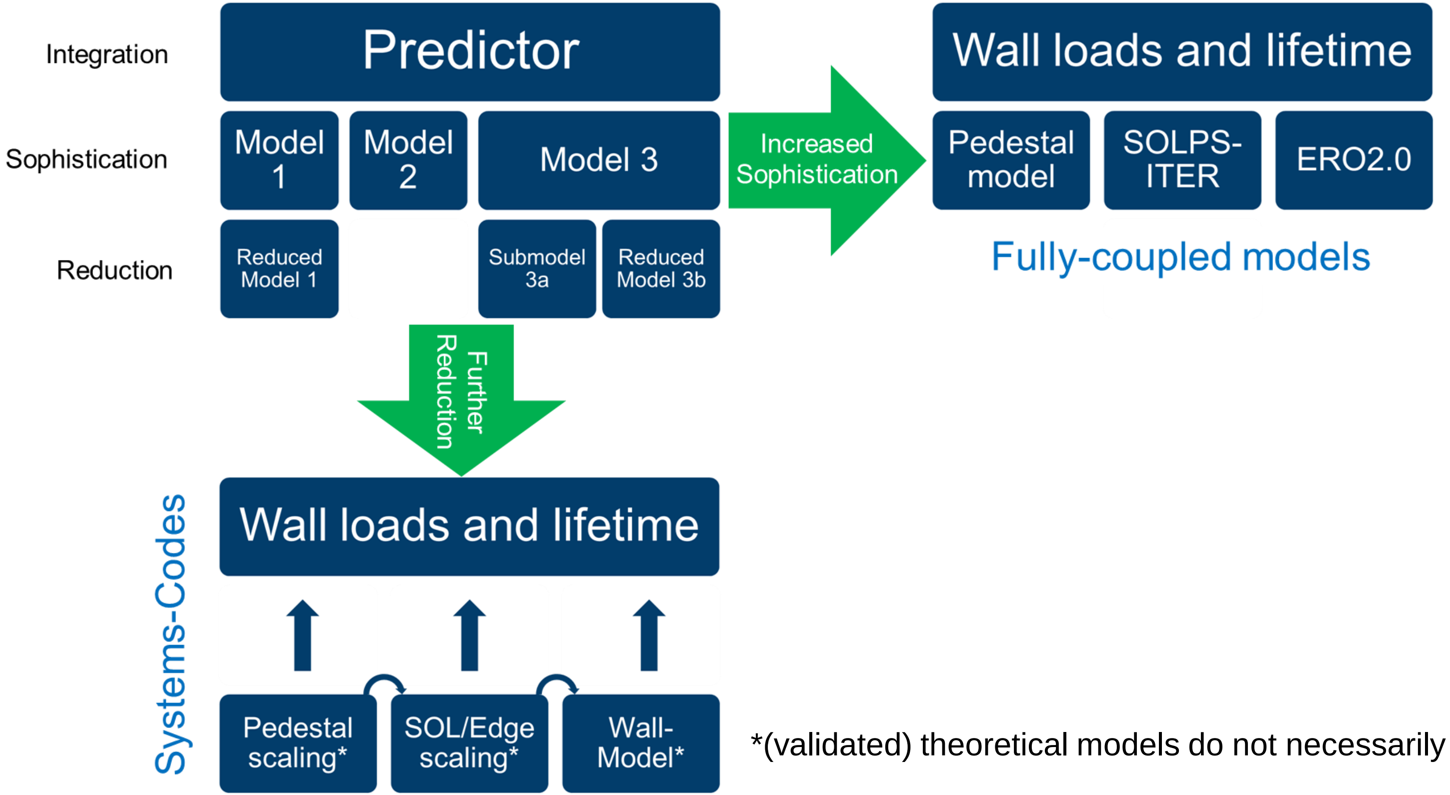
MODEL PREDICTOR SCHEME



MODEL PREDICTOR SCHEME - EXAMPLE

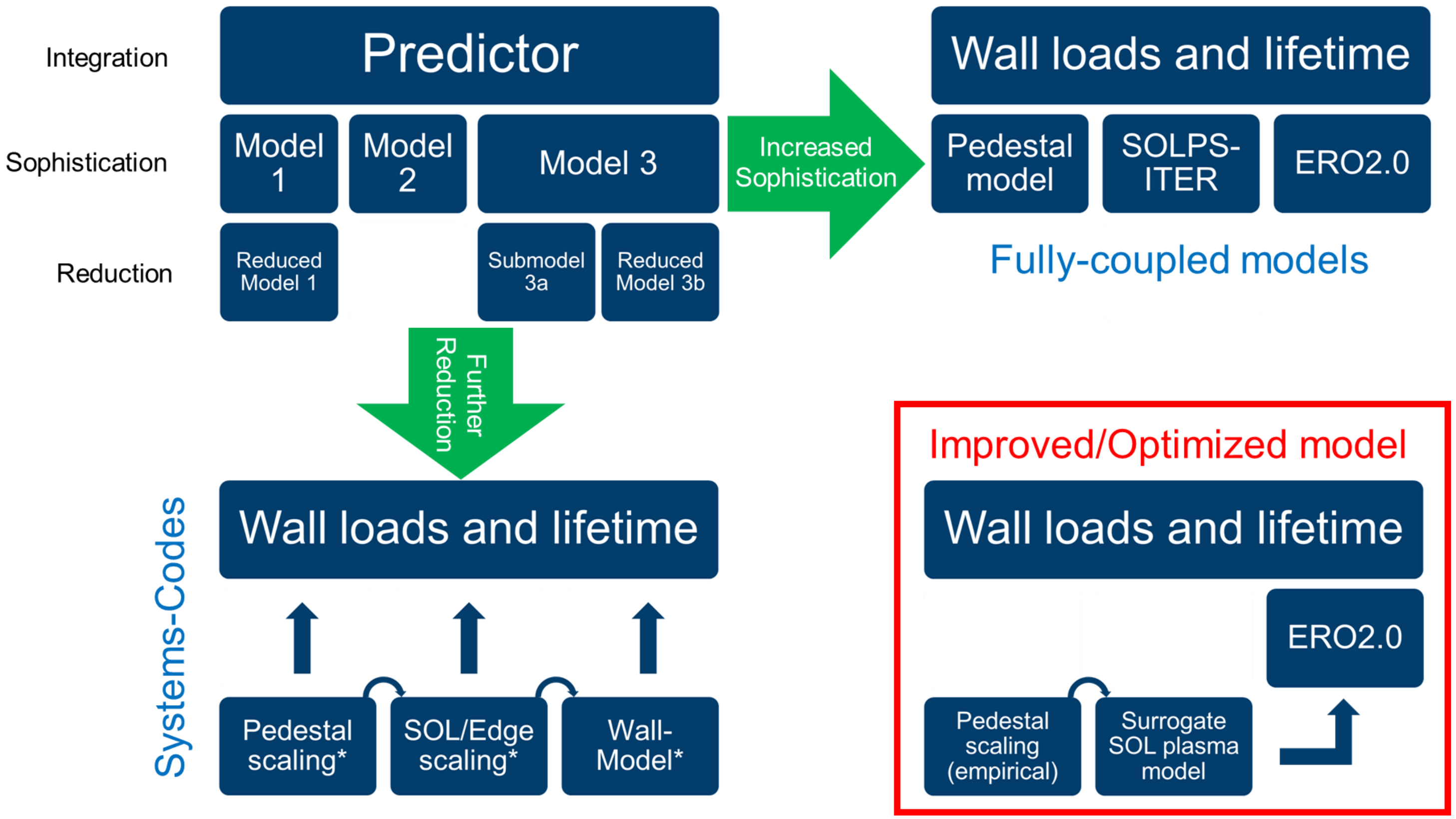


MODEL PREDICTOR SCHEME - EXAMPLE



*(validated) theoretical models do not necessarily exist

MODEL PREDICTOR SCHEME - EXAMPLE



RATIONALE OF ENR

- **Enable and facilitate optimized and improved modelling** that allows a more flexible integration of physics models in the light of extrapolations towards future fusion devices.

- **Demonstrate the applicability of Machine-Learning (ML) and Artificial Neural Network (ANN) methods in fusion** with a special focus on plasma-exhaust (scrape-off layer and pedestal region) and PWI.

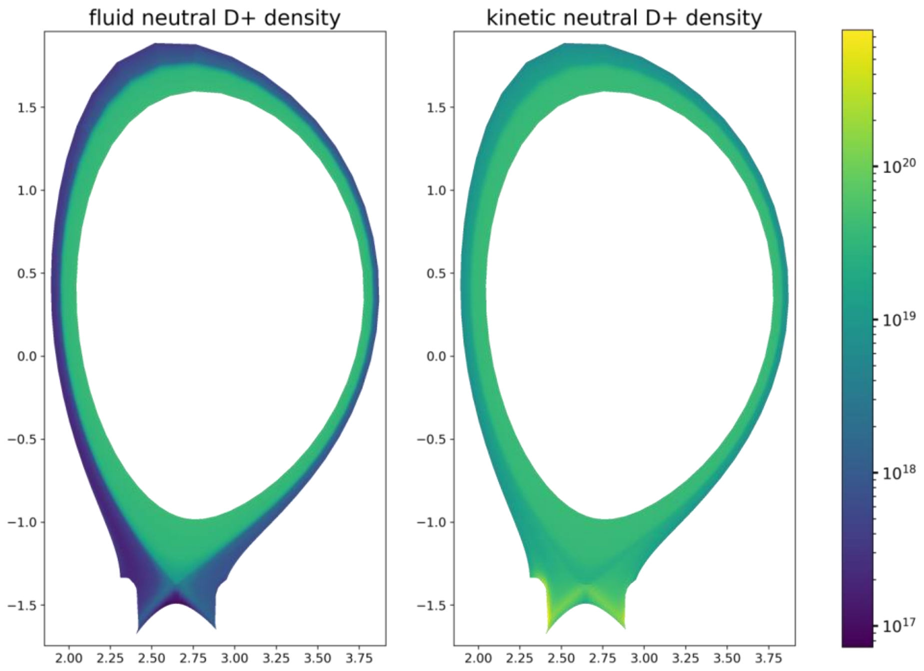
- **This ENR project elaborates on the conceptual basis for an improved model predictor scheme** involving new methods and computational technologies based on **ML/ANN for exploitation in fusion device design studies**.

- Include **uncertainty quantification (UQ)** to enable an efficient selection of the numerical data, i.e. its cardinality, on which the training must be based and **how reduced models are efficiently and quantifiably calibrated**

- **This ER project aims at expanding and disseminating new expertise & knowledge in the field of ML/ANN into the fusion community.**

SP1 NEUTRAL PHYSICS MODEL

- Kinetic neutral theory is closer to reality
- Using fluid neutrals drastically reduces simulation runtime, allowing for more simulations
- Simply disabling the kinetic theory yields vastly different results
- Fluid neutral settings have to be fine tuned by comparing with kinetic neutral simulation
- Especially gas puffs and pumps have to be mimicked by boundary conditions



SP1 SIZE SCALING

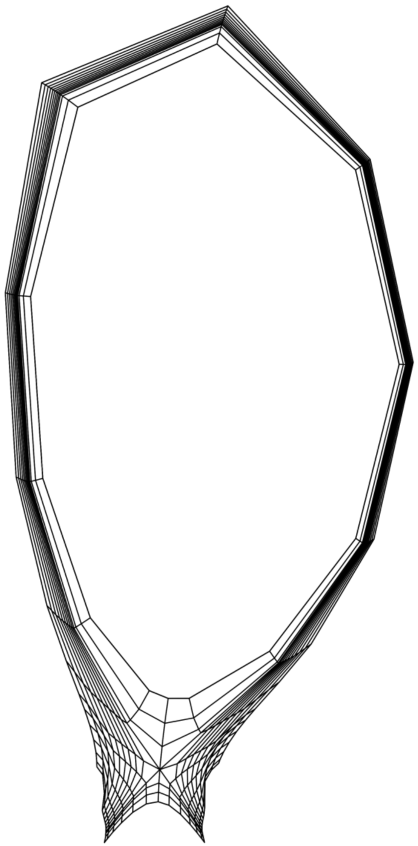
B2 GRID AND THE GRAD-SHAFRANOV EQUATION

- The layout of the computational grid should remain unchanged except the size
  - Changes to grid geometry would be a hidden parameter

- The computational grid has to be aligned to the magnetic field

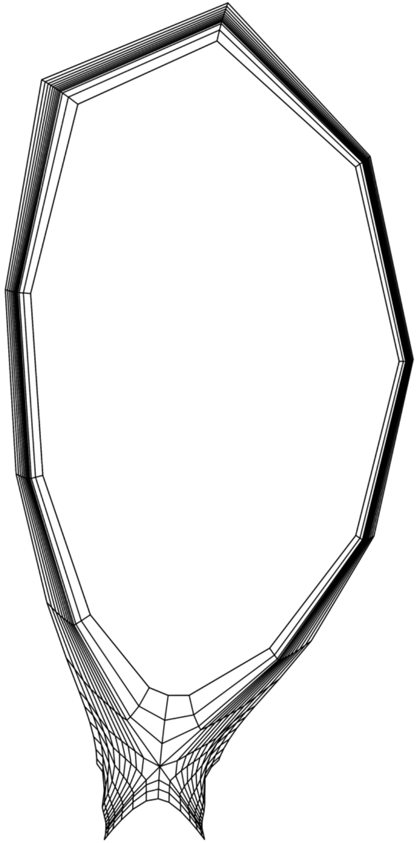
- The magnetic field is determined by the Grad-Shafranov (GS) equation, so any transformation has to result in a valid solution to the GS equation

$$\frac{\partial^2\psi}{\partial R^2} - \frac{1}{R}\frac{\partial\psi}{\partial R} + \frac{\partial^2\psi}{\partial Z^2} = -\mu_0 R^2 \frac{dp}{d\psi} - \frac{1}{2}\frac{dF^2}{d\psi}$$



SP1 SIZE SCALING

B2 GRID AND THE GRAD-SHAFRANOV EQUATION



- Undimensionalizing the equation yields the possible transformations

$$\frac{\partial^2\overline{\psi}}{\partial r^2}-\frac{1}{r}\frac{\partial\overline{\psi}}{\partial r}+\frac{\partial^2\overline{\psi}}{\partial z^2}=-r^2\frac{R_0^4B_0^2}{\psi_0^2}\frac{dp'}{d\overline{\psi}}-\frac{1}{2}\frac{R_0^4B_0^2}{\psi_0^2}\frac{df'^2}{d\overline{\psi}}$$

- Keeping p', f' and $\frac{R_0^4B_0^2}{\psi_0^2}$ constant leaves the shape of the solution intact

- This allows for scaling the size and magnetic field independently but with the constraints of constant aspect ratio and constant safety factor:

$$\frac{R_0}{a}=const \qquad \frac{B_t}{B_p}=const$$

- The real physical pr… ent flux functio… ngly:

$$p=p'\cdot B_0^2/\mu_0 \quad F^2=R_0^2B_0^2+R_0^2B_0^2f'^2$$

SP1 CURRENT STATUS

In correspondence with SP2 decided to use flat profiles for the radial transport coefficients and vary all coefficients simultaneous during simulation farming with single scaling parameter

Currently testing different boundary conditions and other options proposed in Coster et al. (2014) to keep the fluid neutral simulation results closer to kinetic neutral results

It was decided the first machine learning model to test on the dataset will be a (deconvolutional) neural network

Python scripts for simulation farming were developed/improved: Now includes ability to check simulations automatically for convergence and resubmit or run post-processing depending on the outcome

SHORT TERM ACTIVITY

Meeting with KU Leuven group on 1.12. to discuss whether the not yet released Advanced Fluid neutral option could be used for our simulations

The generation of the first training database is expected to be done by end of december

Methods:

- Model Discovery based on Kuramoto-Sivashinski model regression
- Pattern identification by neural networks
- Noise reduction and displacement correction
  by Kalman-Filter or Neural Networks

Goal:

- automatic detection of structures and models for
  two-dimensional surface stuctures
- analysis and extension of microscopic erosion models
- application to experimental data or atomistic simulations

SP4 INPUT AND OUTPUT OF ML MODEL

Different choices

Option 1

- Input: code parameters n_X, $q_{||,X}$, L
  equilibrium solution at t= 0
  n_X ramp rate

Output: n_{target}, T_{target}, T_X as functions of time

'time dependent 2 Point Model'

Option 2

- Input: full profiles at time t

Output: full profiles at time $t + \Delta t$

BACKUP: FORWARD VS INVERSE-UQ

"Forward UQ process always starts with characterization of the input uncertainties. Unfortunately, such information is not always readily available to the code users. Such condition is known as the *lack of input uncertainty information* issue"
[…]
"The backward problem asks whether we can reduce the output uncertainty by updating the statistical model using comparisons between computations and experiments"

→ belongs to sub-group of Bayesian calibration techniques

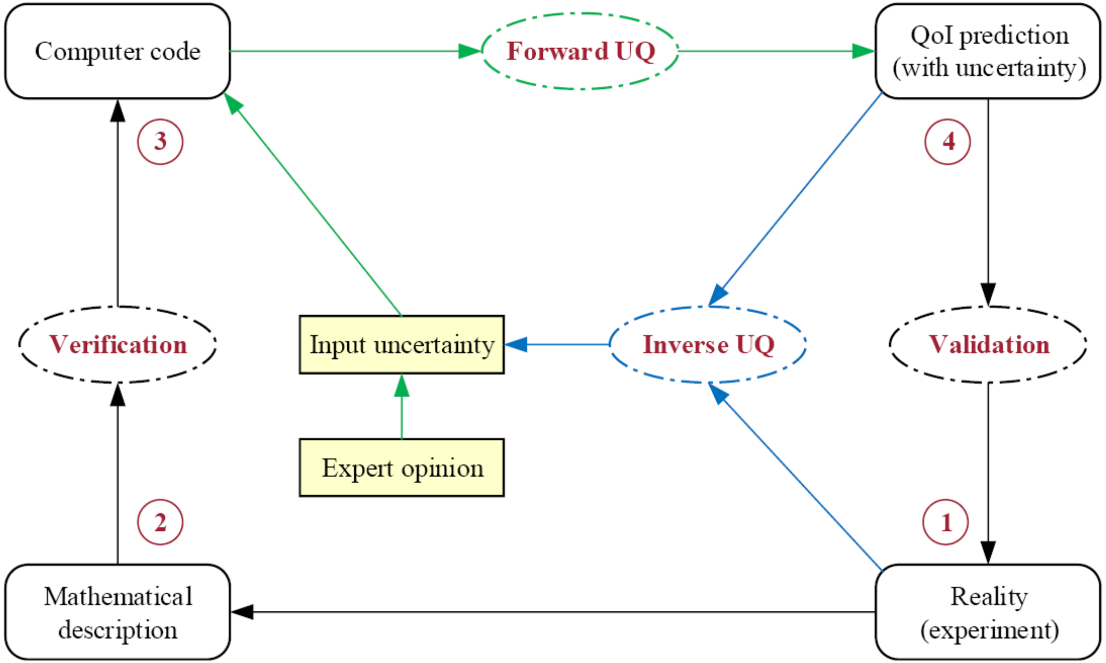


Figure 1: Some essential parts of computer modeling (a non-exclusive list)

X. Wu et al, Nucl. Eng. Des. (2018)
"Inverse Uncertainty Quantification using the Modular Bayesian Approach based on Gaussian Process, Part 1: Theory"