Investigation and perspectives of using GNN* to model complex systems

the simulation of the helium II bayonet heat exchanger in the LHC

*Graph Neural Networks

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CERN – Technology Department

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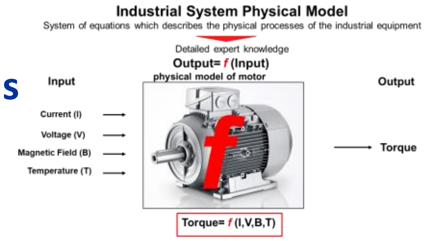
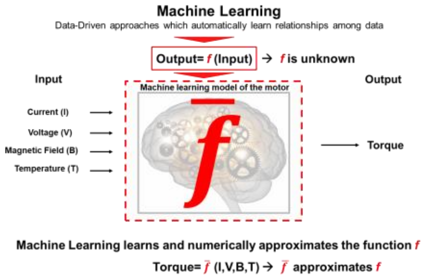
Modelling and prediction of complex systems

Model-based approaches are usually adopted to provide simulations, early identification of **failures** and to reveal **hidden dependencies** among **critical systems**



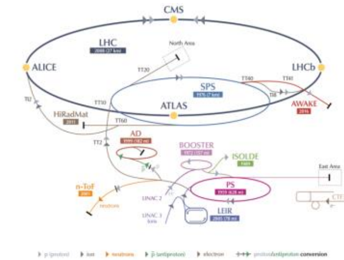
Novel approaches are now available combining **Big Data analytics** and **machine learning techniques** to extract descriptive and predictive models directly from data

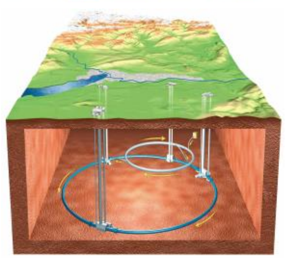
- Suitable for **complex systems** and variable conditions
- **Efficient** when it is difficult to develop an analytical model
- Allow to identify **patterns in data**, anomalies or failures
- Allow to **discover** “hidden” **dependencies**
- Reveal **new information** from available data (a.k.a. data-mining)



CERN has a complex system of systems, e.g. the LHC superfluid helium cryogenic system, with very stringent requirements in terms of availability and reliability

- **Requiring tools for**: quality control, faults analysis, prevention, prediction & mitigation, modelling
- **Providing a complete test bed for**: modelling, complex fault trees, systems dependencies, risks and failures propagation, data and images analysis and interpretation





We present our investigation of using Graph Neural Networks (GNN) to build a model of the helium II bayonet heat exchanger operating in the LHC at CERN

Outline

- Introduction to GNN and the LHC SHe helium loop
- Modelling of the helium II bayonet HX
- GNN training & testing on LHC prototypes data
- Validation of the model on the LHC standard cell
- Conclusions and perspectives

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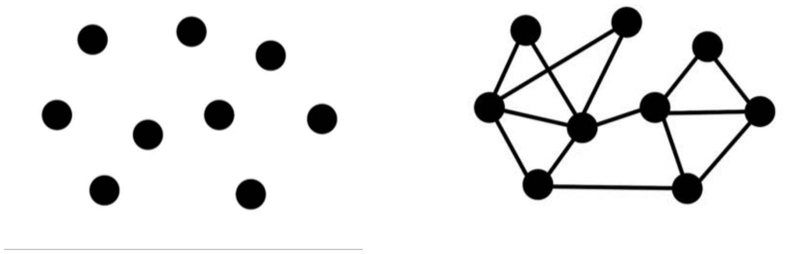
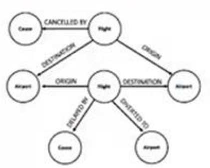
Why Graphs

Graphs are a general language for describing and analyzing entities with relations/interactions



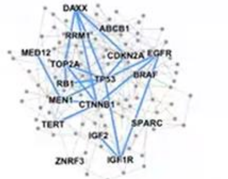
Many types of data are graphs: events, networks, pathways, neurons, molecules, 3D shapes, etc



Event Graphs

Image credit: SalientNetworks

Computer Networks



Disease Pathways

Graphs can represent relational structures: molecules, 3D shapes, physics simulations

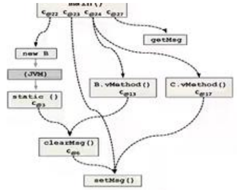


Image credit: ResearchGate

Code Graphs

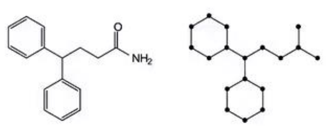


Image credit: MDPI

Molecules

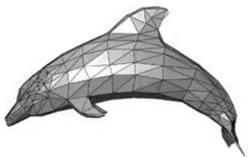


Image credit: Wikipedia

3D Shapes

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
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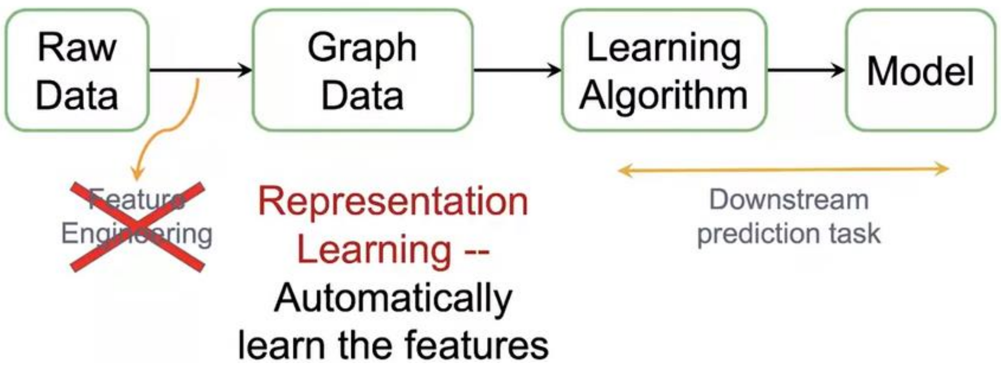
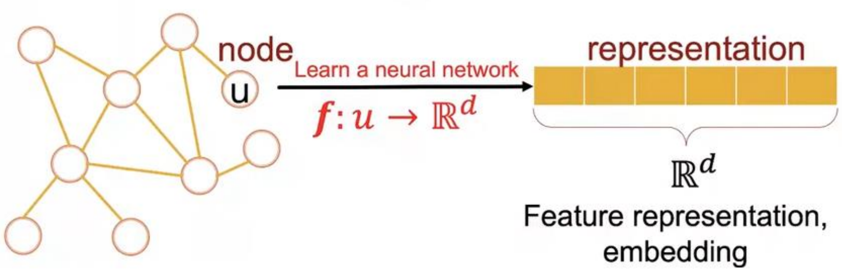
Complex domains have a rich relational structure, which can be represented as a **relational graph**



Map nodes to d-dimensional **embeddings** such that similar nodes in the network are embedded close together



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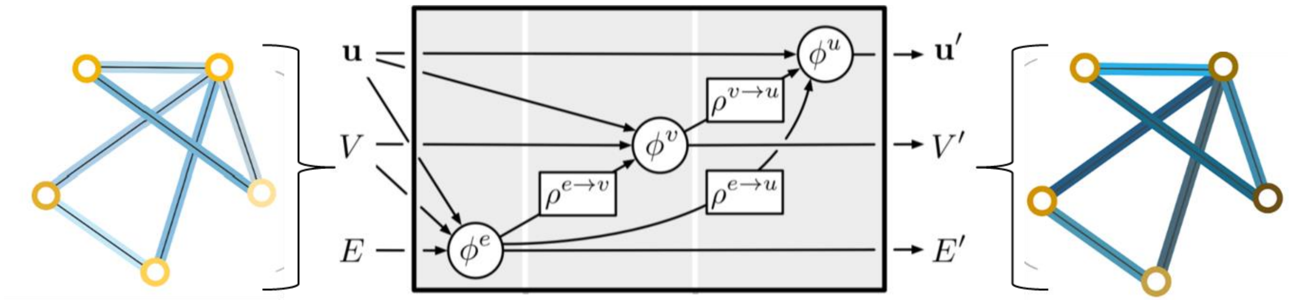
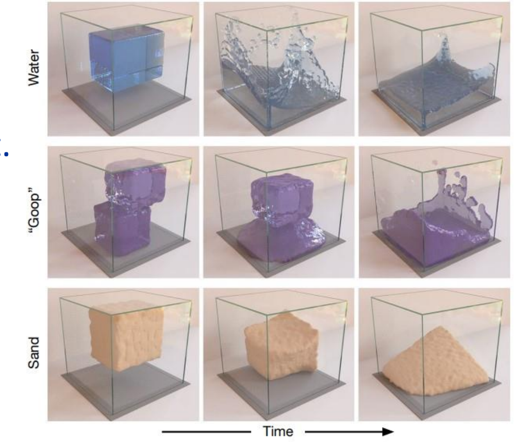
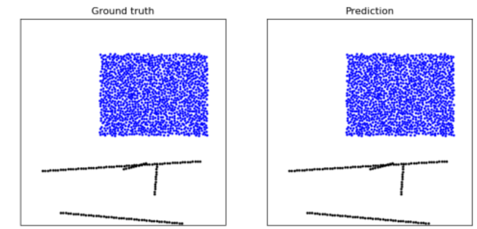
Neural Network that operates on **graph data (GNN)**

A graph network takes a graph as input and returns a graph as output.

The output graph has the same structure, but updated attributes.







- **V**: node set
- **E**: edge set
- **u**: global attributes

- **Φ**: Update functions
- ***ρ***: Aggregation functions

Proved to be able to learn interactions (and physics) **just by "observing" the real world**

Many real-world objects and phenomena can be represented as graphs

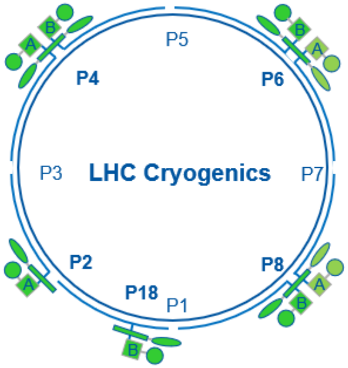
E.g.: Simulations [Sanchez-Gonzalez at al. 2020]

Useful in complex simulations, can speed-up and optimise computation

They can learn relations ("physics") just based on observations

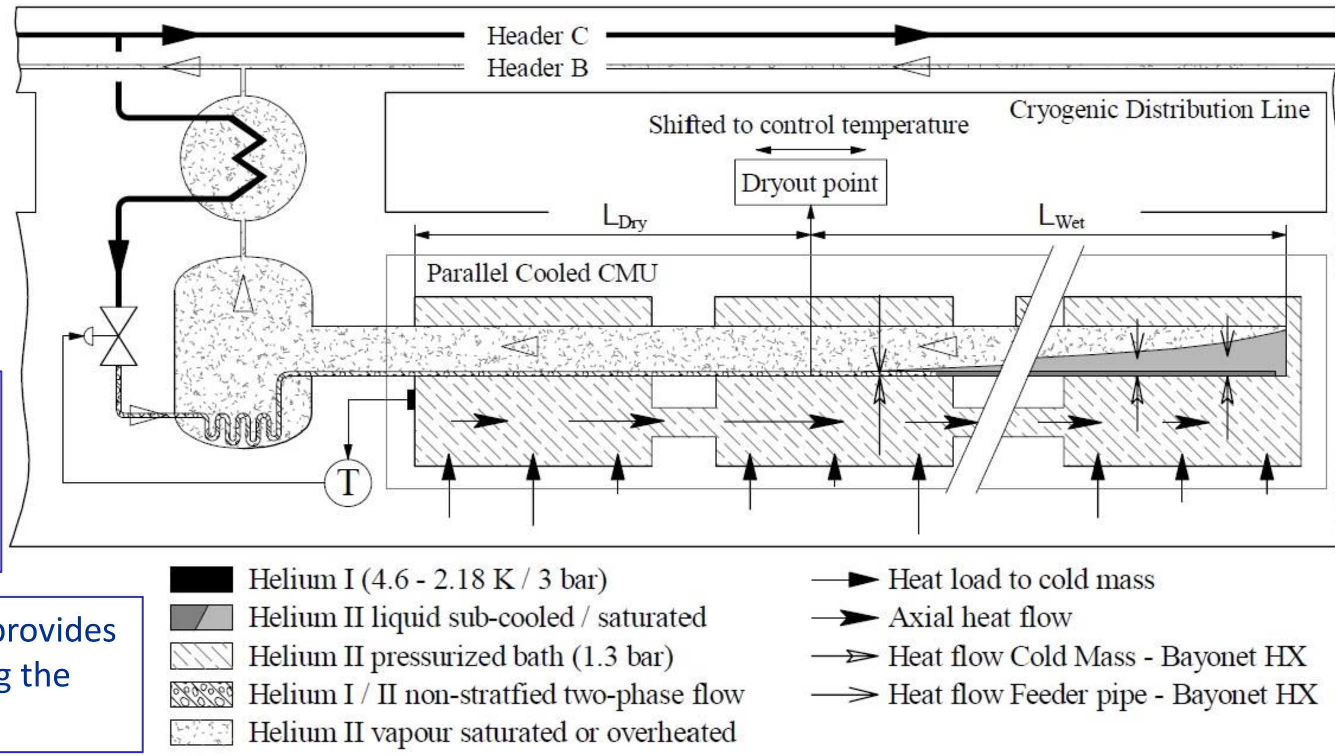
=> They have the potential to find new *(yet unknown)* relations

The LHC Superfluid Helium Loop



The LHC cryogenic system at CERN is designed to distribute a cooling power along a 3.3 km-long sector of the LHC machine

a bayonet heat exchanger (BHX) provides a quasi-isothermal heat sink along the magnet string in a bath of SHe II



The cooling scheme underwent extensive studies and testing on dedicated test loops and partial/full-scale prototypes of the magnet string, called String-1 and String-2

The knowledge gained from the experiments facilitated the definition of the control parameters for the safe and efficient operation of the 27-km LHC machine at temperatures below 1.9 K over several years

This valuable data has also been utilized for training various models, aiding in this intricate cooling scheme's comprehension and diagnostic capabilities, leading to improved operation

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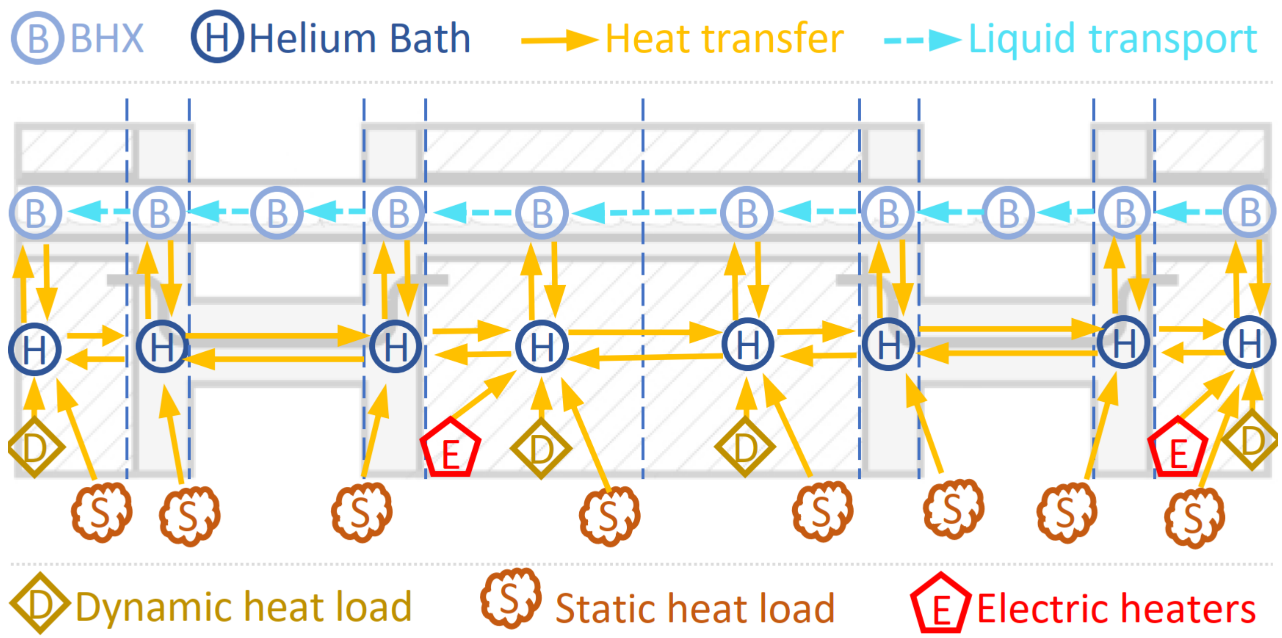
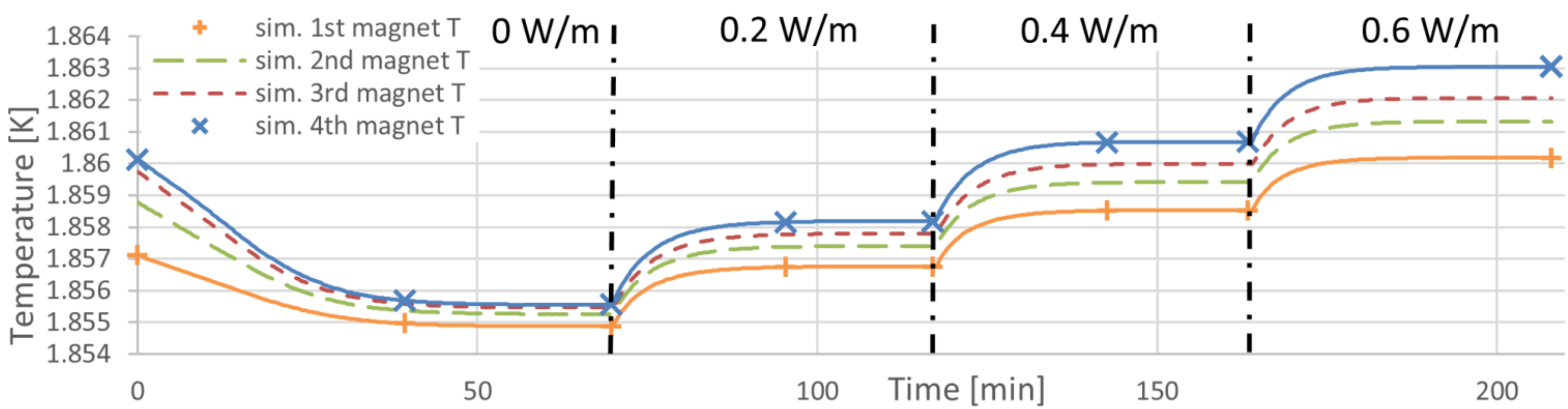
Graph modeling of the LHC SHe cooling loop





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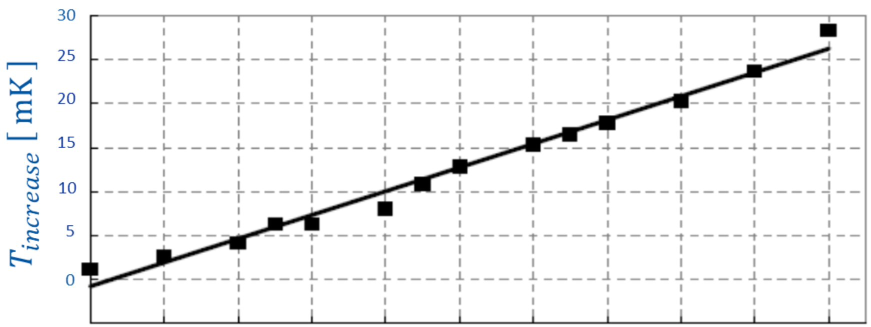
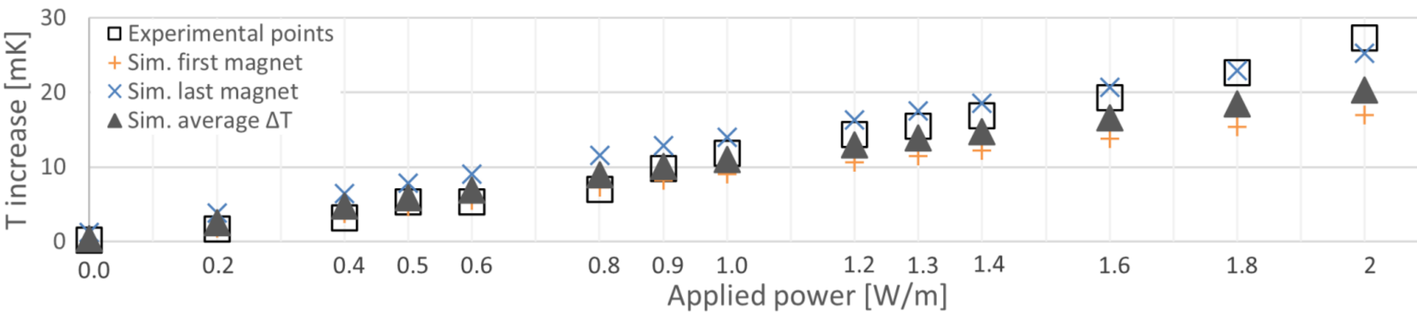
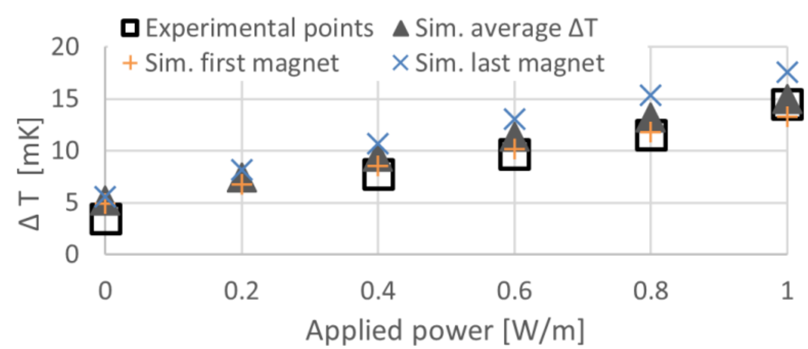
Model training and testing on prototypes data



simulated experiments performed to measure the heat conductivity of BHX on the prototype LHC magnets

- applied heat load is set
- system left to find new equilibrium temperature state
- temperature difference is measured





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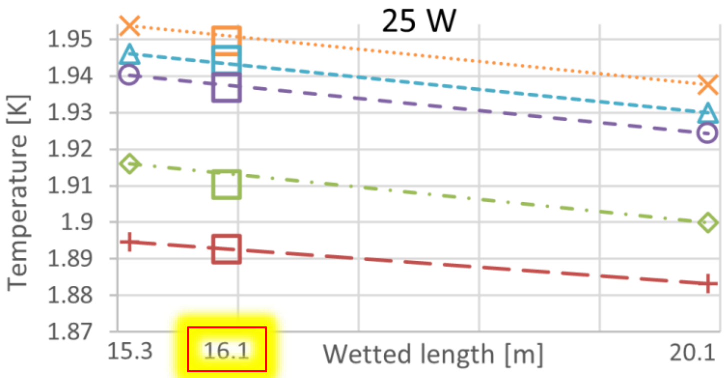
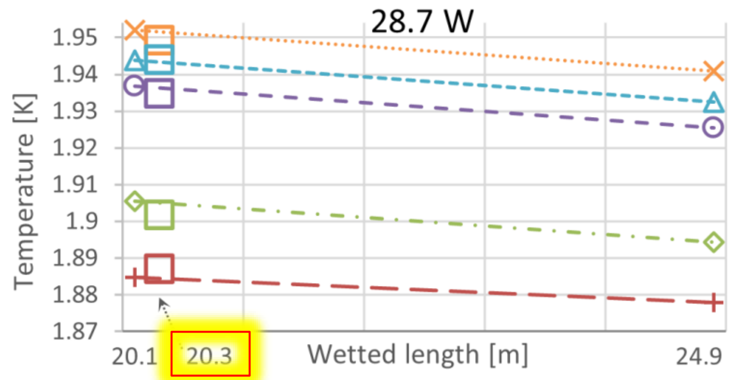
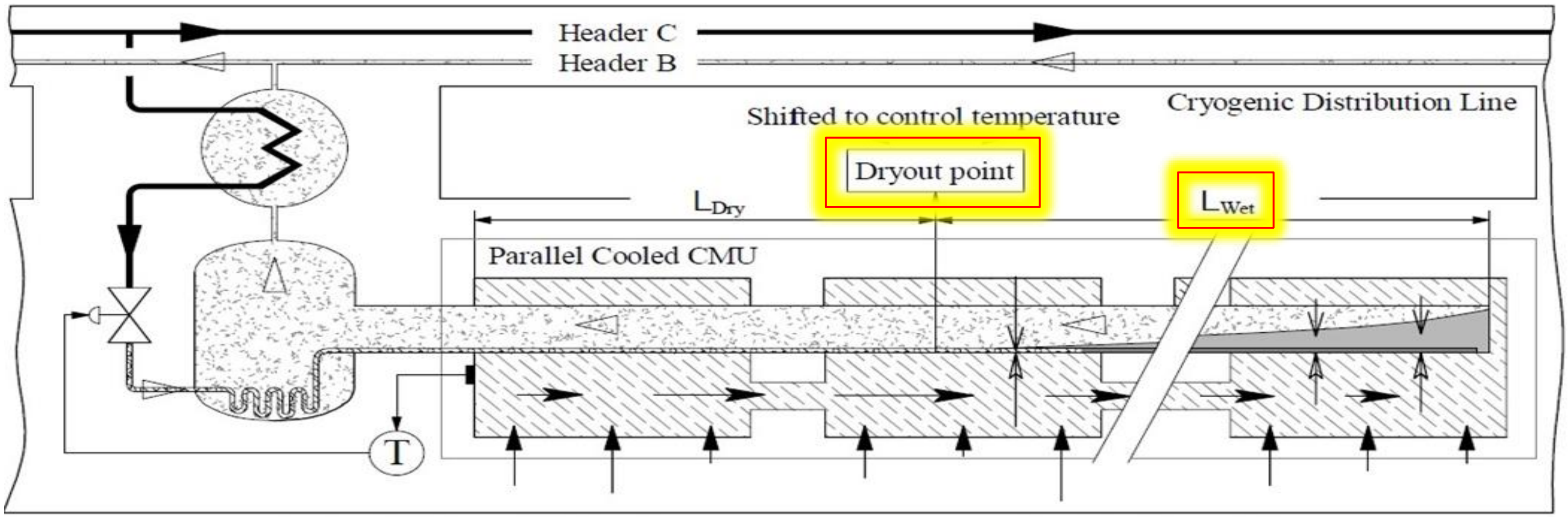
Simulation of the LHC accelerator operation







The distribution of temperatures is predicted within sensor's overall absolute accuracy of 5 mK
The derived wetted lengths match the temperature distribution along the magnet string

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Conclusions and perspectives

The developed model is:

- accurate despite some simplifications
- inspectable and explainable
- provides the time evolution of all internal variables
- is easily scalable to simulate various system configurations

The model can be used to

- test and validate existing and future designs
- perform diagnostics (twin model)
- support advanced predictive control

We plan to further improve it by removing current simplifications

- modelling non-linear characteristics of superfluid helium II
- proper simulation of gaseous flow to predict the inverse response