Multivariate meta-modelling for Human-interpretable, dynamic **AI** with an eye for the physics

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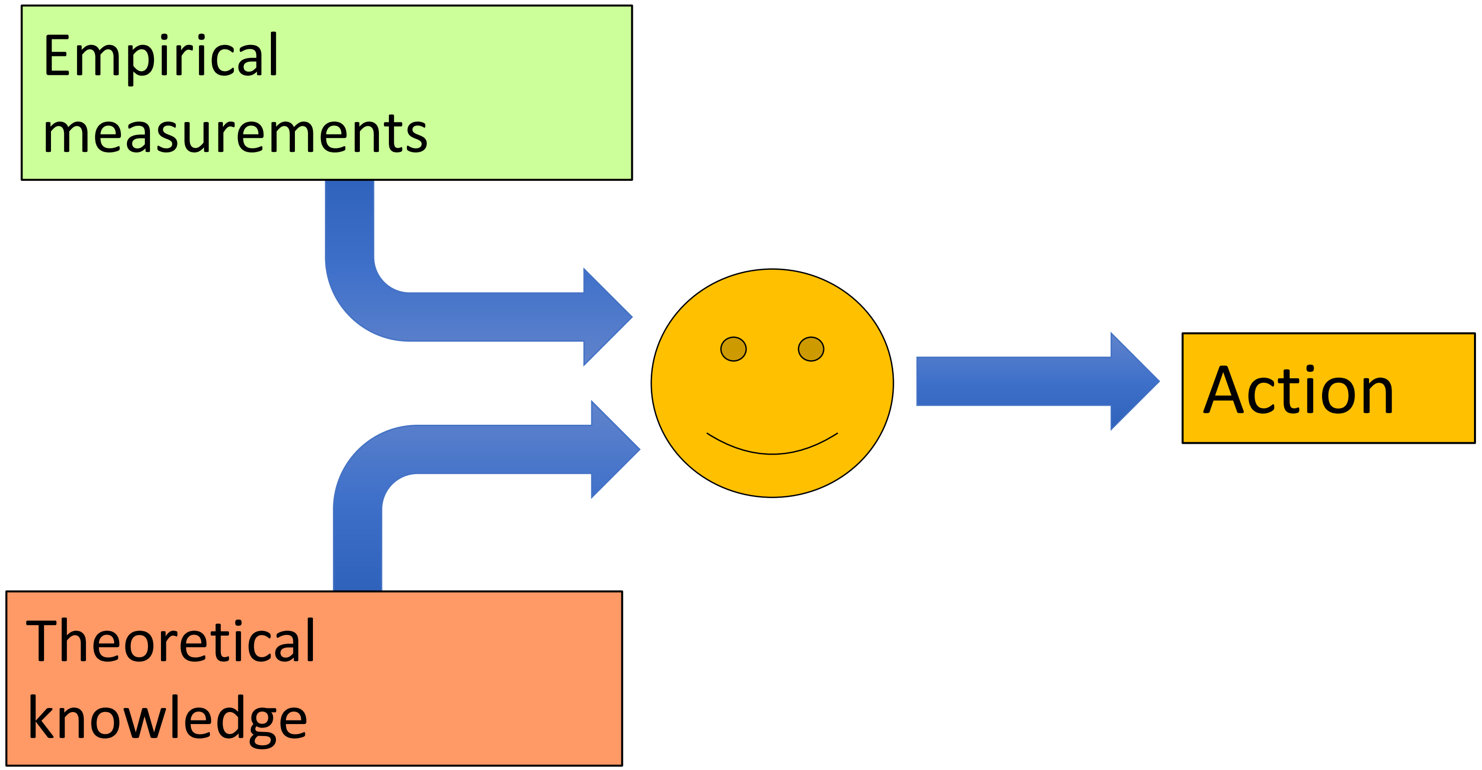
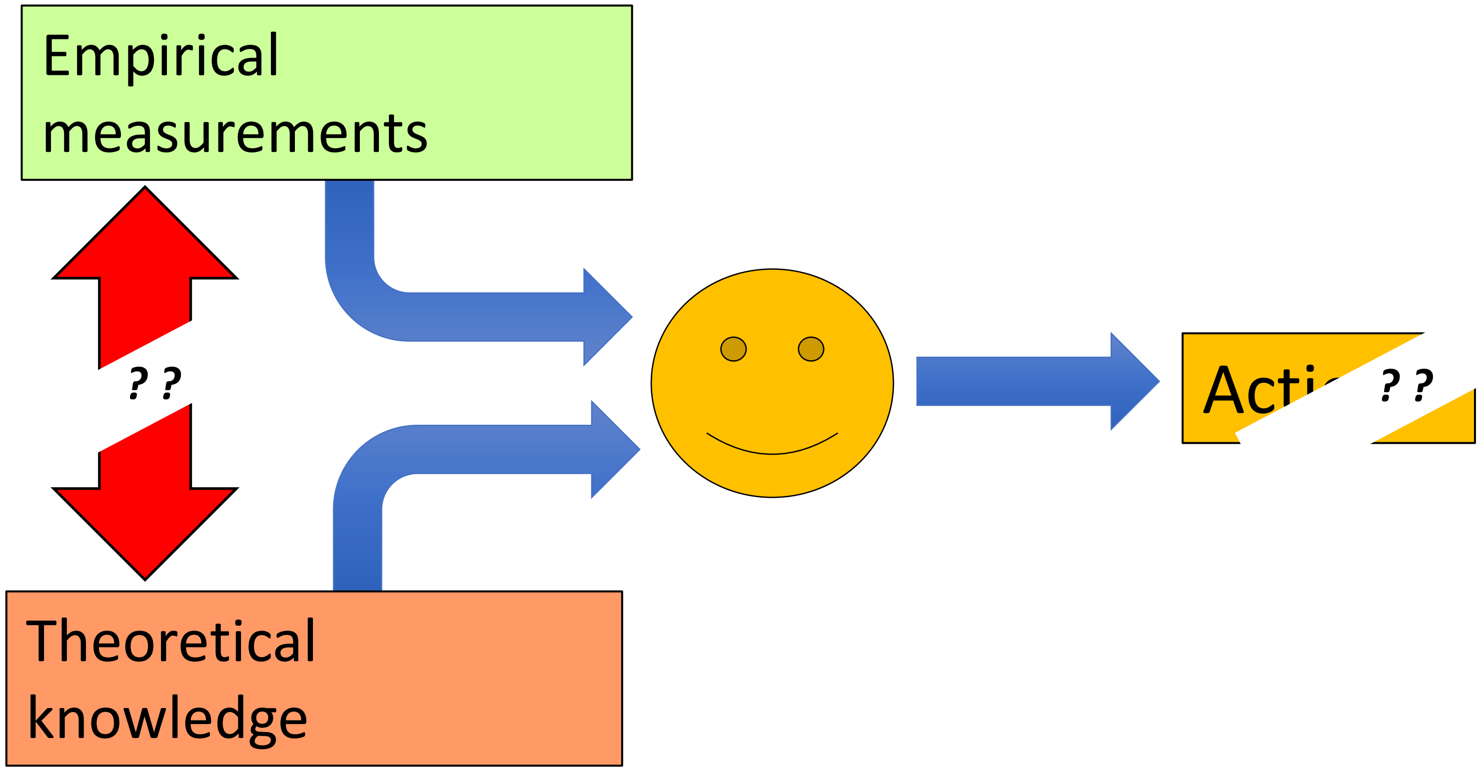
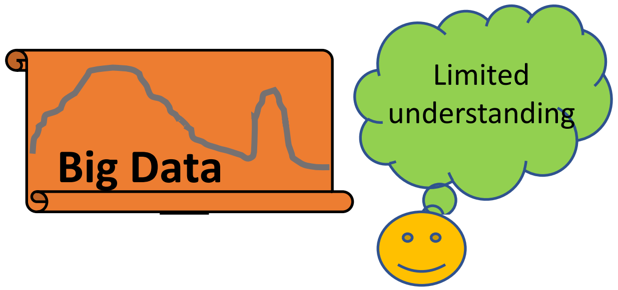
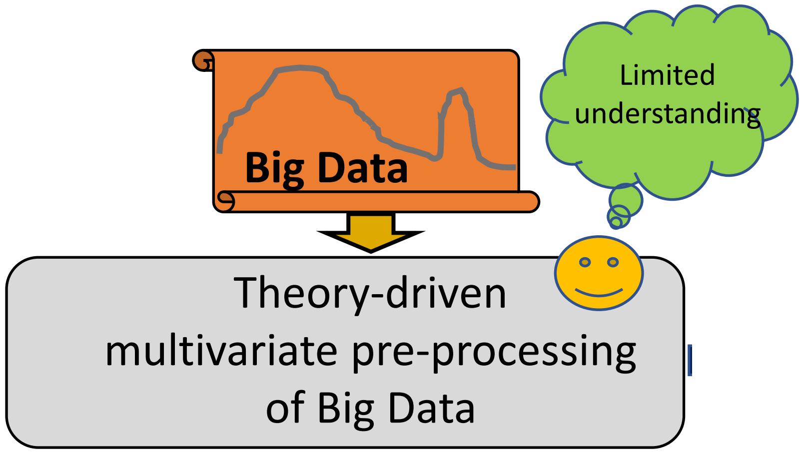
Two source of knowledge

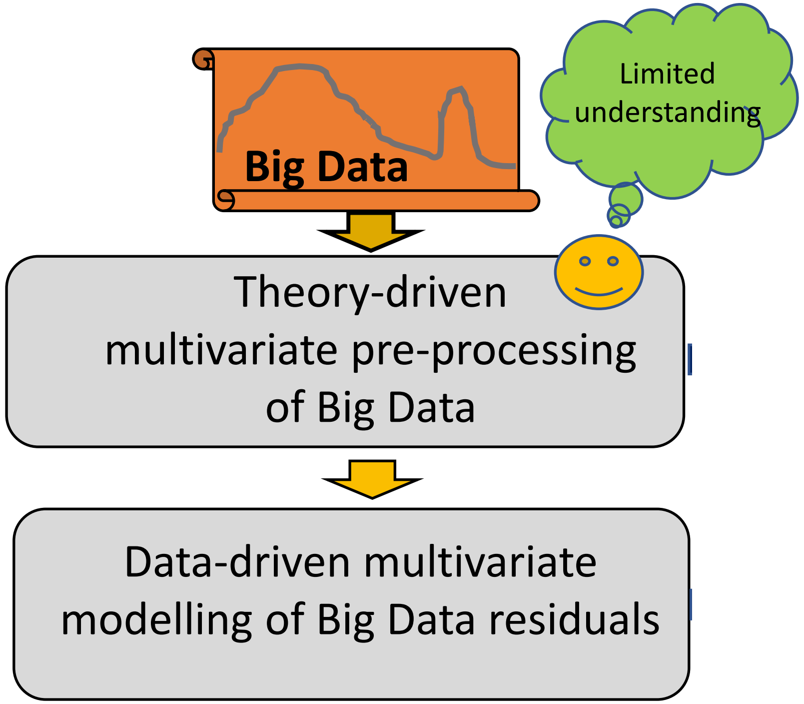


Two incompatible cultures ?




Big Data
Limited understanding


Big Data
Limited understanding
Theory-driven multivariate pre-processing of Big Data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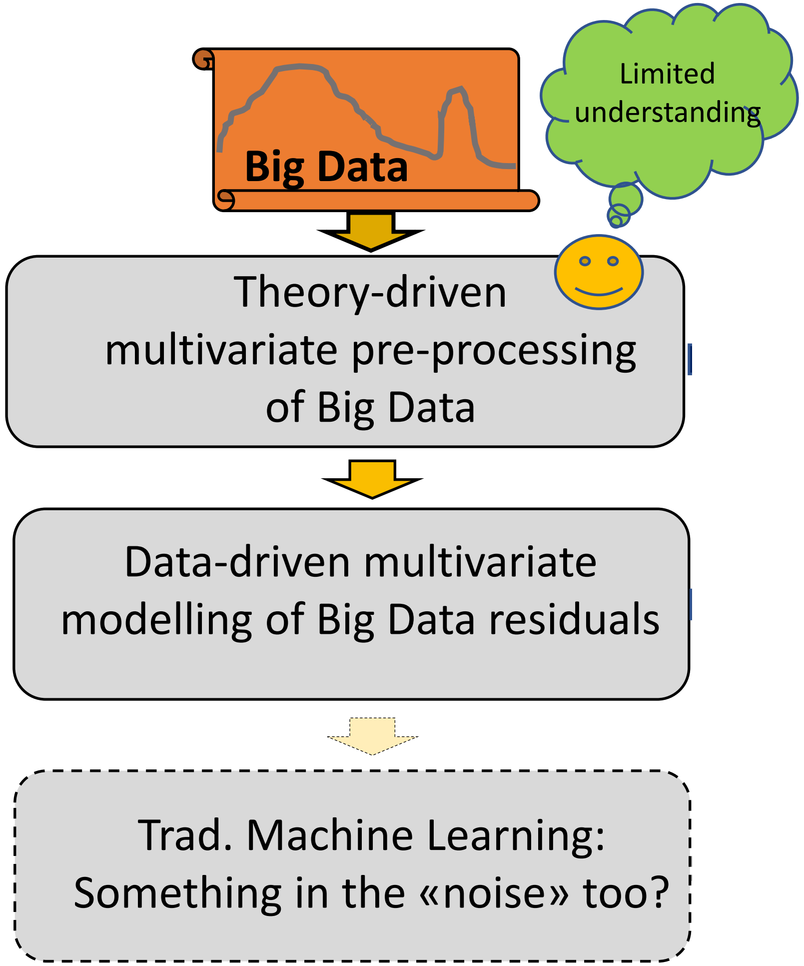
Data-driven multivariate modelling of Big Data residuals



Big Data
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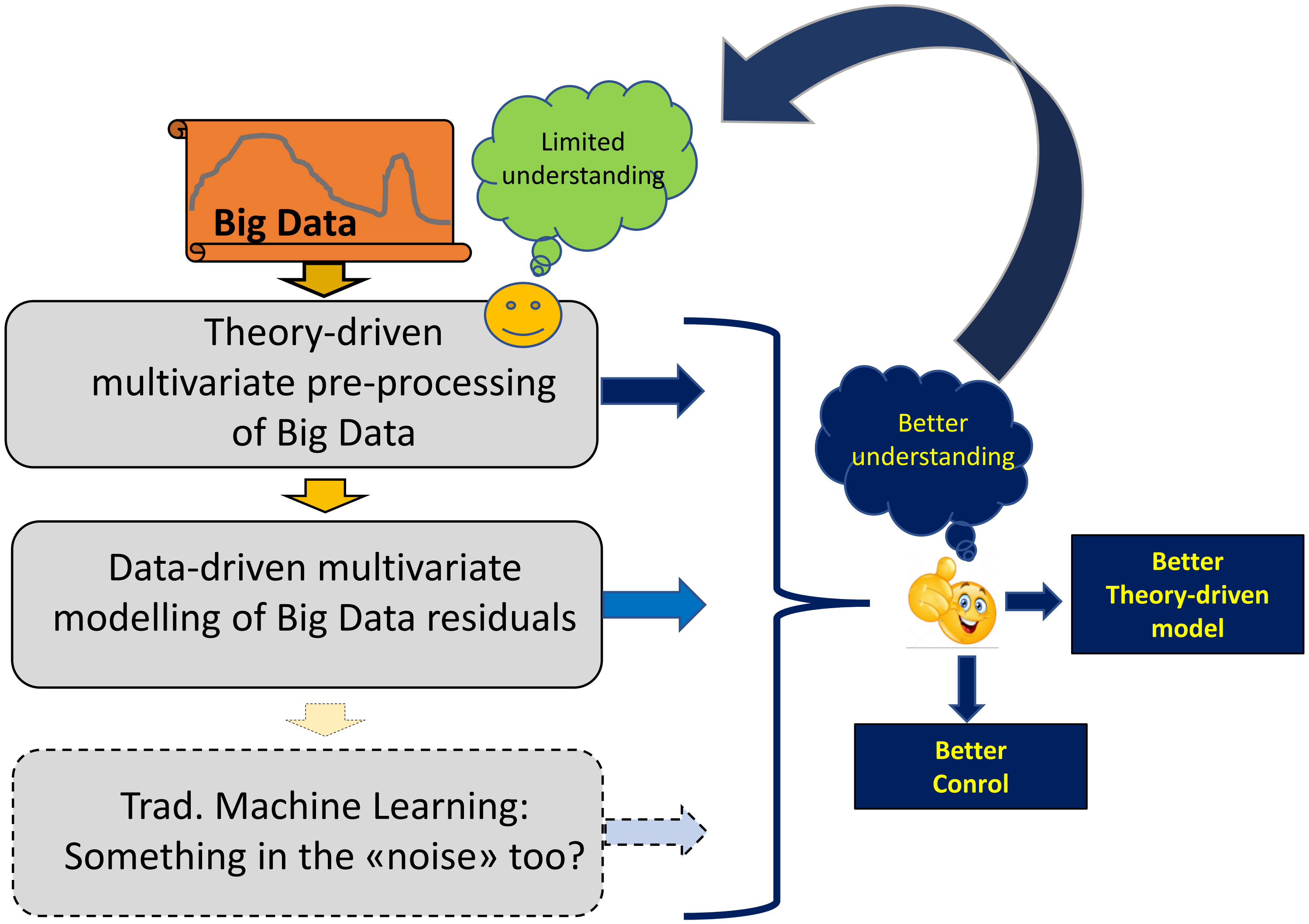
Trad. Machine Learning: Something in the «noise» too?



Big Data
Limited understanding
Theory-driven multivariate pre-processing of Big Data
Data-driven multivariate modelling of Big Data residuals
Trad. Machine Learning: Something in the «noise» too?
Better understanding
Better Theory-driven model
Better Conrol

Problem:
Shadows and other illumination effects

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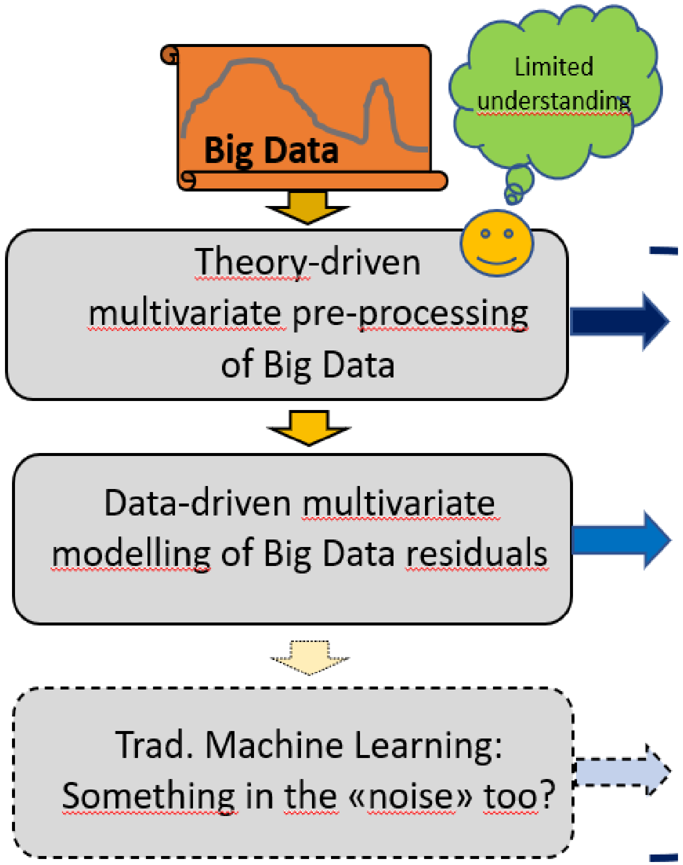
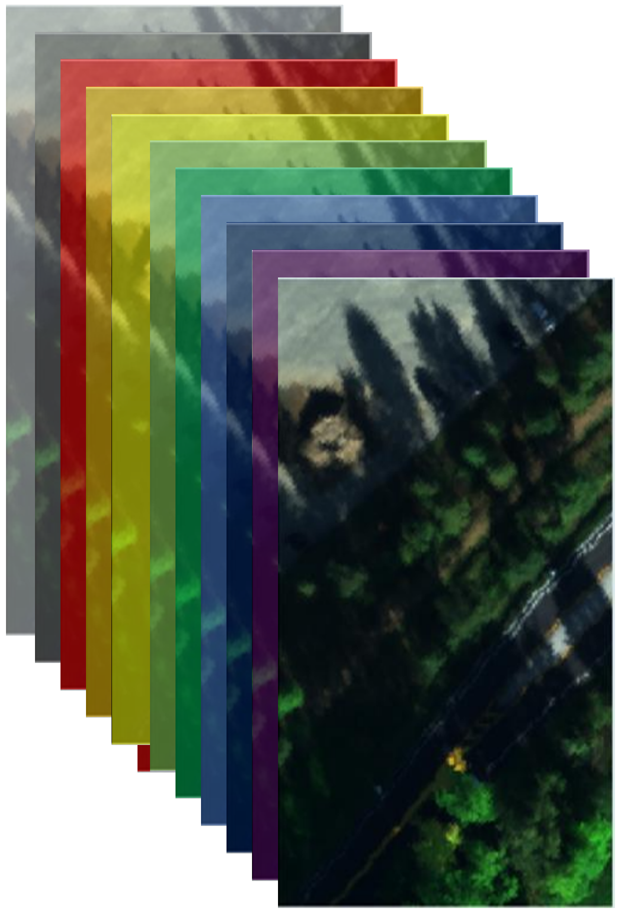
1. Multi-channel or «hyperspectral» imaging





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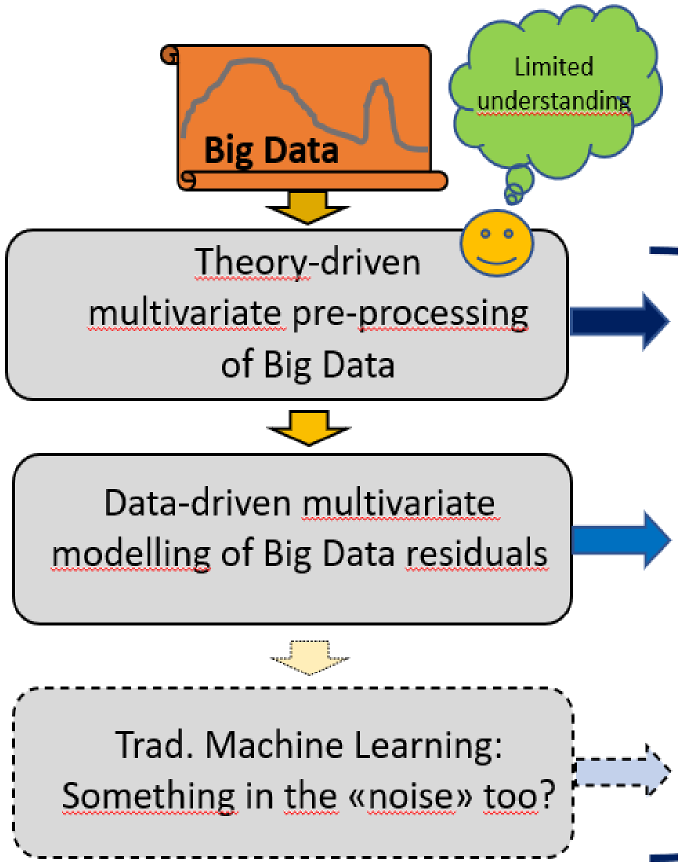
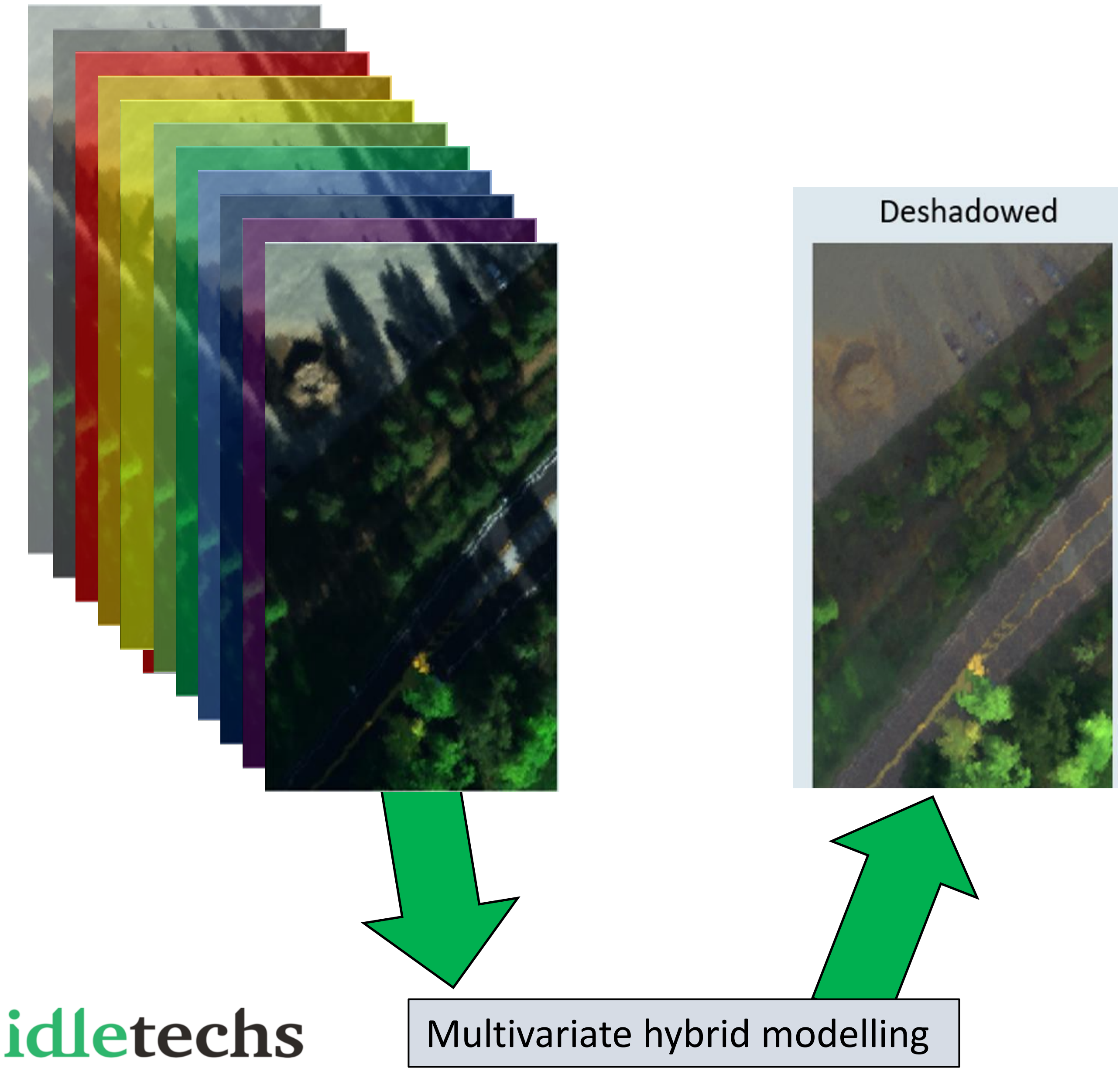
2. Multivariate spectral pre-processing





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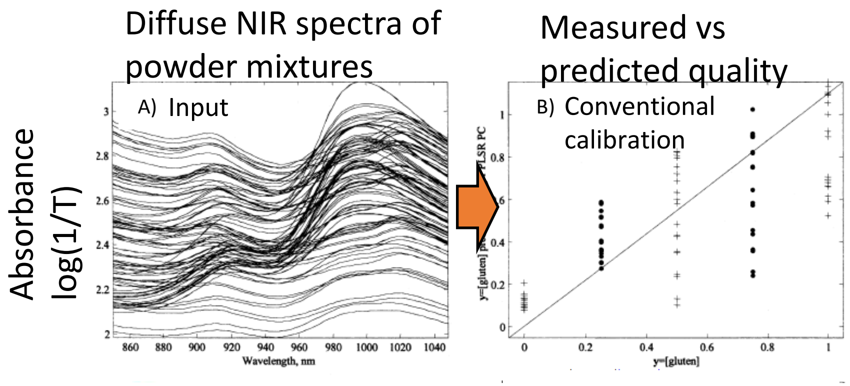
High-speed spectroscopic profiling of powder mixtures



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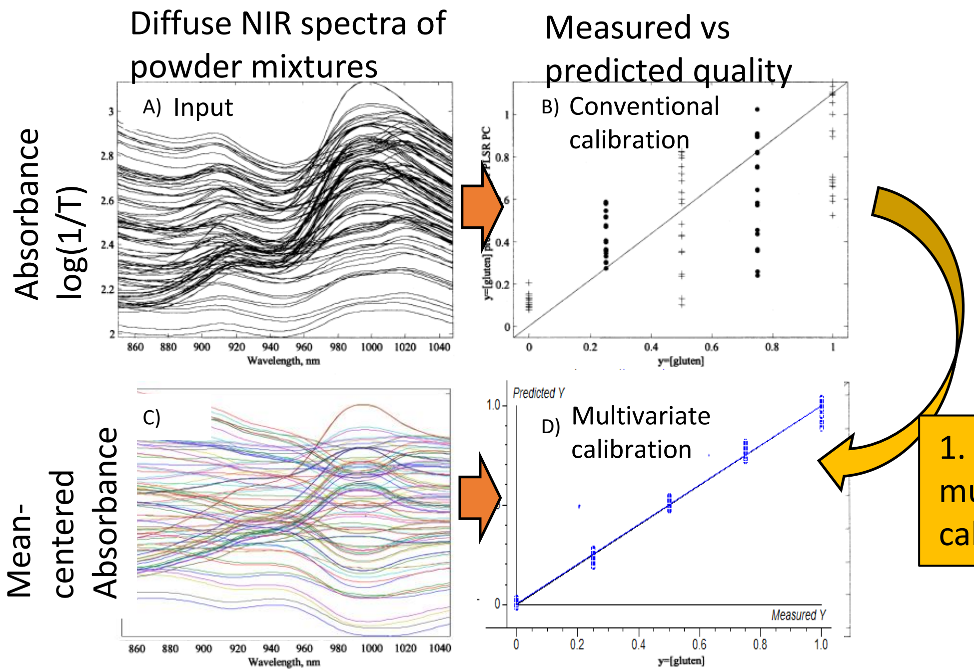
High-speed spectroscopic profiling of powder mixtures



1. Purely empirical multivariate calibration model

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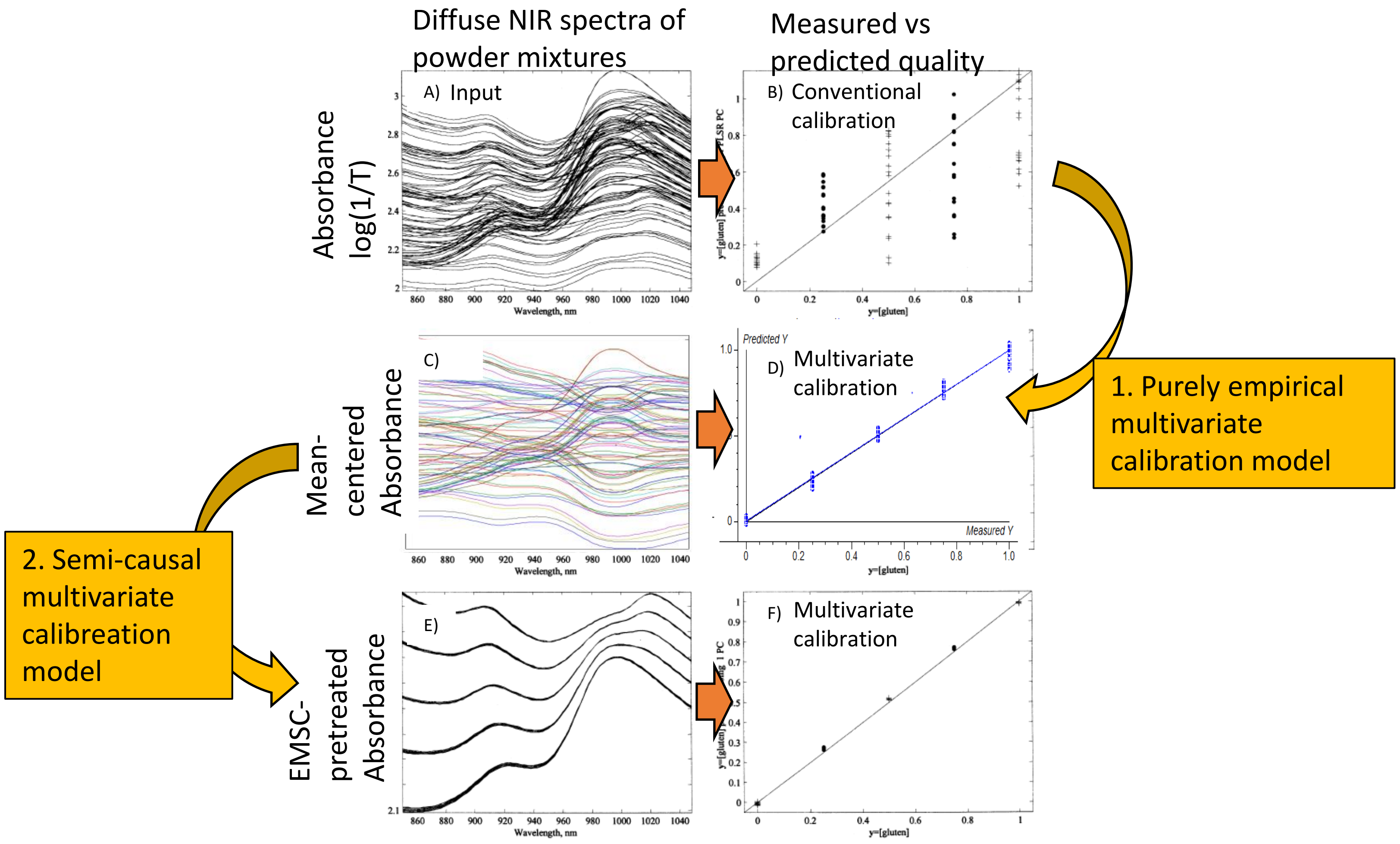
High-speed spectroscopic profiling of powder mixtures



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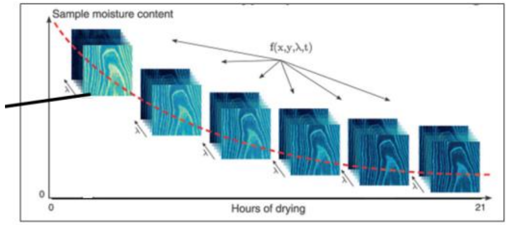
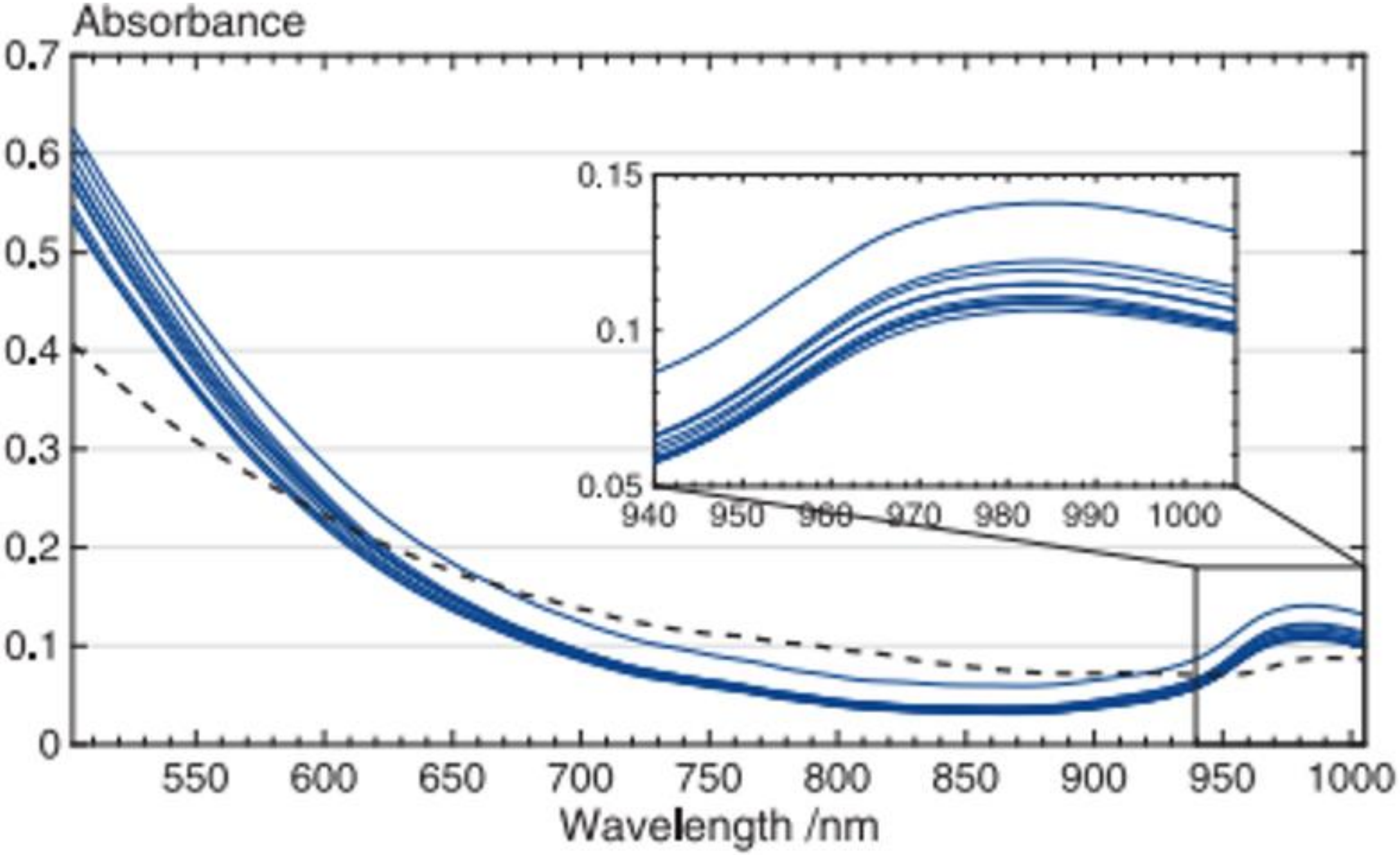
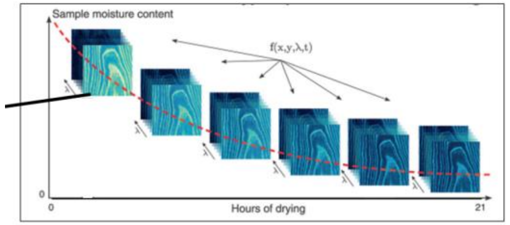
Hyperspectral NIR video



Drying of wet wood



Hyperspectral NIR video



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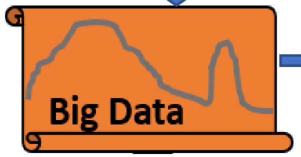

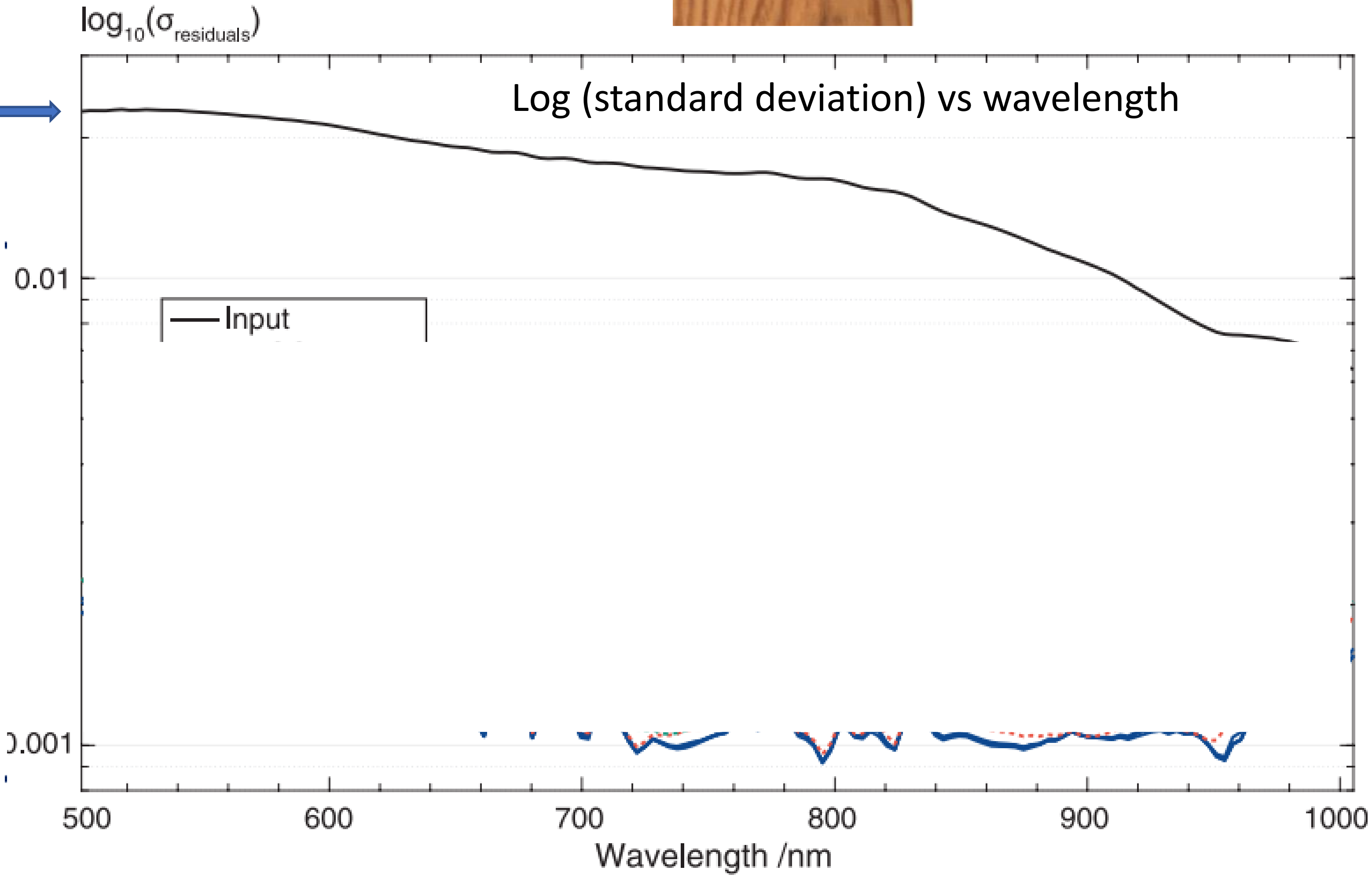

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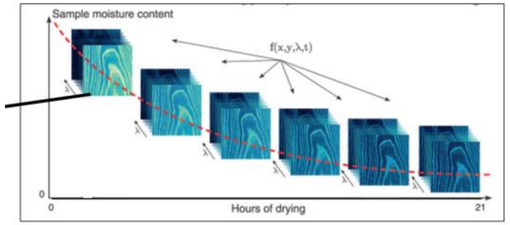

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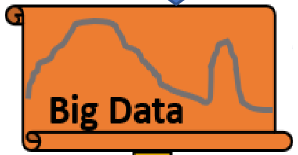
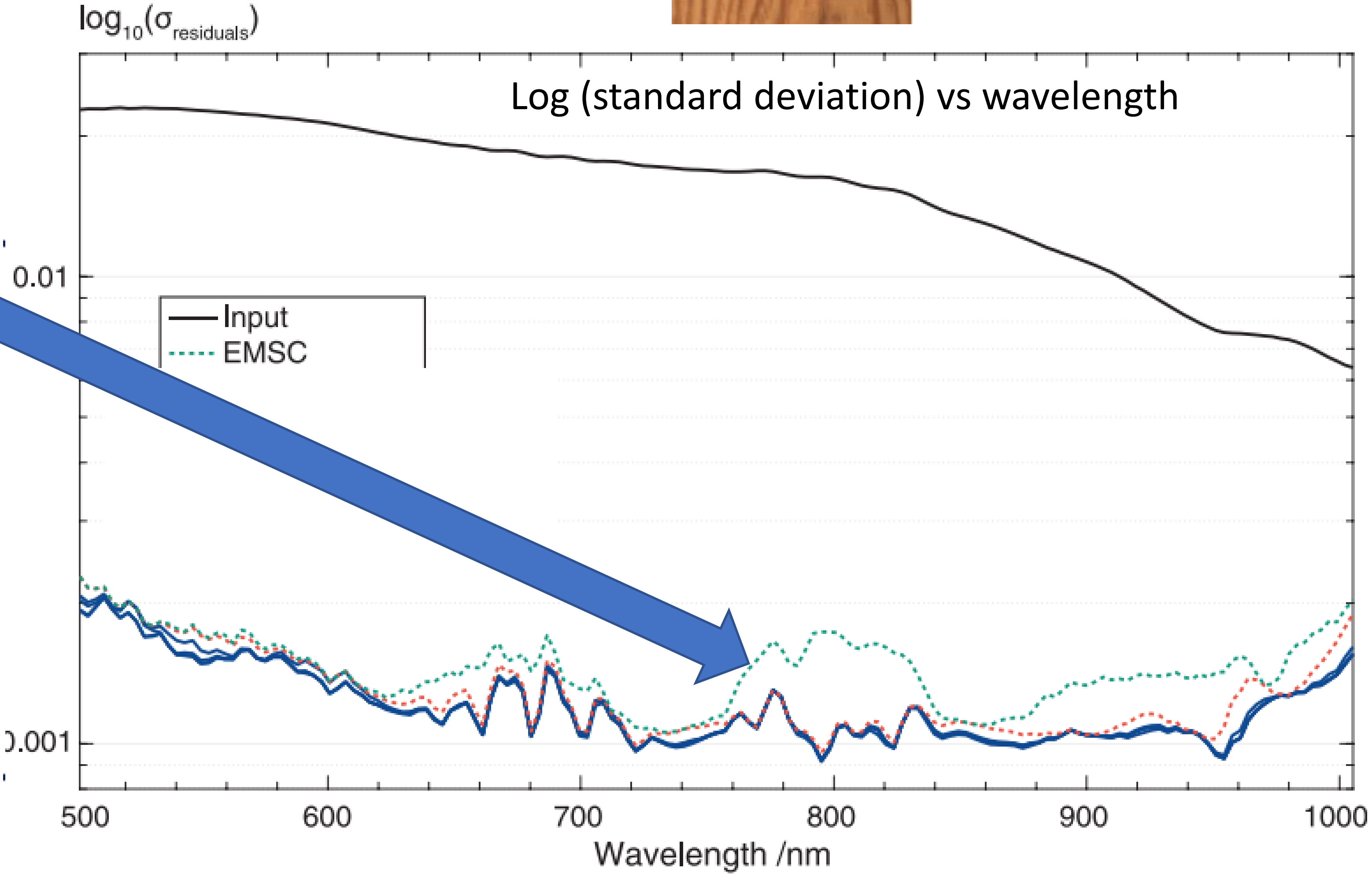
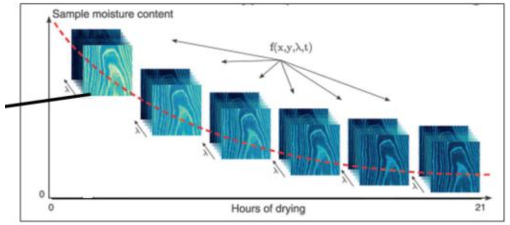


Theory-driven multivariate pre-processing of Big Data



Hyperspectral NIR video



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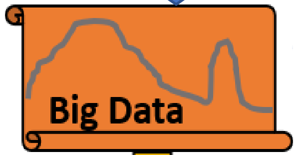
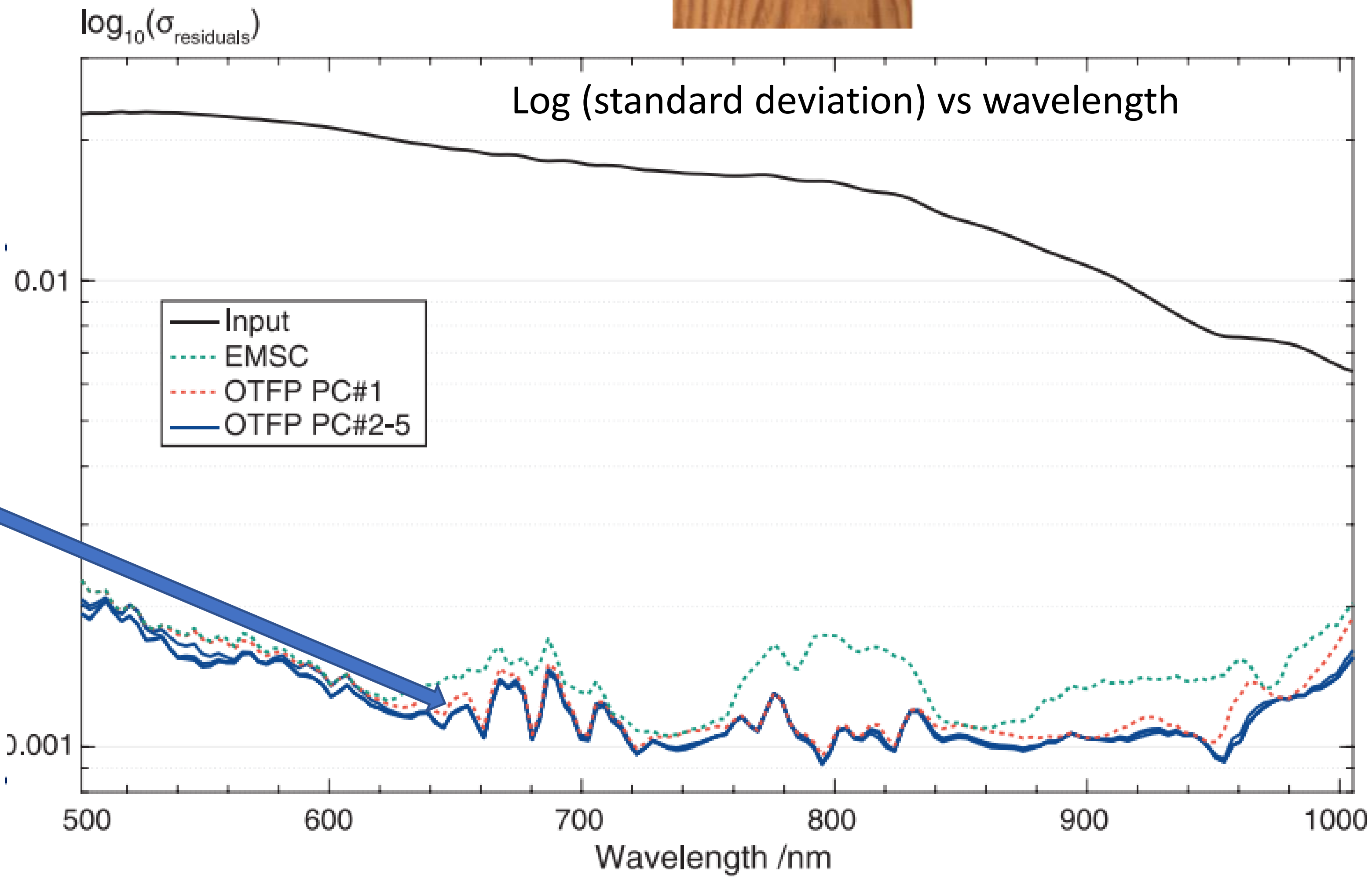
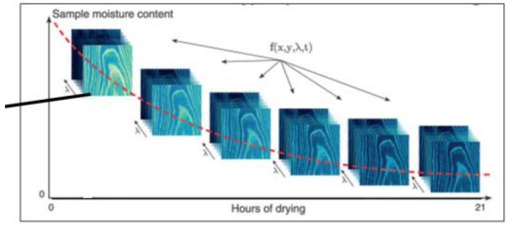


Theory-driven multivariate pre-processing of Big Data

Data-driven multivariate modelling of Big Data residuals



Hyperspectral NIR video



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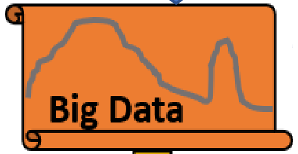
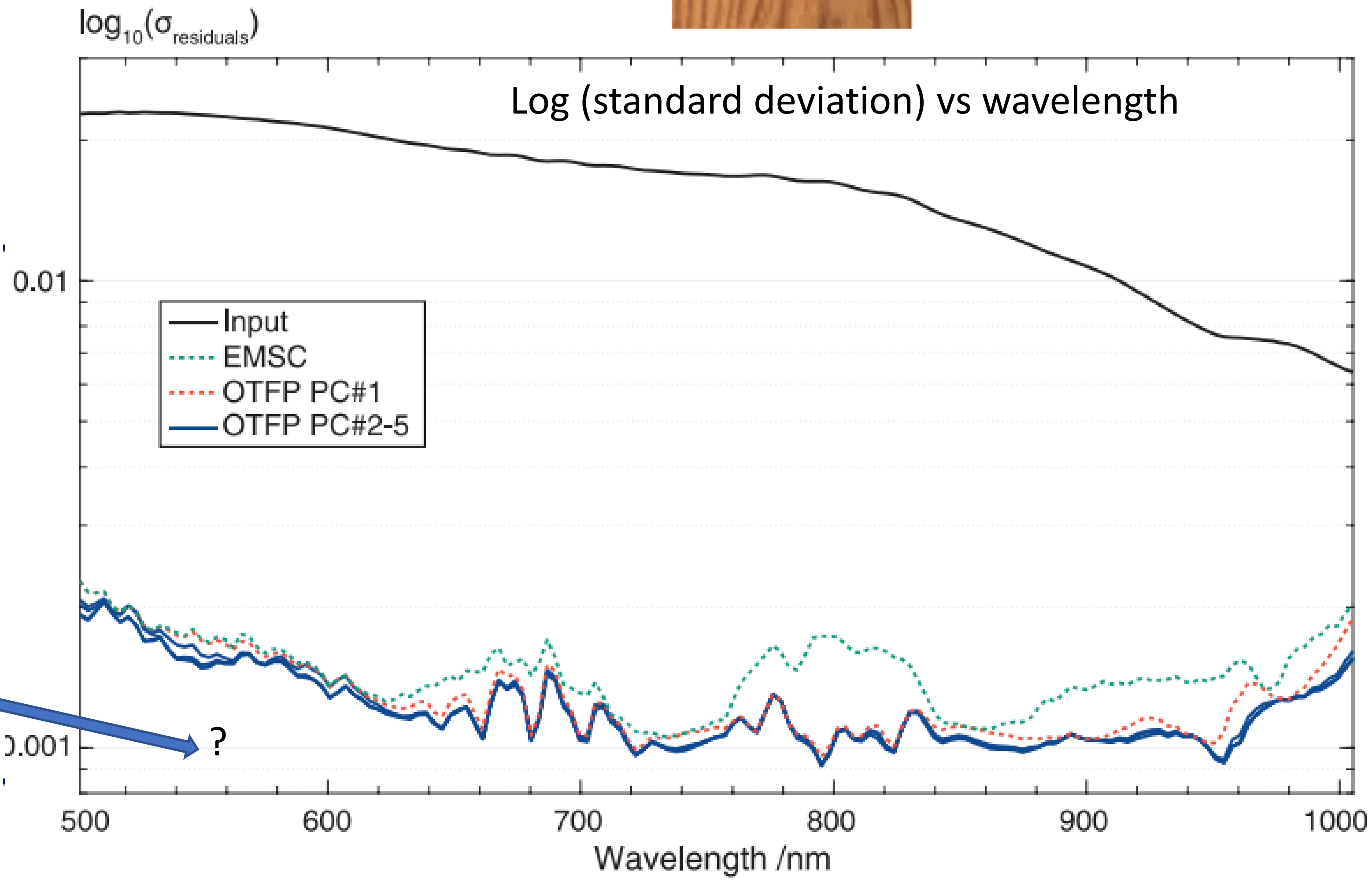


Theory-driven multivariate pre-processing of Big Data

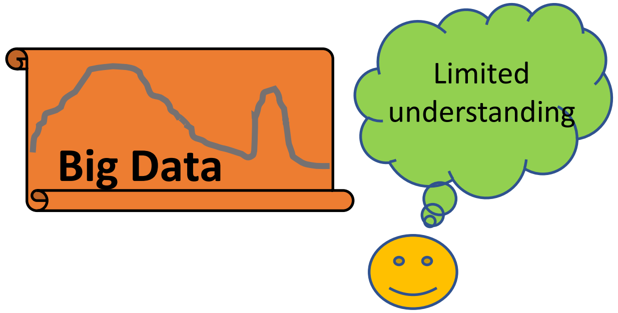
Data-driven multivariate modelling of Big Data residuals

Trad. Machine Learning: Something in the «noise» too?

?



Human-interpretable, dynamic **AI** with an eye for the physics



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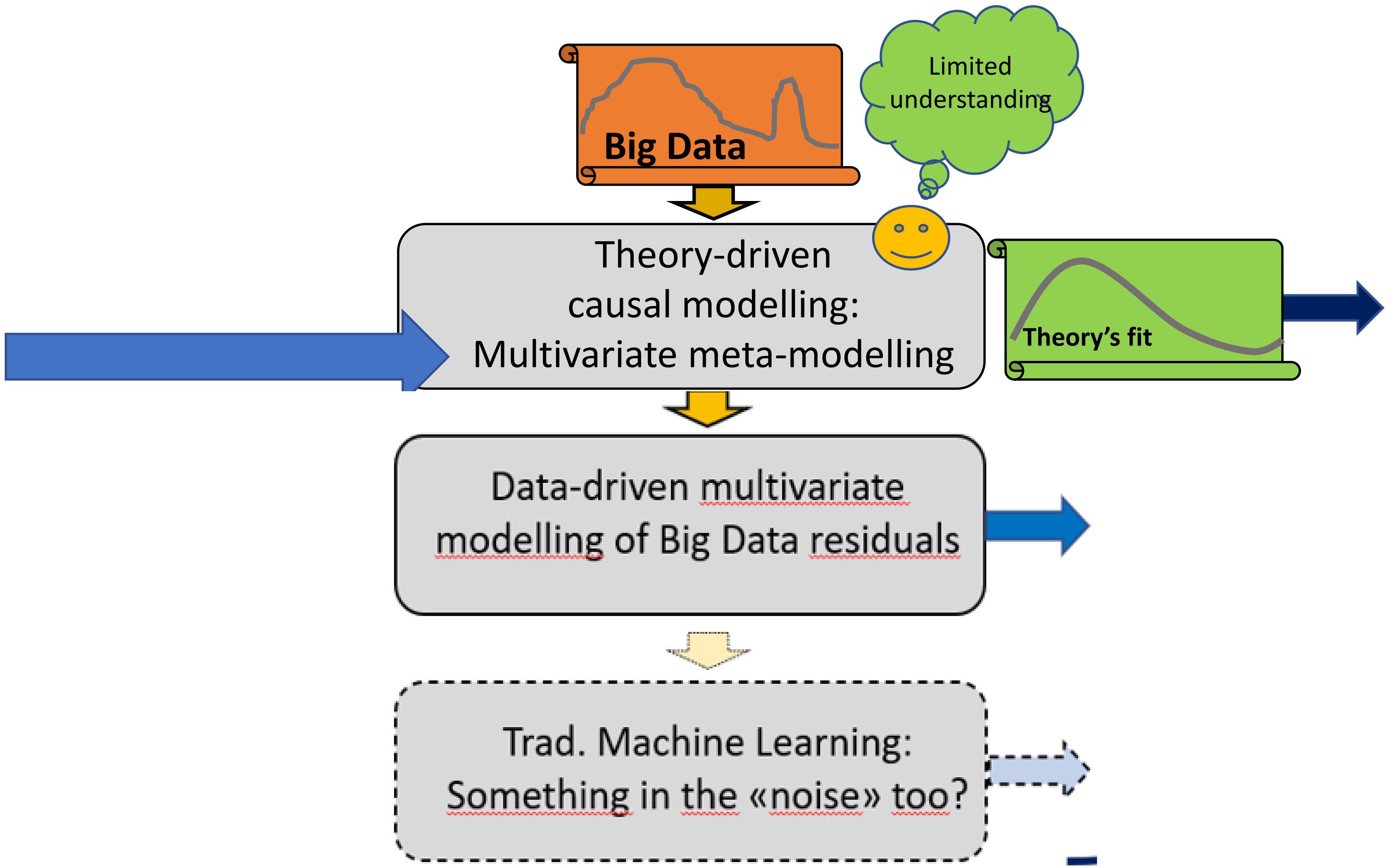
Multivariate meta-modelling:

Fast, interpretable statistical "surrogate" model of a slow model



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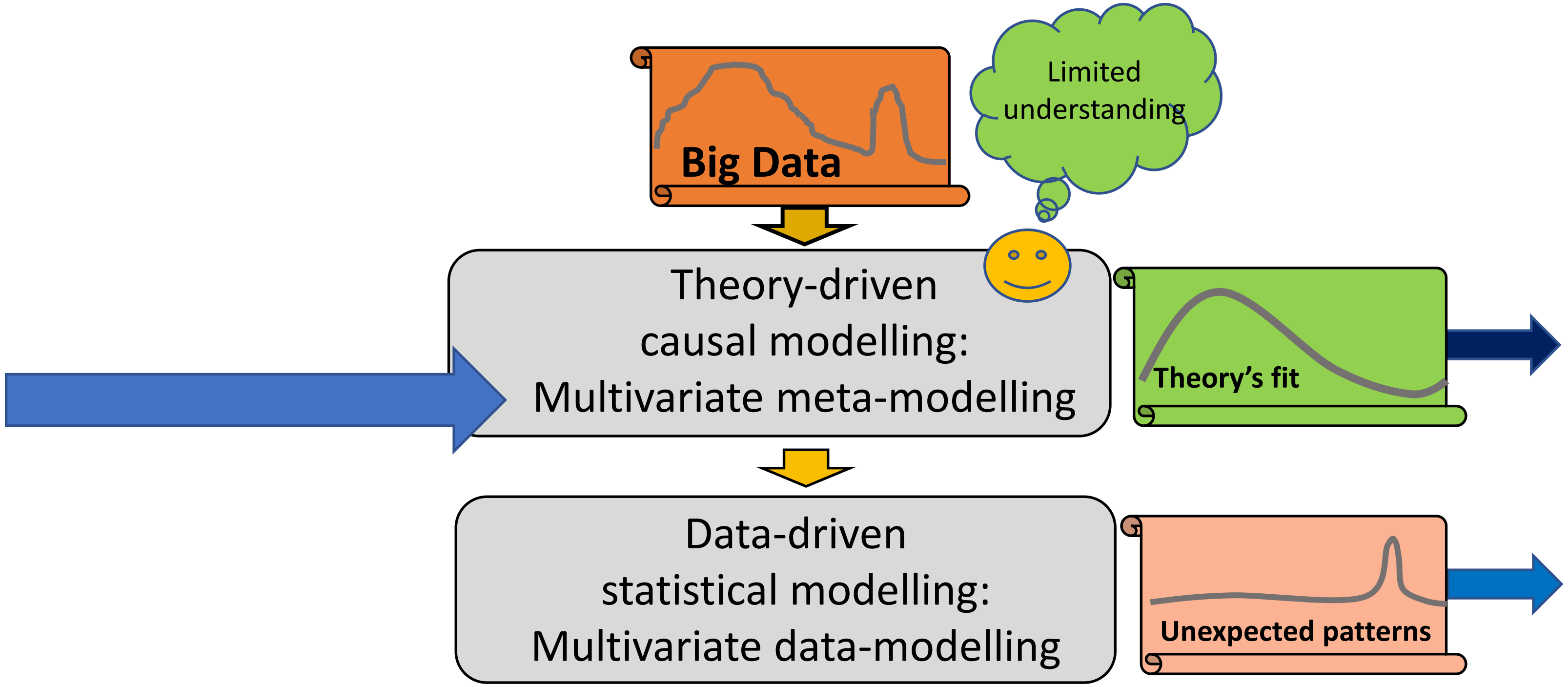
Fast, interpretable statistical "surrogate" model of a slow model



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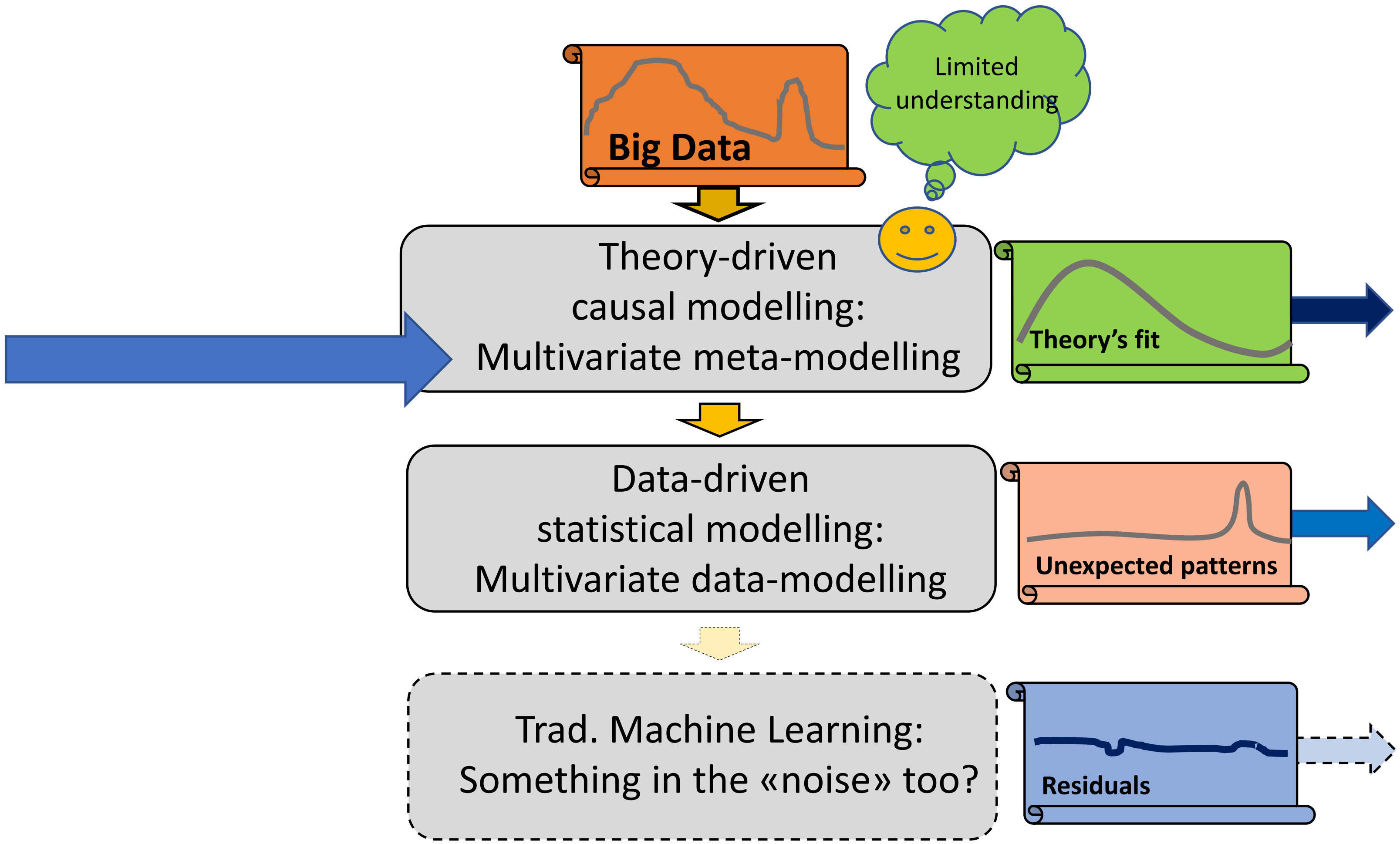

Multivariate meta-modelling:

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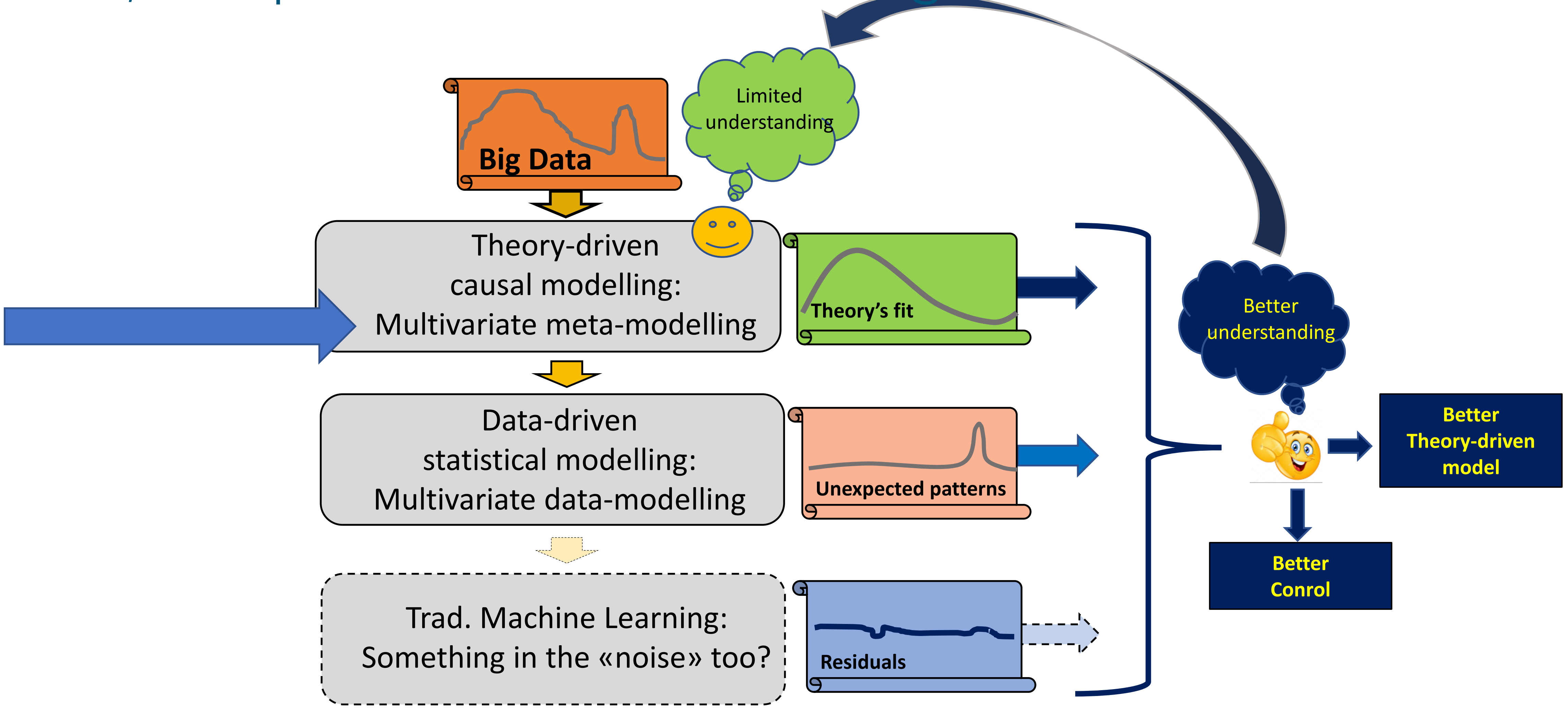
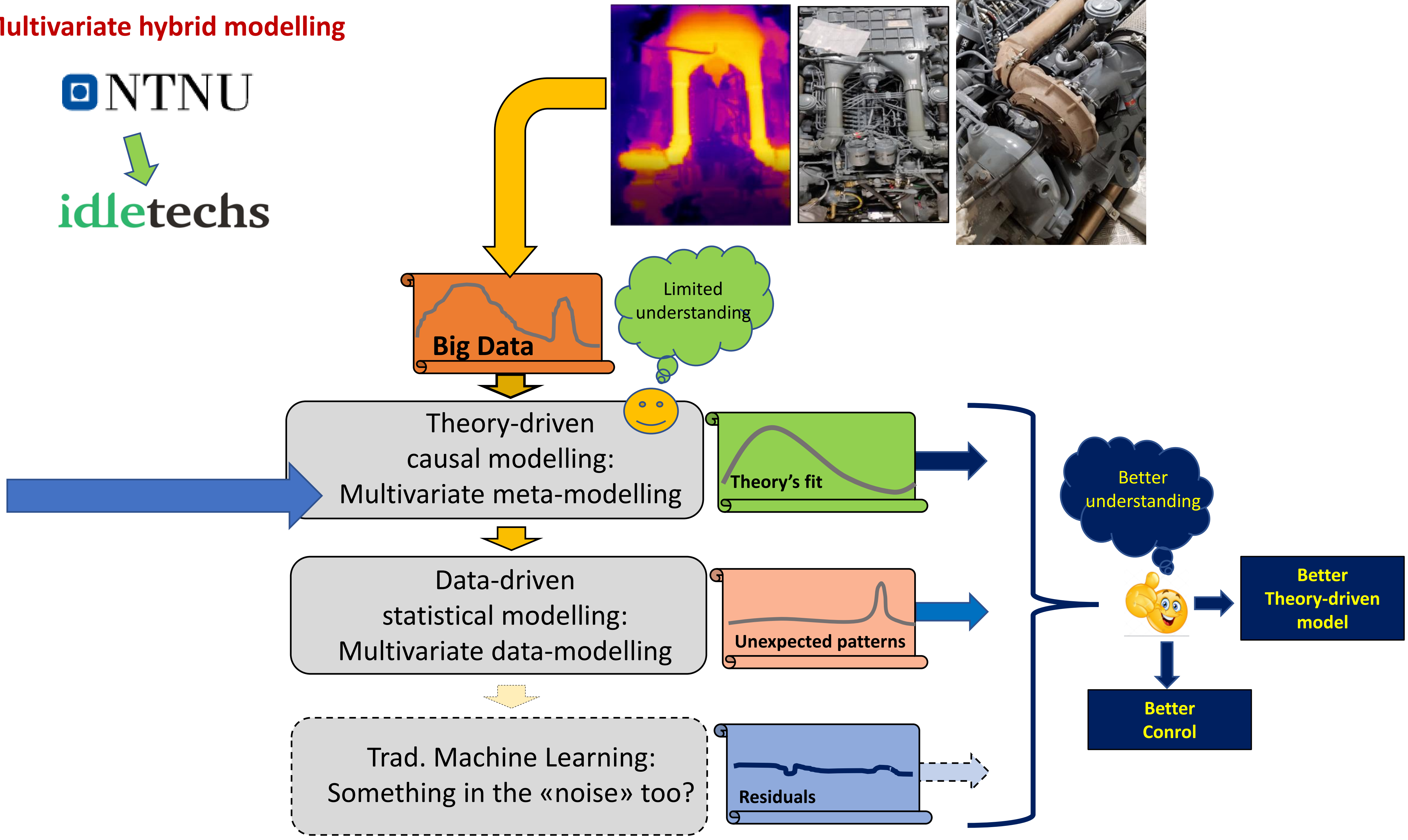


Multivariate hybrid modelling



Metamodelling in metallurgy

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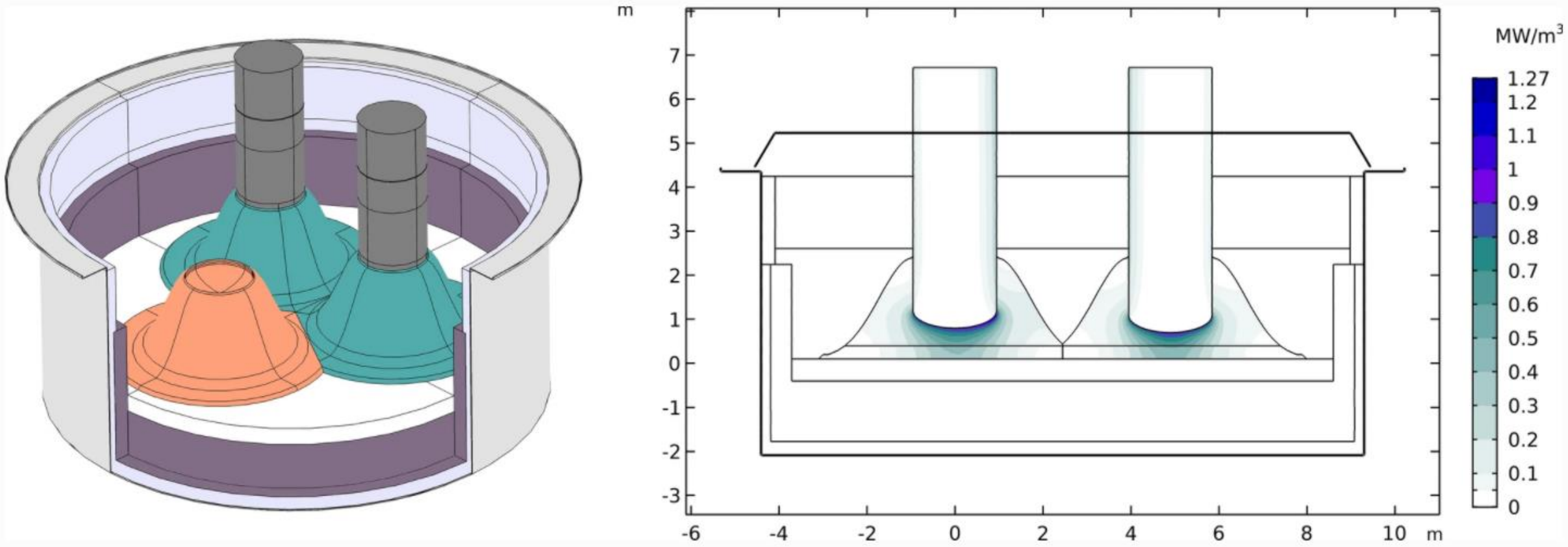
Metamodeling of the Electrical Conditions in Submerged Arc Furnaces

Manuel Sparta, Damiano Varagnolo, Kristian Stråbø, Svenn Anton Halvorsen, Egil Vålandsmyr Herland & Harald Martens

Metallurgical and Materials Transactions B **52**, 1267–1278 (2021) | Cite this article

Fig. 1

From: Metamodeling of the Electrical Conditions in Submerged Arc Furnaces



FEM model. Left panel: 3D rendering of the furnace where charge and other sections are hidden to reveal the coke beds (orange and green), two electrodes (dark gray), the metal pool (white), the furnace linings (light and dark purple) and the steel shell (silver). Right panel: 2D slice showing a typical power dissipation density (Color figure online)

Metamodelling in metallurgy

Springer Link

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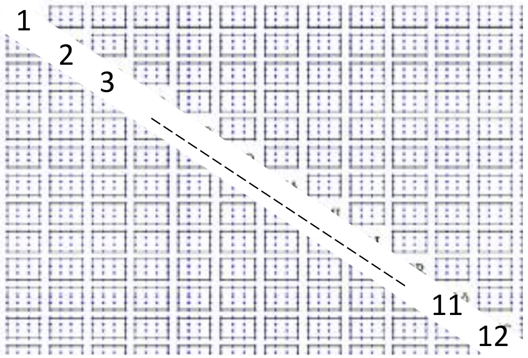
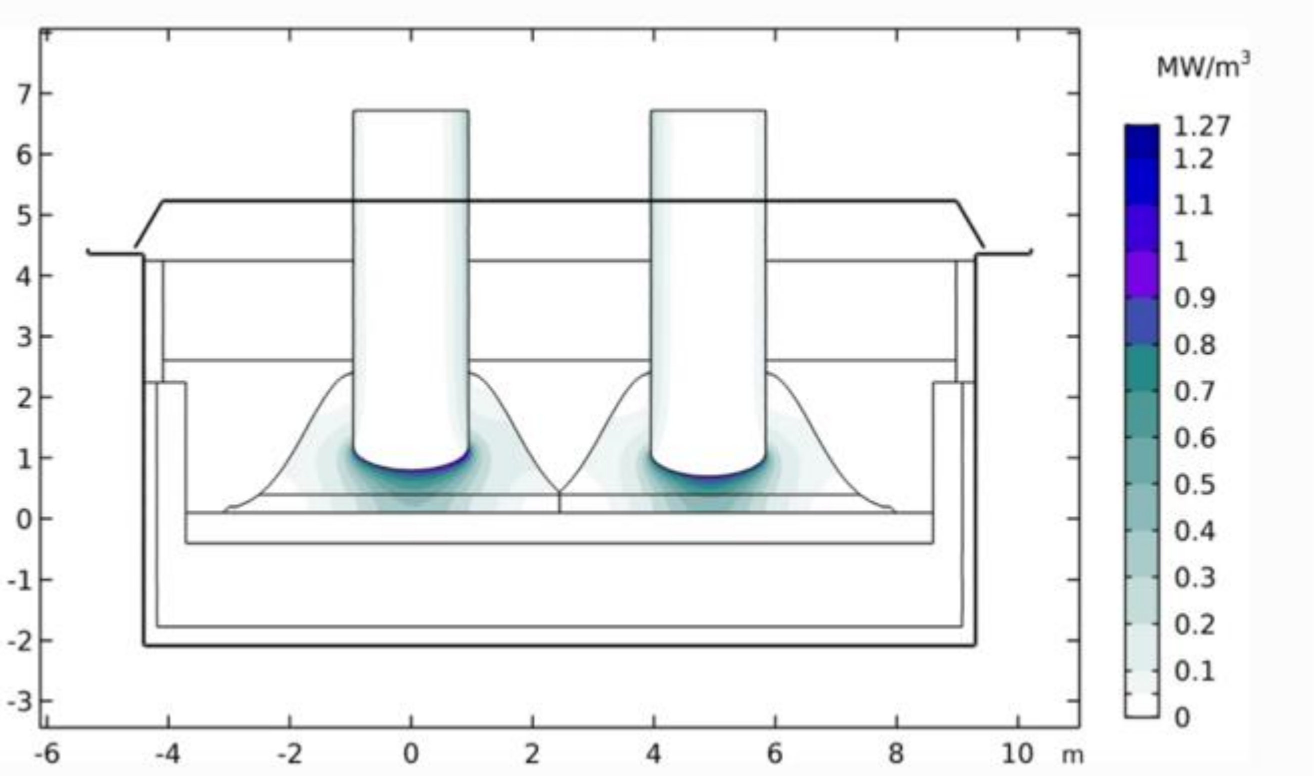
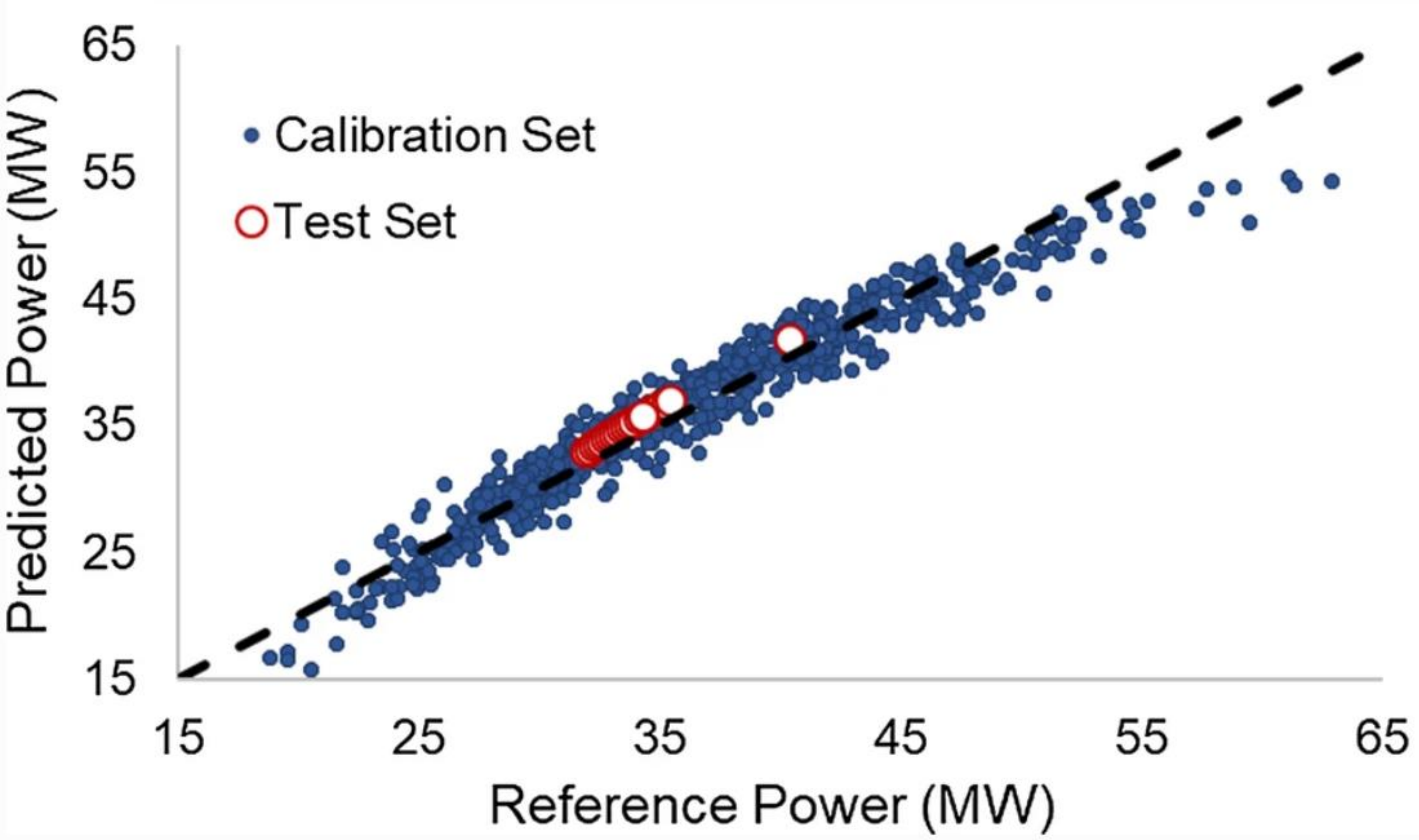
Sparse factorial design in 12 input parameters

→ ≈ 500 simulations (instead of 4^{12}=17 000 000)



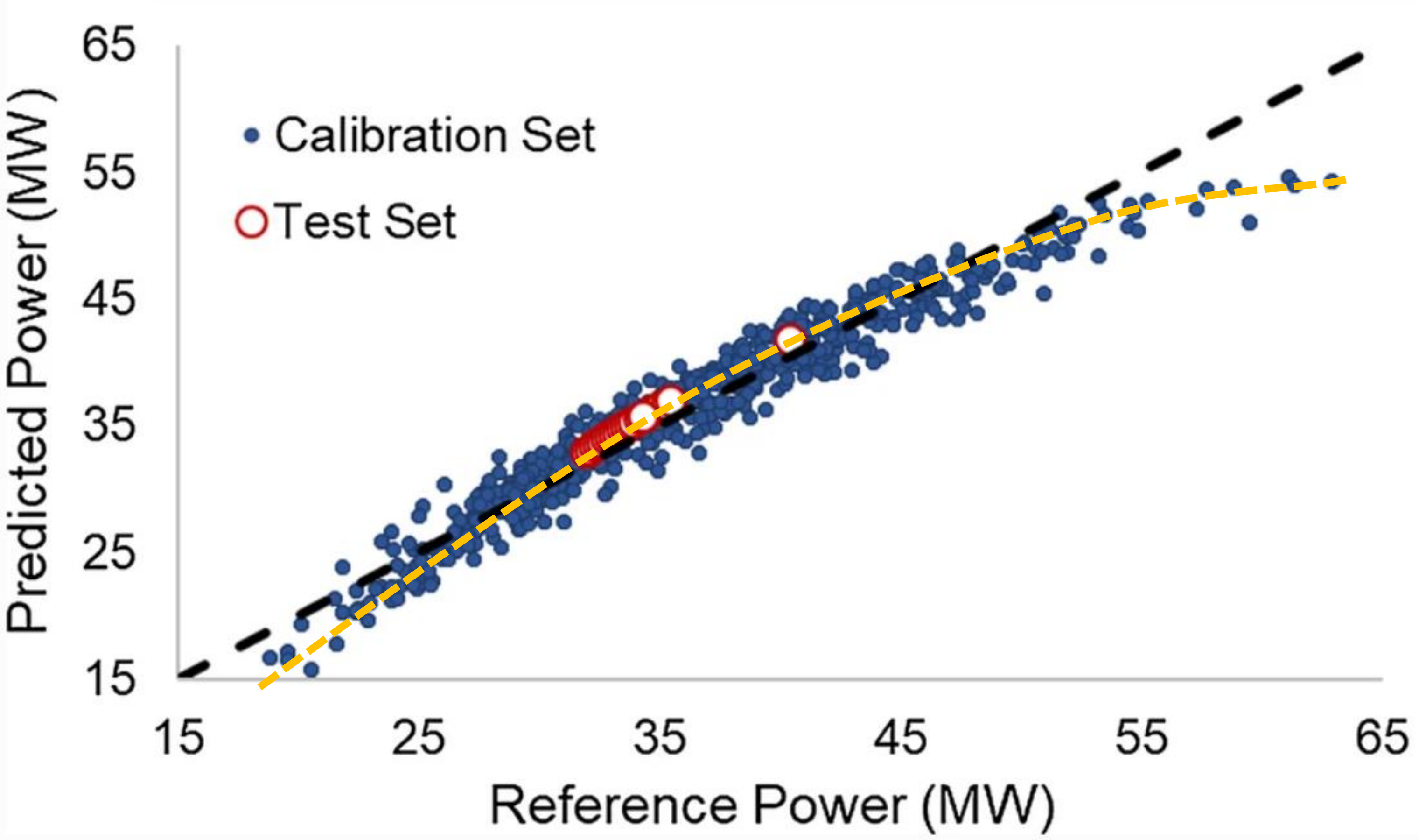


From: Metamodeling of the Electrical Conditions in Submerged Arc Furnaces



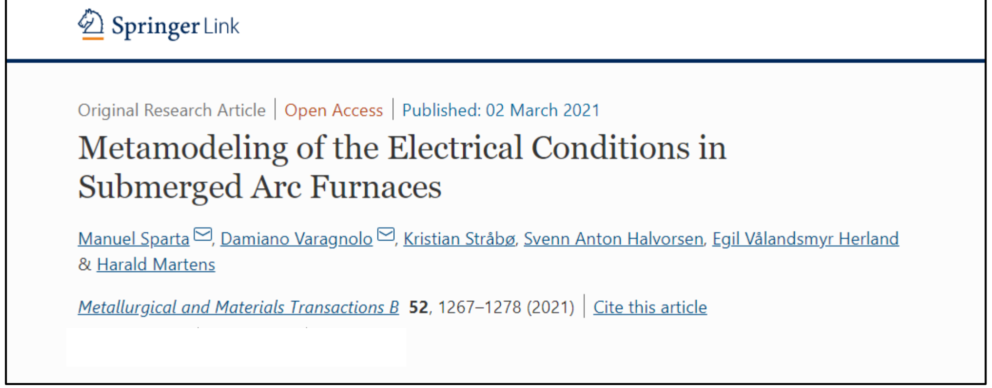
Calibration (blue) and Test (red) sets in the Predicted vs Reference Power plot (Color figure online)

From: Metamodeling of the Electrical Conditions in Submerged Arc Furnaces



Calibration (blue) and Test (red) sets in the Predicted vs Reference Power plot (Color figure online)

Summary: Fast causal modelling by **multivariate metamodelling**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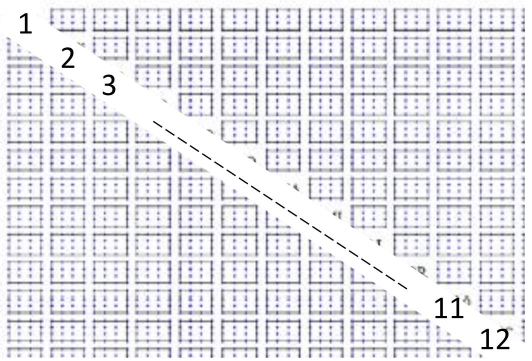
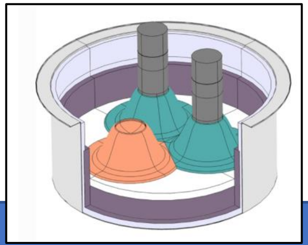
Furnace model: 12 input parameters

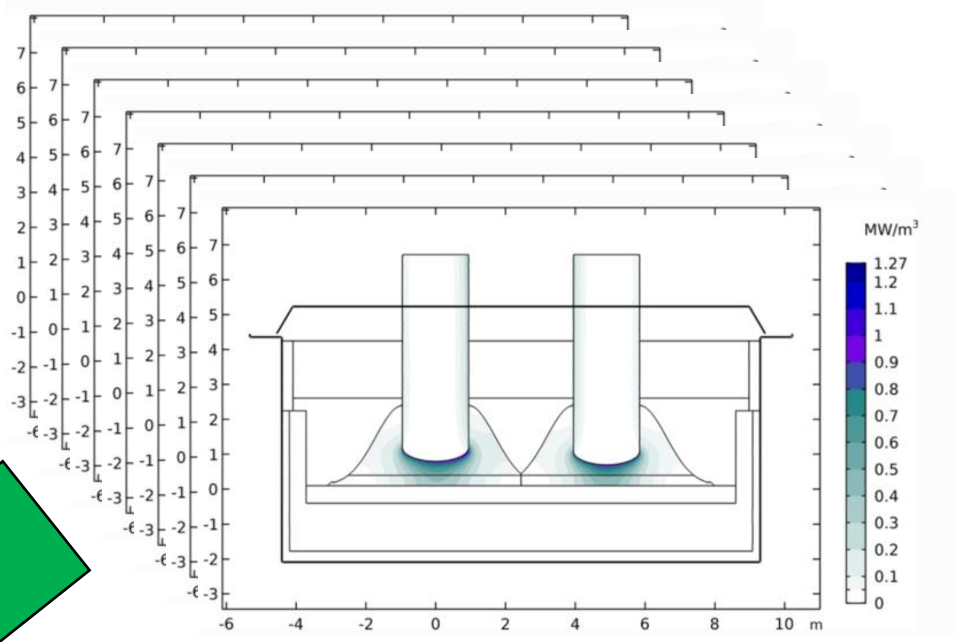


Sparse factorial design in the 12 input parameters

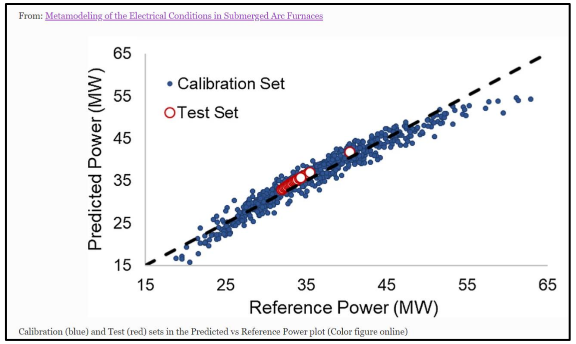
→ ≈ 500 simulations (instead of 4^{12}=17 000 000)



Slow mechanistic model



Fast multivariate meta-model



Faster Digital Twins
by
multivariate metamodelling

Take-home messages:

- Two good process cultures: Measurements, Theory. But cultural math gap
- Multivariate data-modelling: Find actual variation patterns from measurements

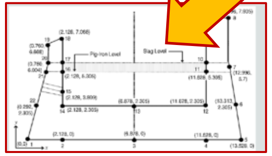
To develop a good digital twin of an industrial plant requires mathematical modelling at several levels of detail

Mechanistic model often too slow or impractical for real-time use

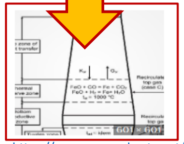
https://www.goodfreephotos.com/cache/wales/other-wales/blast-furnace-at-corus-talbot-works_800.jpg?cached=1522496786

https://thumbs.dreamstime.com/b/blast-furnace-29646421.jpg

https://www.forg… …ext/resources/Issues/2018/October/fg1018-modeling-…



https://www.researchgate.net/profile/Luis-Verdeja/publication/225729039/figure/fig6/AS:668616995393540@1536422122298/The-characteristics-of-blast-furnace-crucibles-analyzed-by-the-NWM-Twenty-two-points-are.png



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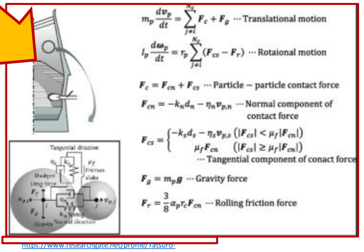

https://www.researchgate.net/profile/Tatsuro-Ariyama/publication/287993041/figure/fig1/AS:614014438629399@1523403858539/Element-of-discrete-element-model-in-blast-furnace-and-fundamental-equations-of-DEM.png

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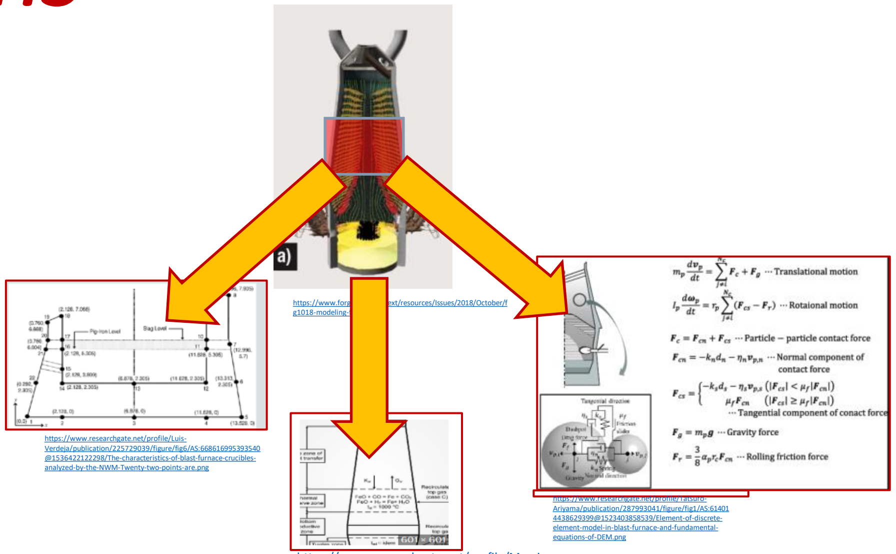
Not only too slow or impractical for real-time use:

Other problems too:

- unexpected convergence problems
-human interpretation problems
- difficult to integrate with measured data streams



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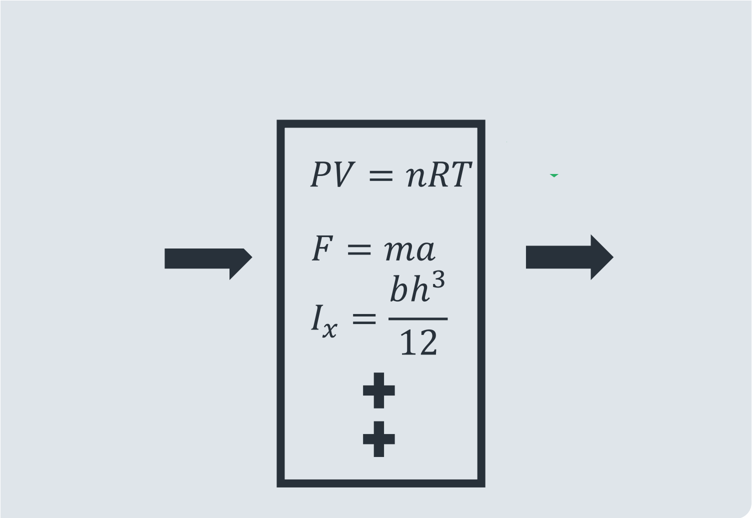
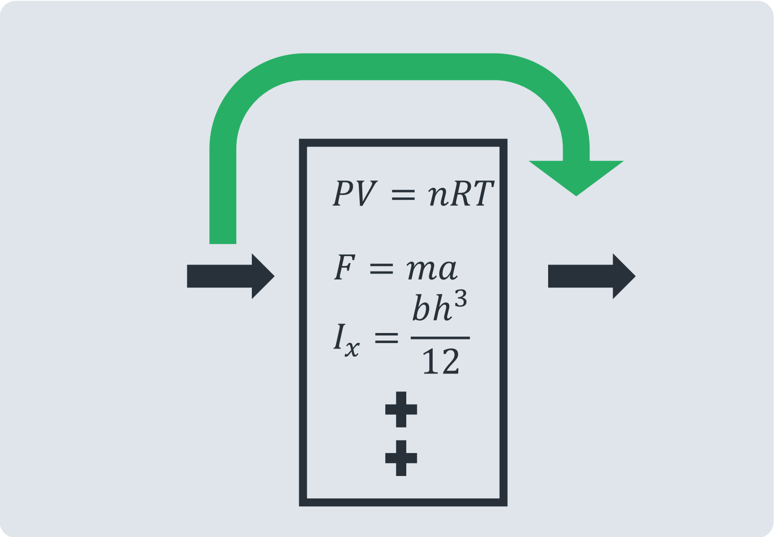
A mechanistic mathematical model:



Modelling

Multivariate metamodelling:
Simpler and safer use of mechanistic mathematical models



Metamodelling

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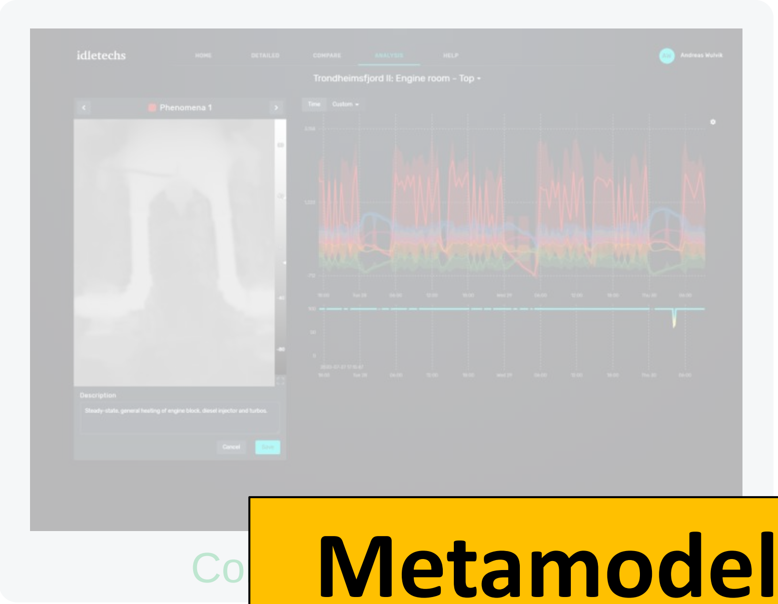

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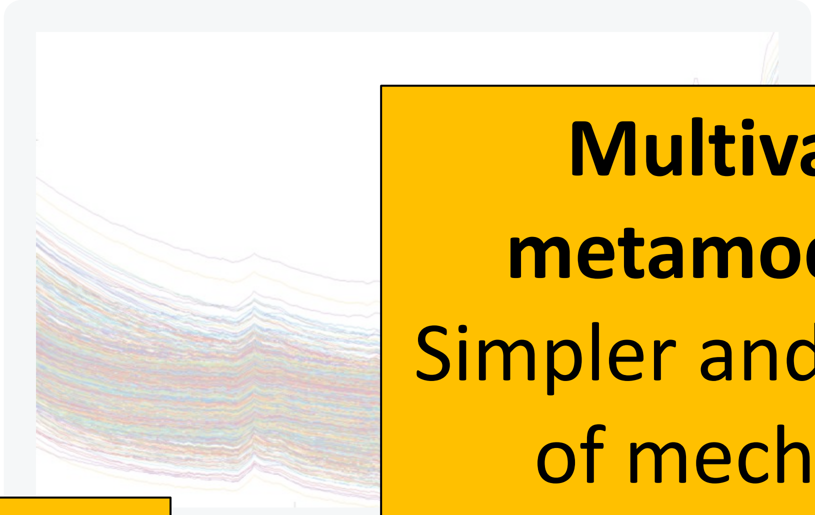
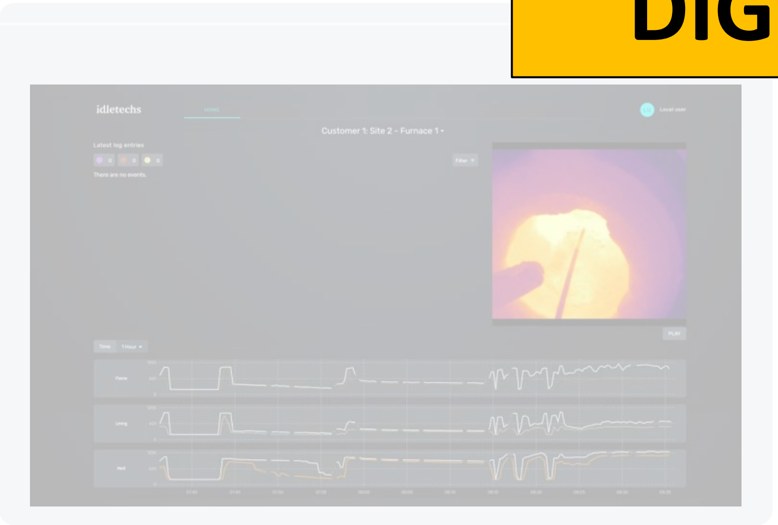


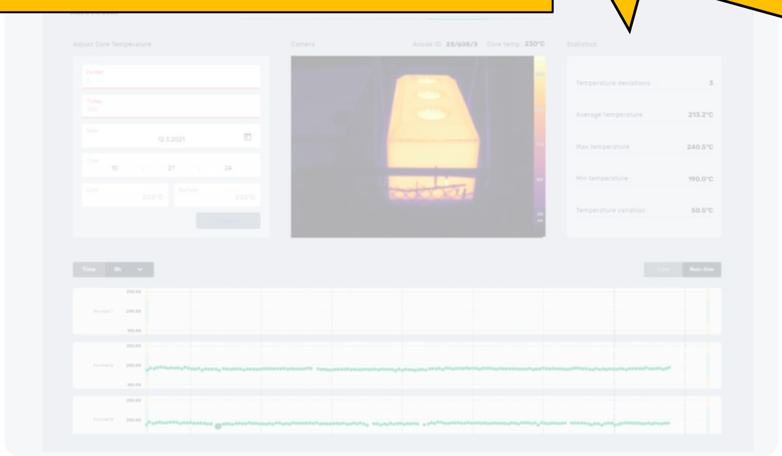
Hyperspe

Metamodelling in DIGITAL TWINS

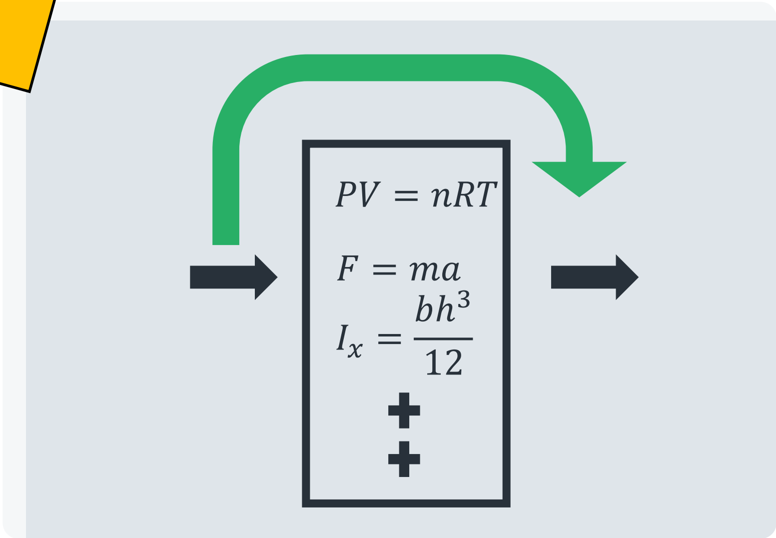
Multivariate metamodelling:
Simpler and safer use of mechanistic mathematical models



Furnace Monitoring



Anode Quality Monitoring



Metamodelling

idletechs


Condition Monitoring
Trondheimsfjord II: Engine room - Top
Hyperspectral Toolbox
Furnace Monitoring
Customer 1: Site 2 - Furnace 1
Anode Quality Monitoring
Metamodelling
$PV = nRT$
$F = ma$
$I_x = \frac{bh^3}{12}$
+
+

idletechs

Example of a mechanistic mathematical model :

A Finite Element Model of human face muscles.

Multivariate metamodelling:

- Study the model's input/output behavior by designed simulations
- Make a simpler, faster but sufficiently rich **statistical model** of the input/output behavior of the mechanistic mathematical model
- **Later, use this fast statistical model to predict new model outputs from new model inputs**

INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN BIOMEDICAL ENGINEERING
Int. J. Numer. Meth. Biomed. Engng. (2014)
Published online in Wiley Online Library (wileyonlinelibrary.com). DOI: 10.1002/cnm.2646

Emulating facial biomechanics using multivariate partial least squares surrogate models

Tim Wu[1,*,†], Harald Martens[2], Peter Hunter[1] and Kumar Mithraratne[1]

[1]*Auckland Bioengineering Institute, The University of Auckland, Auckland, New Zealand*
[2]*Department of Engineering Cybernetics, Norwegian University of Science and Technology, Trondheim, Norway*

The original FEM model:

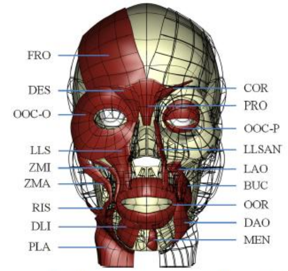


Figure 1. Finite element geometries of the facial muscles. See Table I for the list of abbreviated terms.

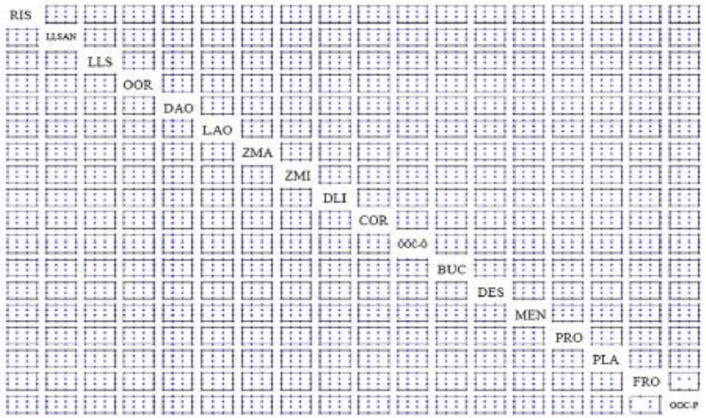
2 hrs CPU time
per facial expression

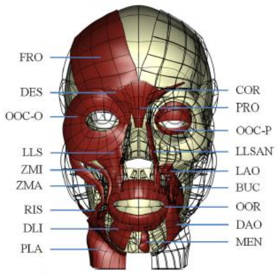
VERY SLOW TO COMPUTE !
Many simulations failed !

Planning the simulation study

Multivariate metamodelling:

- Study the model's input/output behavior by designed simulations
- Make a simpler, faster but sufficient **statistical model** of the input/output behavior of the mechanistic mathematical model
- **Later, use this fast statistical model to predict new model outputs for new model inputs**





e 1. Finite element geometries of the facial muscles. See Table I for the list of abbreviated terms.

Experimental design:

18 model parameters - to probe the relevant repertoire of the model
4 levels of each - to catch nonlinear effects on the output
Factorial design - to catch interaction effects on the output
$\Rightarrow$ $4^{12} \approx 10^{10}$ desired parameter combinations

Instead: Only 128 informative parameter combinations

Planning the simulation study

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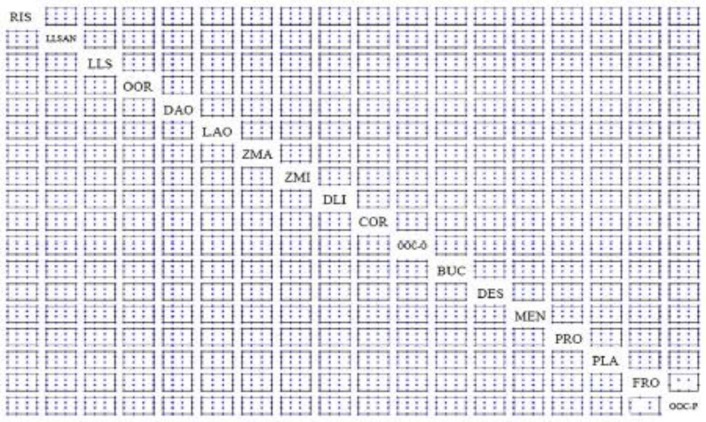

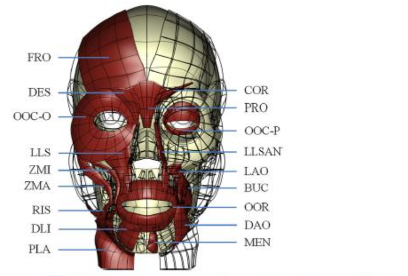

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6 of the 128 simulations:

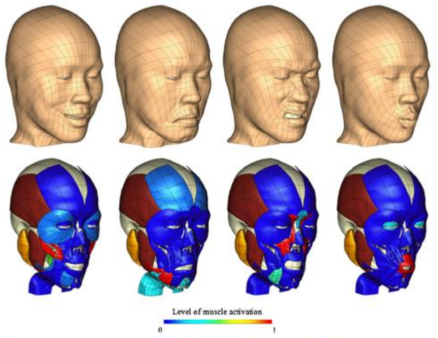


Figure 2. Biomechanical simulations of the expressions of (from left to right) joy, sadness, snarl and the kissing gesture, by activating the corresponding facial muscles.

Making the multivariate metamodel

Multivariate metamodelling:

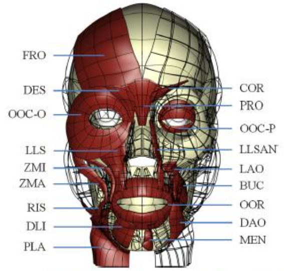
- Study the model's input/output behavior by designed simulations
- Make a simpler, faster but sufficient **statistical model** of the input/output behavior of the mechanistic mathematical model
- **Later, use this fast statistical model to predict new model outputs for new model inputs**

Experimental design: from 4^{18} to 128 parameter combinations:

Multivariate metamodelling:

Partial Least Squares Regression (PLSR) $\Rightarrow$ «model of the model»

CPU time in FEM: 2 hrs each



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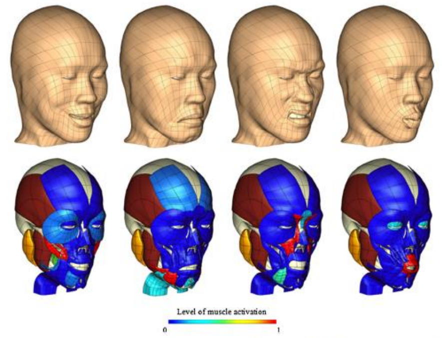

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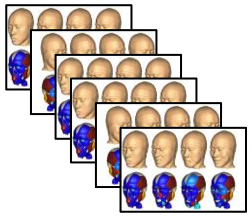
CPU time in FEM via meta-model: < 10 ms each

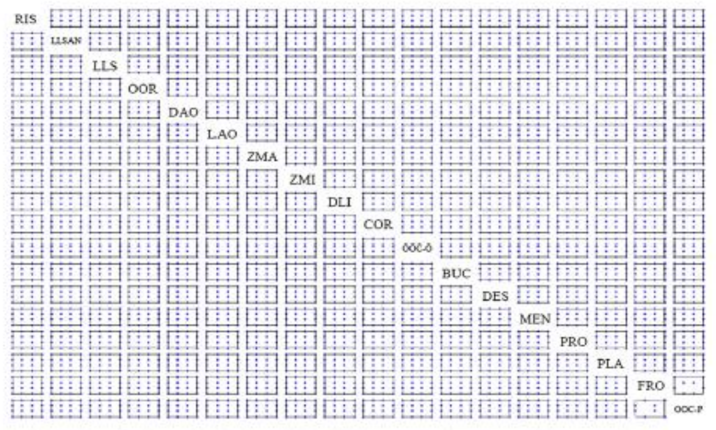


Using the multivariate metamodel

Multivariate metamodelling:

- Study the model's input/output behavior by designed simulations
- Make a simpler, faster but sufficient **statistical model** of the input/output behavior of the mechanistic mathematical model
- **Later, use this fast statistical model to predict new model outputs for many new model inputs**

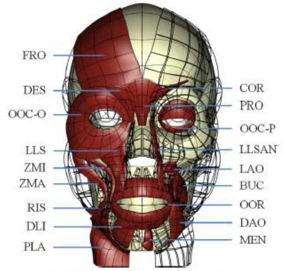
Experimental design: from 4^{18} to 128 parameter combinations:



Multivariate metamodelling:

Partial Least Squares Regression (PLSR) ⇒ «model of the model»

CPU time in FEM: 2 hrs each



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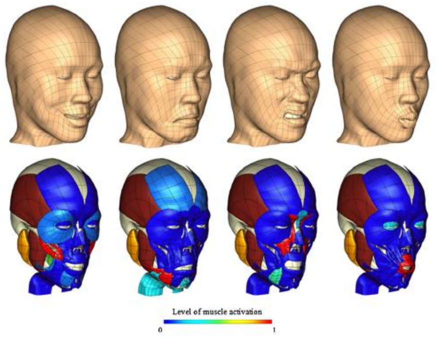

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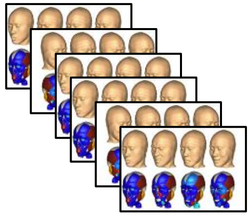


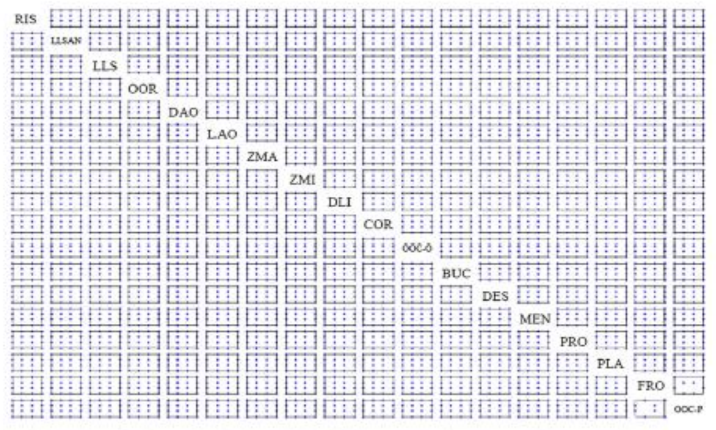
CPU time in FEM via meta-model: < 10 ms each

How are multivariate metamodels developed?
Example : A slow Finite Element Model. Multivariate metamodelling

Multivariate metamodelling:

- Study the model's input/output behavior by designed simulations
- Make a simpler, faster but sufficient **statistical model** of the input/output behavior of the mechanistic mathematical model
- **Later, use this fast statistical model to predict new model outputs for many new model inputs**

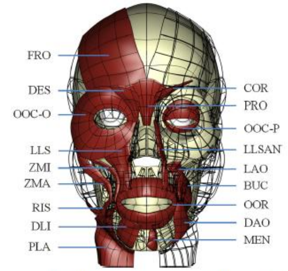
Experimental design: from 4^{18} to 128 parameter combinations:



Multivariate metamodelling:

Partial Least Squares Regression (PLSR) ⇒ «model of the model»

CPU time in FEM: 2 hrs each



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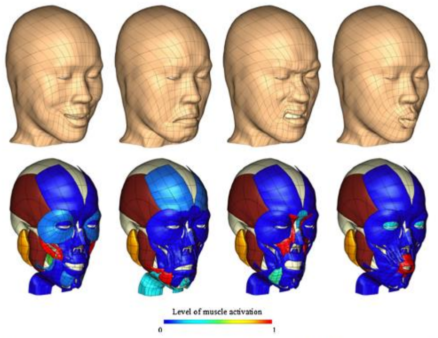

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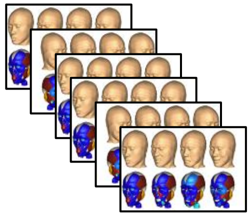
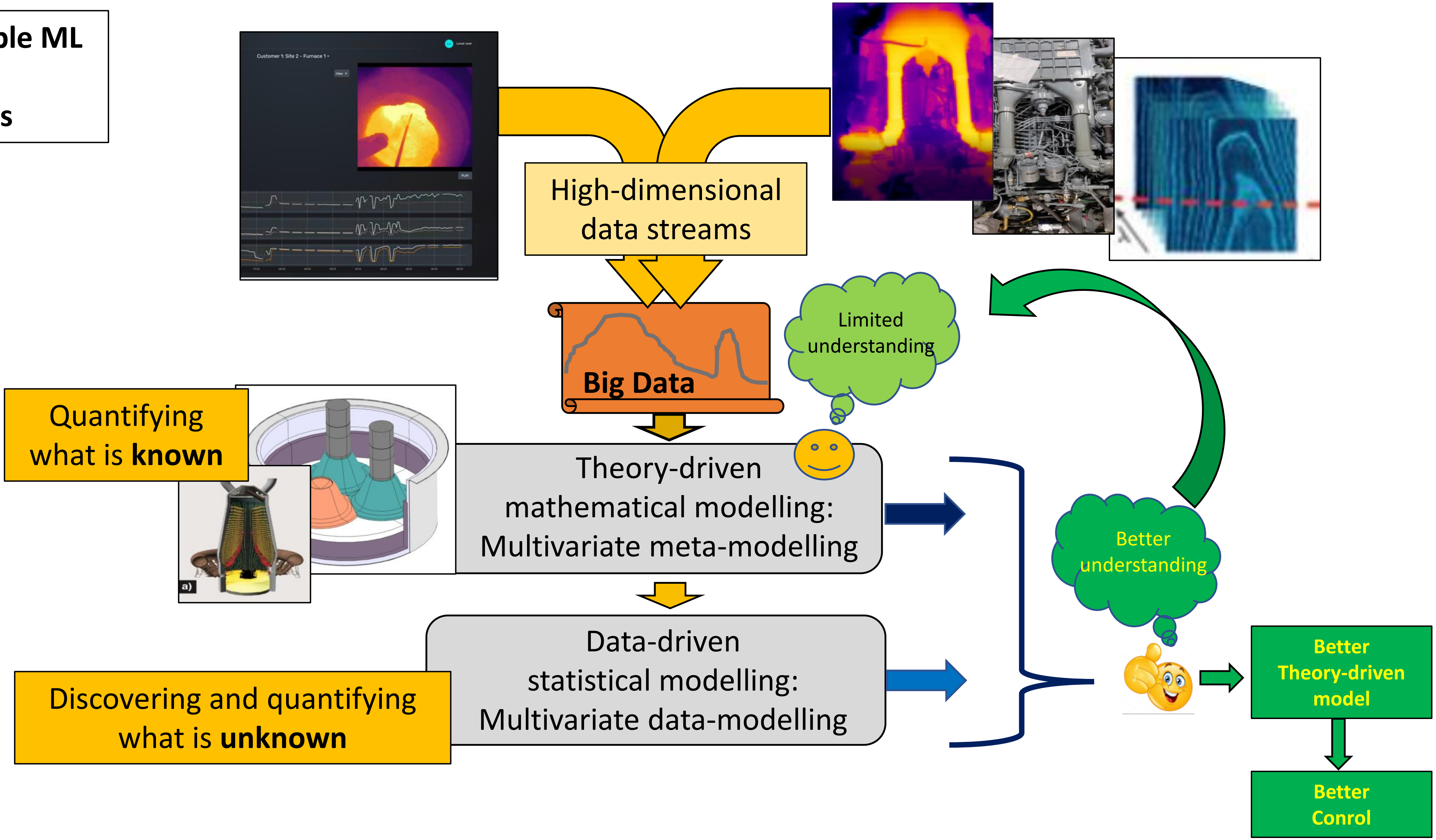


CPU time in FEM via meta-model: < 10 ms each

Conclusion: Metamodelling speeded up the FEM computations more than 1 million times

Human-interpretable ML with an eye for the physics



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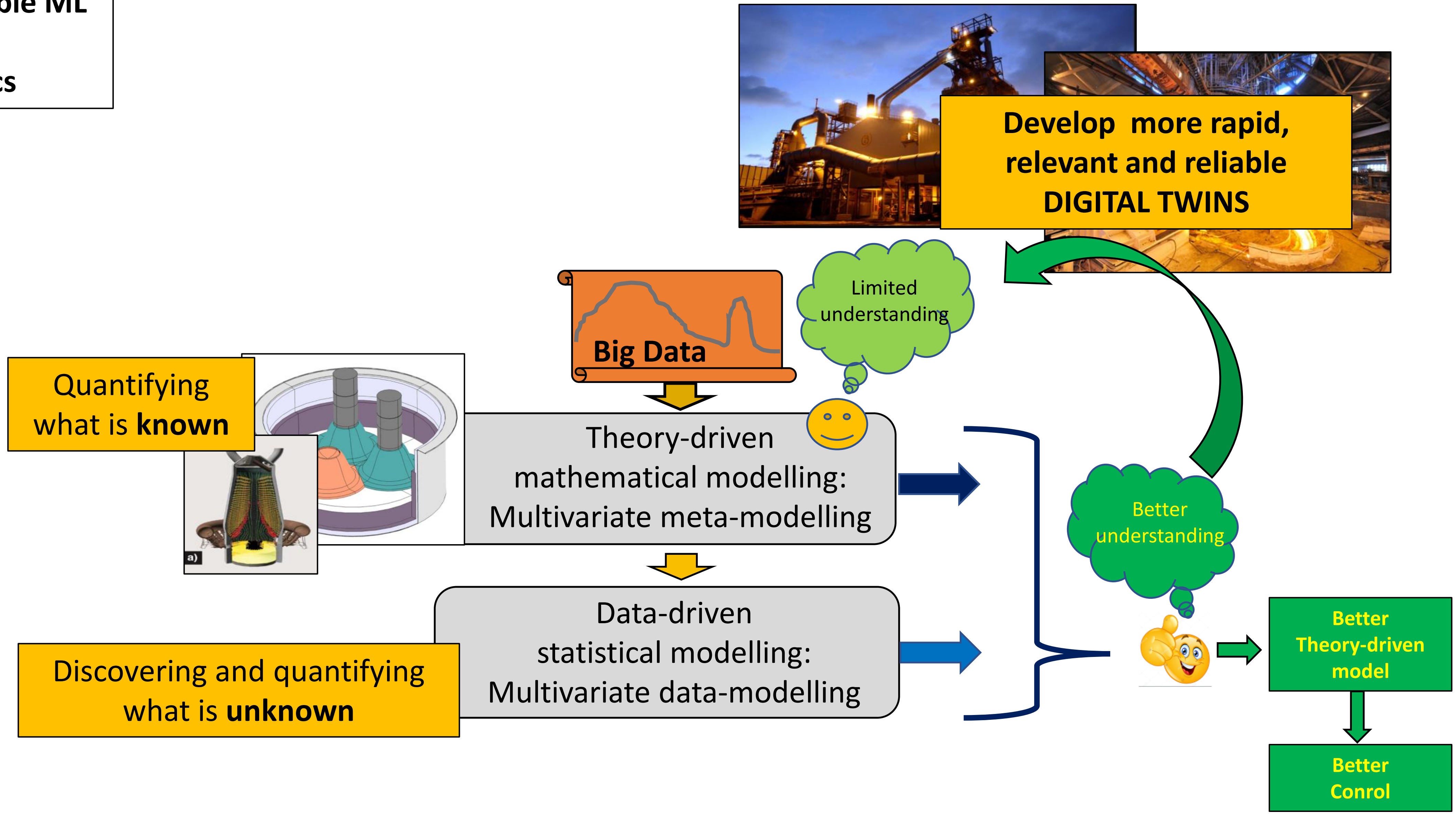

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Faster Digital Twins
by
multivariate metamodelling

<u>Take-home messages:</u>

- Two good process cultures: Measurements, Theory. But cultural math gap
- Multivariate data-modelling: Find actual variation patterns from measurements
- Multivariate meta-modelling: Find possible variation patterns from simulations
- Combine: Multivariate hybrid process modelling

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Bonus: Modeling of time and intensity: IDLE