Paving the Path for Digital Twins on HPC

Introduction

Dirk Pleiter (KTH), 2023-03-21

Goals for this Session

- Create an understanding of the Digital Twin concept within the HPC communicate
- Initiate a discussion on how the design and operation of HPC infrastructures need to change for realising Digital Twin projects
- Discussion of governance and resource allocation aspects

Speakers

General expertise

- Elena Lazovik (TNO)

User communities

- Thomas Geenen (ECMWF)
- DP for Marcella Orwick Rydmark (UIO)
- Tomáš Karásek (IT4I)

Supercomputing centres

- Pekka Manninen (CSC)
- Thomas Eickermann (JSC)
- Tomáš Karásek (IT4I)
- Thomas Geenen (ECMWF)

EuroHPC Summit

2023 Göteborg

Paving the Path for Digital Twins on HPC

Digital Twins: Concepts and Architectures

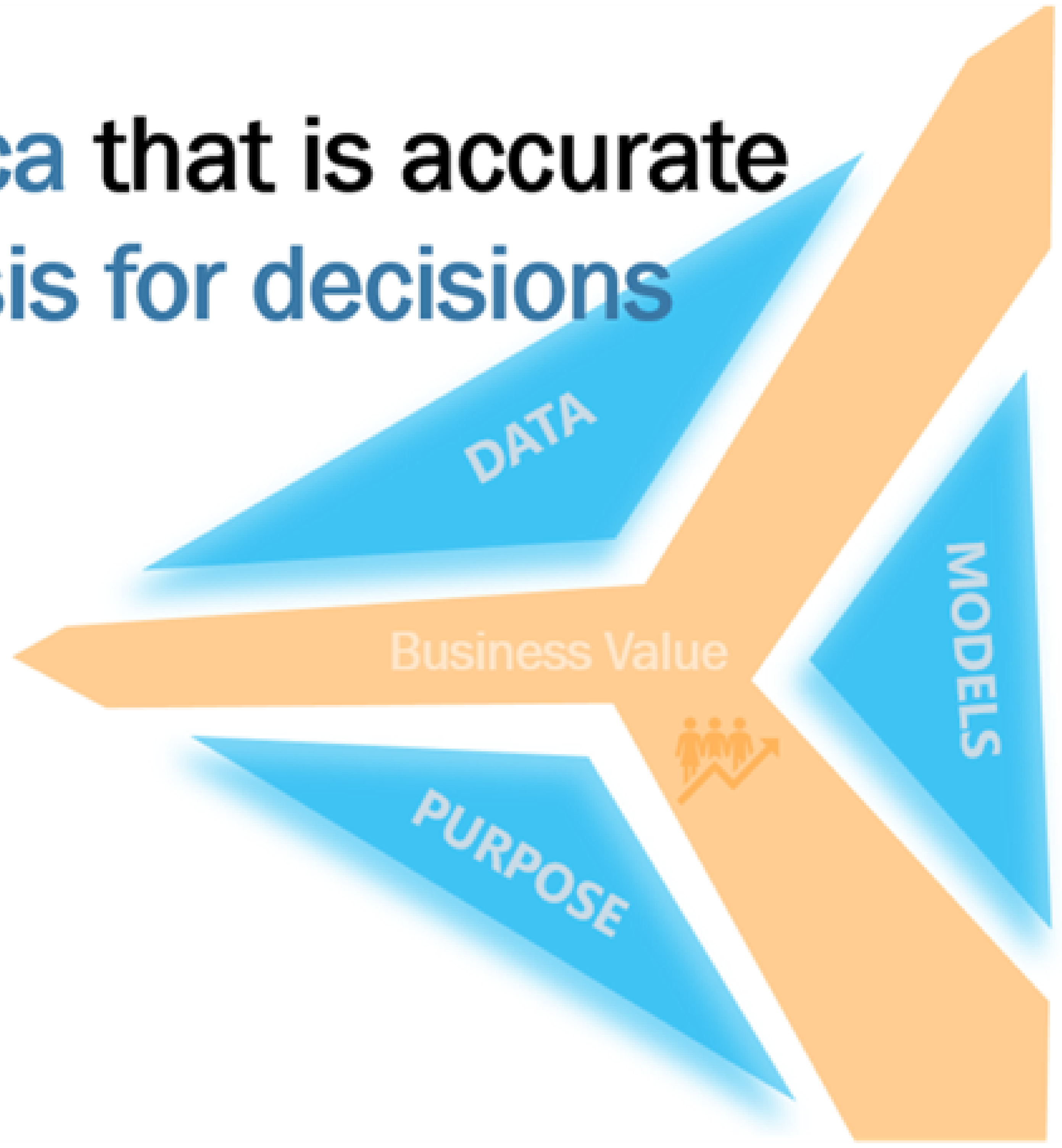
Elena Lazovik (TNO), 2023-03-21

What is a Digital Twin

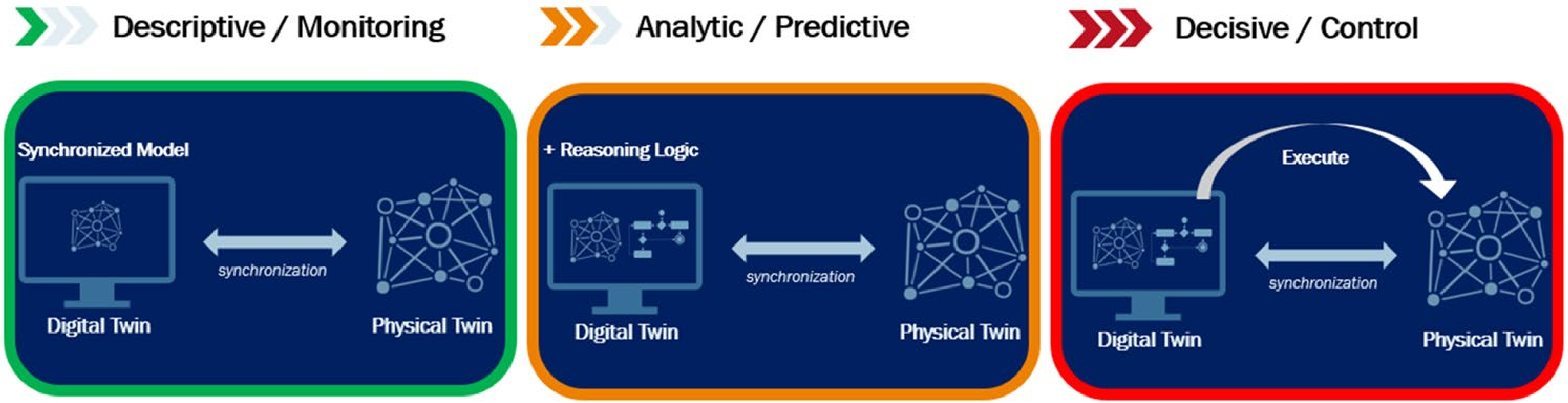
- "The digital twin is the virtual representation of a physical object or system across its life-cycle. It uses real-time data and other sources to enable learning, reasoning, and dynamically recalibrating for improved decision making."

A digital twin is a digital replica that is accurate enough that it can be the basis for decisions given a specific purpose

- Creates value by linking data, models & purpose
- The replica is often connected by streams of data
- The replica is supported by new IT



Gradation of Digital Twins



- Digital model is synchronized so that the model state is up-to-date with that of the physical twin to provide real-time monitoring capabilities
- Additional reasoning logic enables the digital twin to do calculations that give insights underpinning predictive power and supporting decision-making
- Closing the control loop, the digital twin is integrated into the physical twin so that decision-support is provided in an engineered system

Benefits and shortcomings of DT

- Digital Twin Benefits
  - Reduces CAPEX & OPEX enormously with a FIRST-TIME-RIGHT implementation and Physical Twin lifecycle management
  - Reduced time-to-market of product, process, or production system
- Digital Twin Short-comings
  - It is expensive: mostly custom-built & currently silo-ed
  - It does not evolve well with the physical world: Software Development & Lifecycle (SDLC) Management is barely considered or ignored

The hardest part of DT is not a model

"Hidden Technical Debt in Machine Learning Systems ", Google NIPS 2015

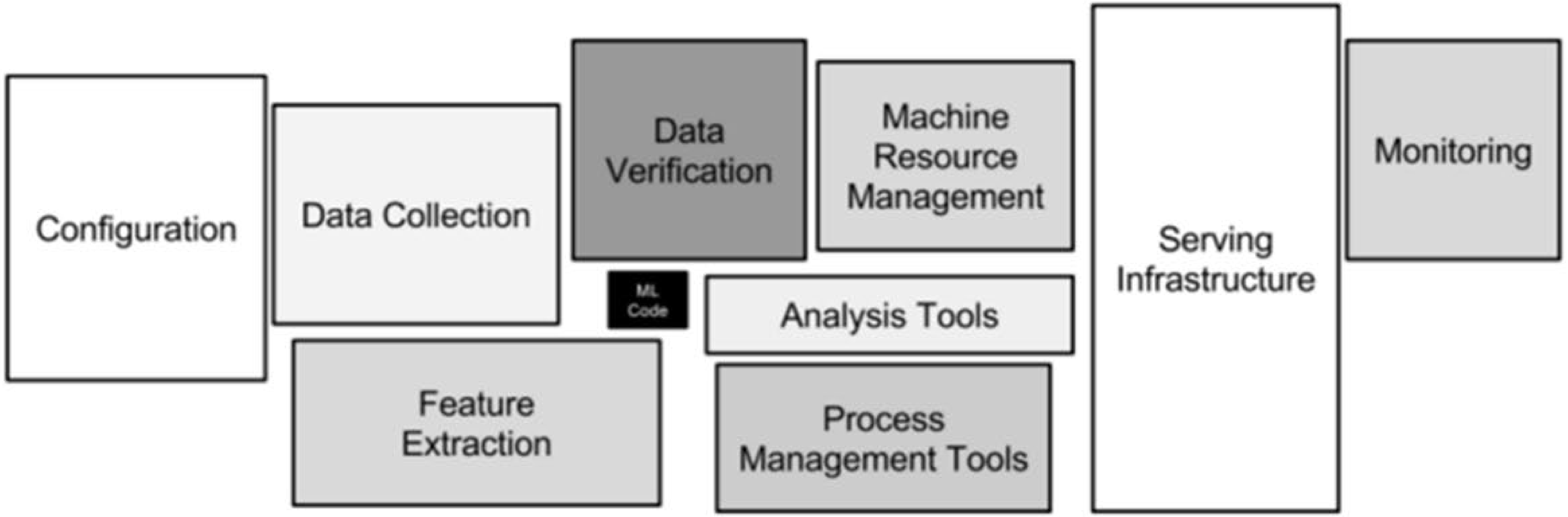
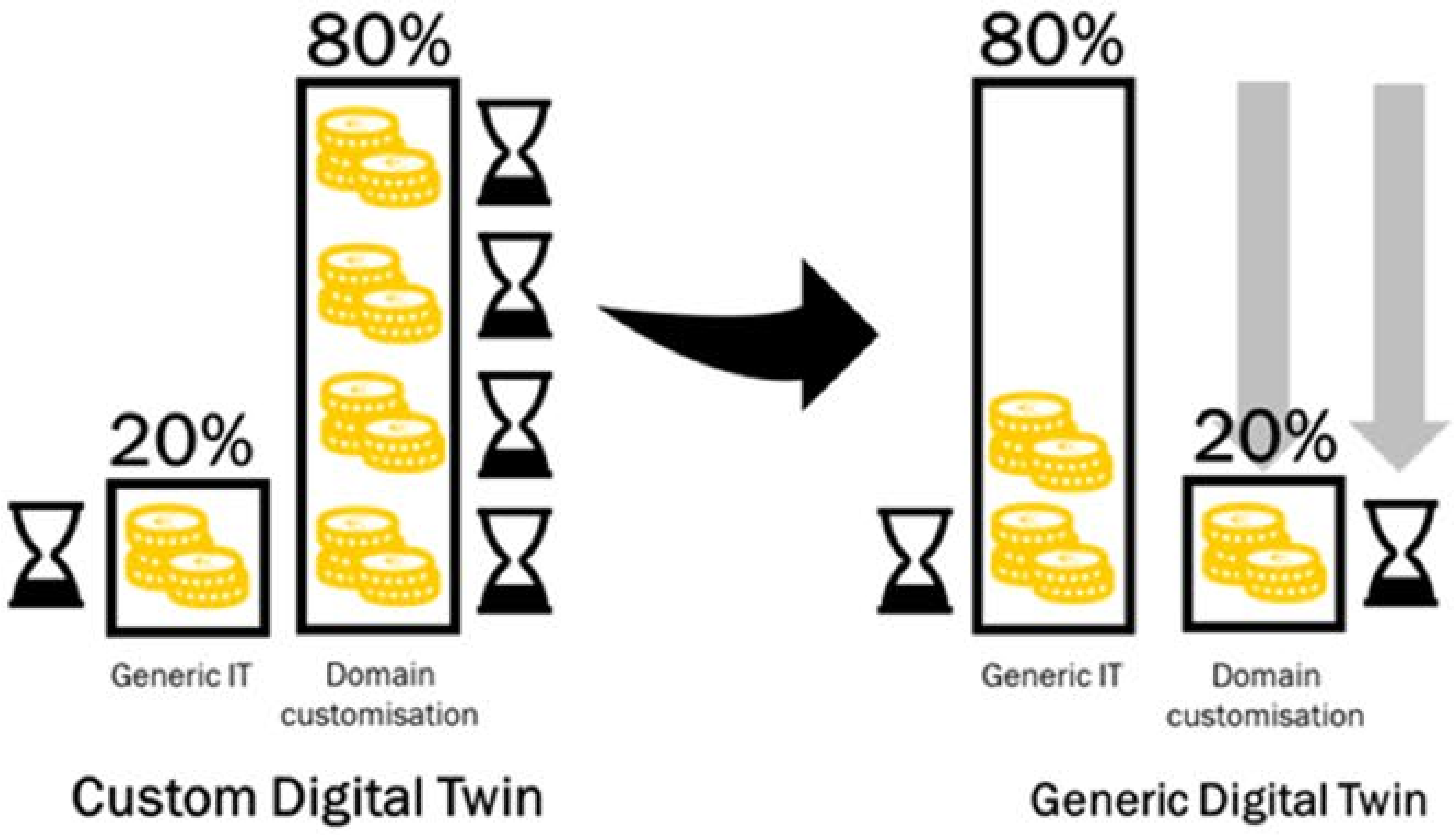
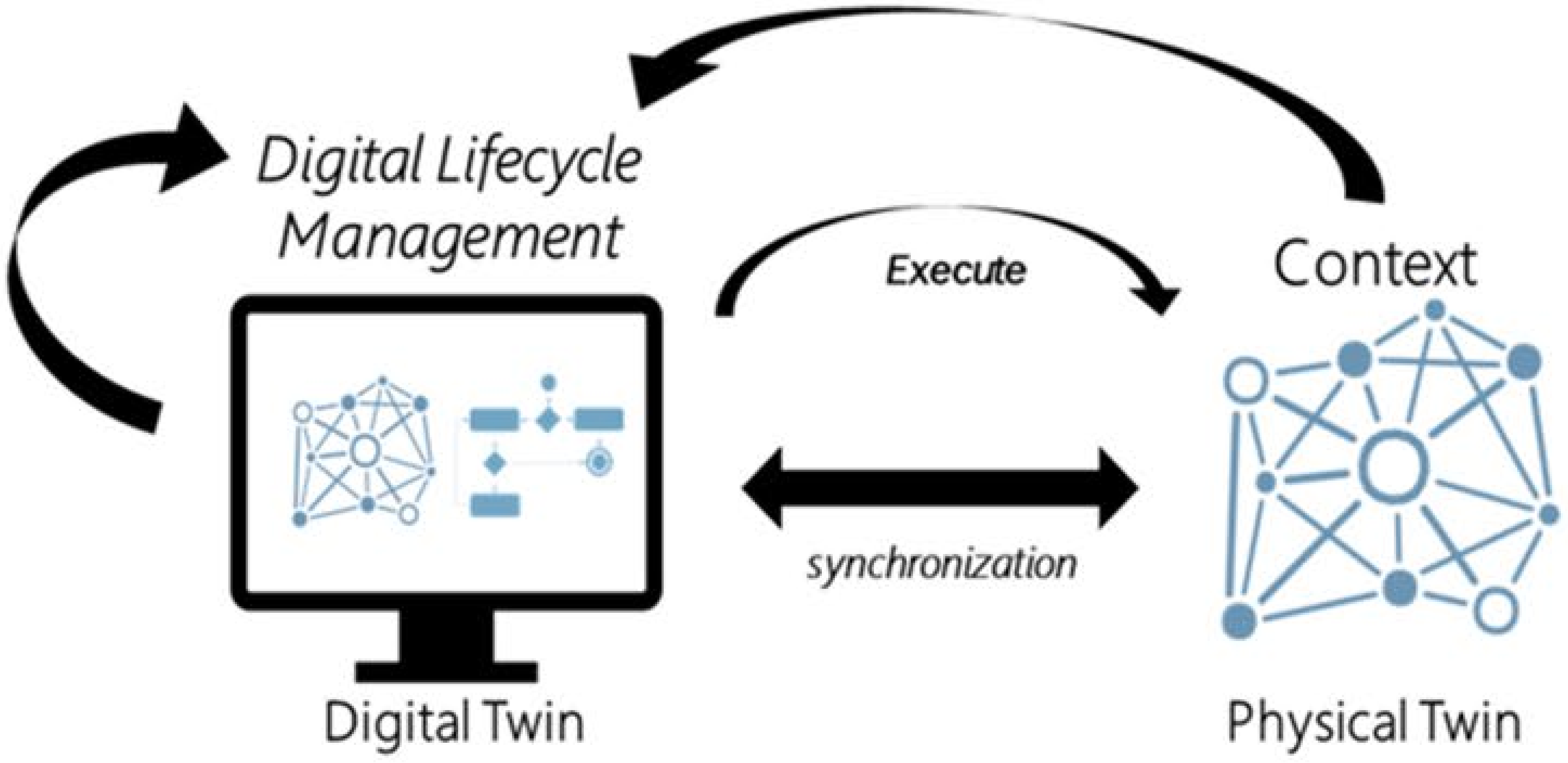


Figure 1: Only a small fraction of real-world ML systems is composed of the ML code, as shown by the small black box in the middle. The required surrounding infrastructure is vast and complex.

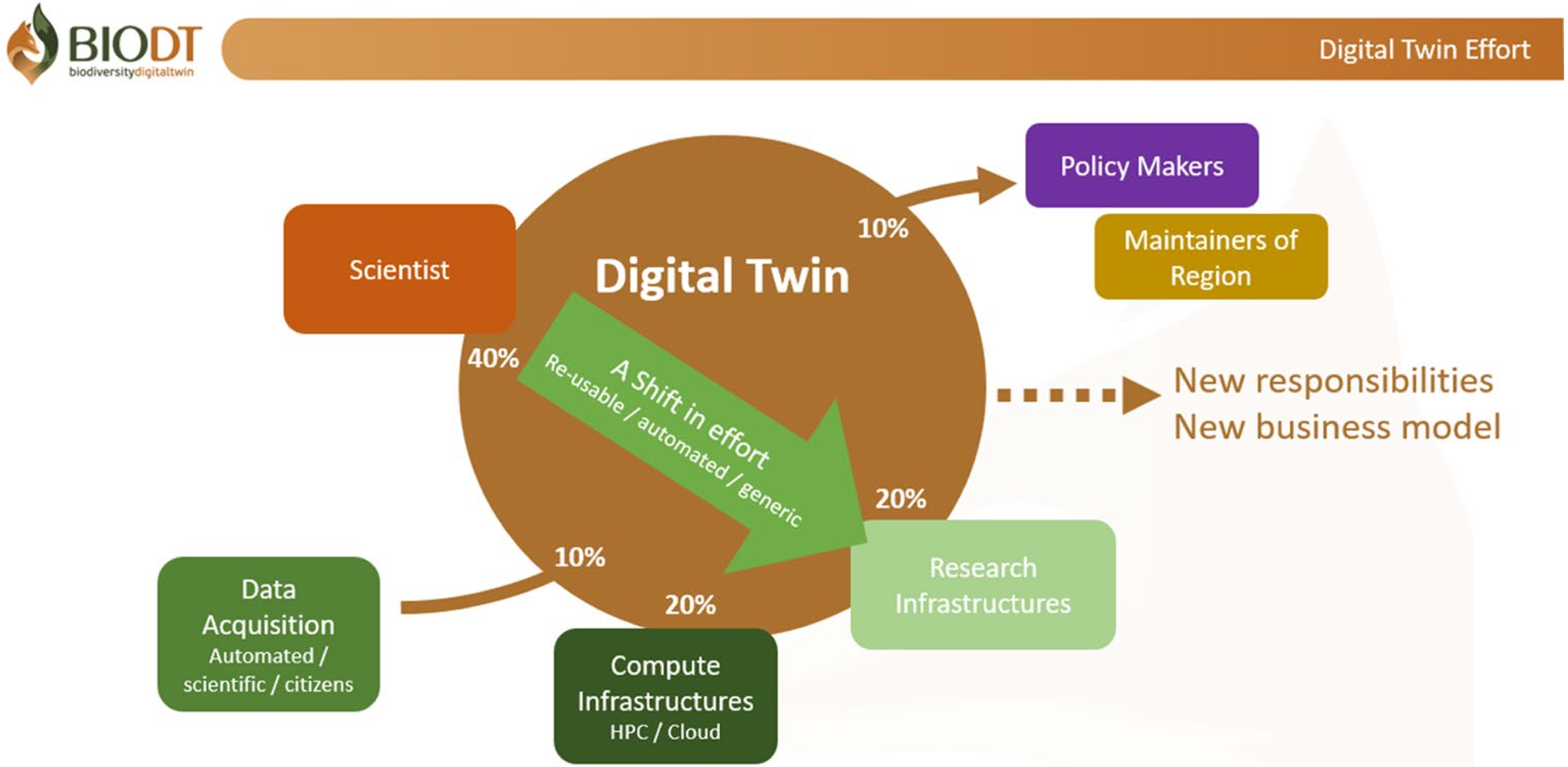
Custom vs. Generic DT

- **Generic IT** for Digital Twin
  - Affordable solution with quick time-to-solution
- **Lifecycle management IT** for Digital Twin
  - Keeping up with our evolving physical world



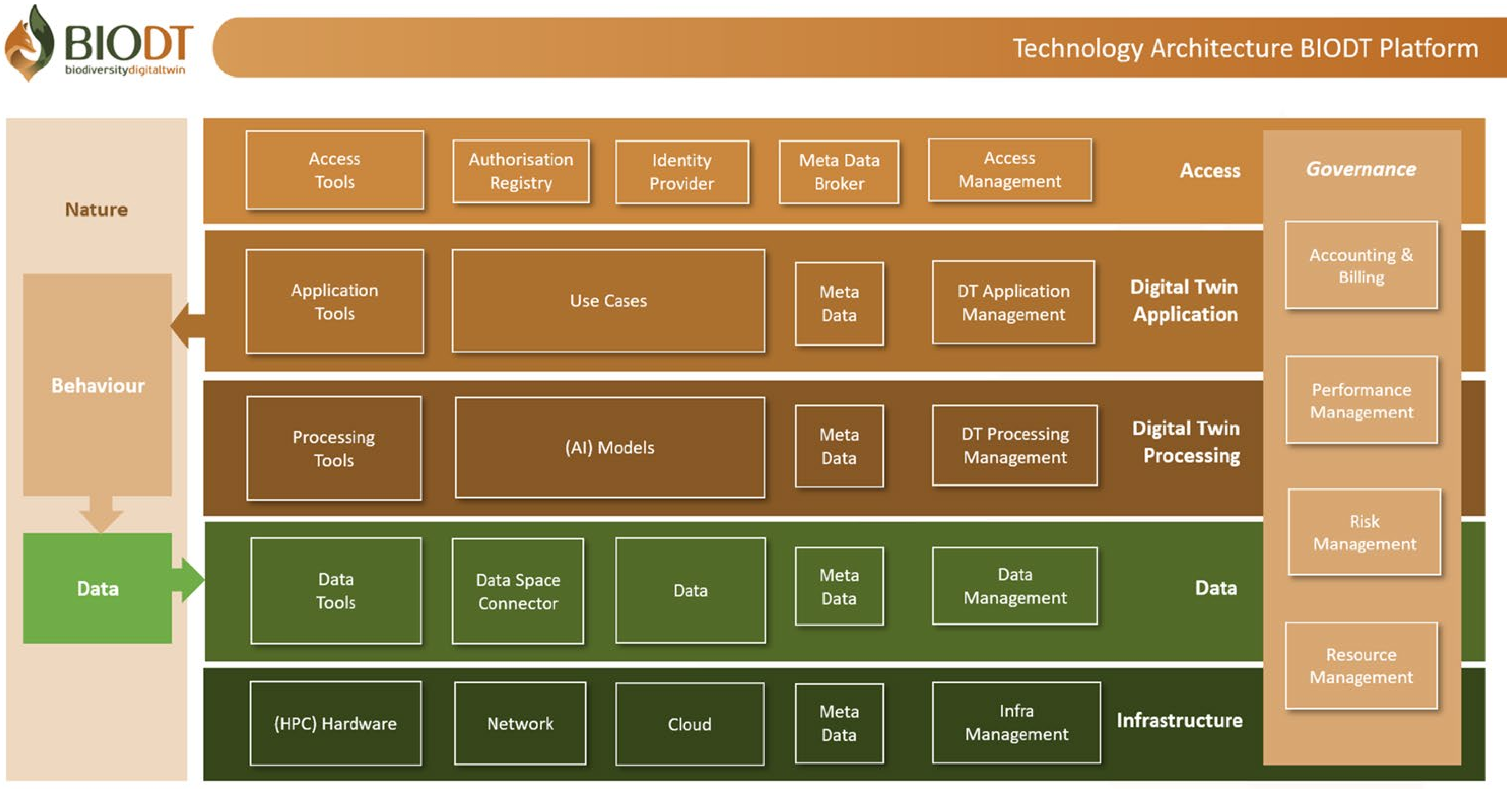


BioDT Digital Twin effort



Digital Twin platform

- **HPC support**
- Different types of infrastructure for different models: CPU, GPU, TPU.
- Offloading of local models to HPC cluster
- Management of different types of data
- Support of models written in very varied languages (R, Python, Java, Rust, Scala, Akka, Erlang, etc.)
- Data ingestion from hundreds and thousands of data sources
- Different types of visualization



EuroHPC Summit

2023 Göteborg

Paving the Path for Digital Twins on HPC

Destination Earth: A Digital Twin on a Global Scale

Thomas Geenen (ECMWF), 2023-03-21

EU's Destination Earth (DestinE) initiative

Towards a Digital Twin Earth

Entrusted entities

ECMWF
esa
EUMETSAT

Key elements

- Digital Twin Engine
- Digital Twins
- Data lake
- Core platform

A European Green Deal (2019)

A European strategy for data (2020)

Shaping Europe's digital future (2020)

2021-2023
- Operational cloud-based platform
- First two digital twins

2023-2025
Platform integrates the next operational digital twins and offers services to public sector users

2025-2027+
Towards a full "digital twin of the Earth" through a convergence of multiple digital twins on the platform

Funded by the European Union

ECMWF's role in EU's DestinE initiative

Towards a Digital Twin Earth

ECMWF is responsible for the delivery of:

The DestinE **Digital Twin Engine** (DTE):
- common approach for a unified orchestration of Earth-system simulations and their fusion with observations, requiring **large-scale HPC** and data handling resources

Weather-induced and Geophysical **Extremes Digital Twin**:
- capabilities and services for the assessment and prediction of **environmental extremes (a few days ahead)**

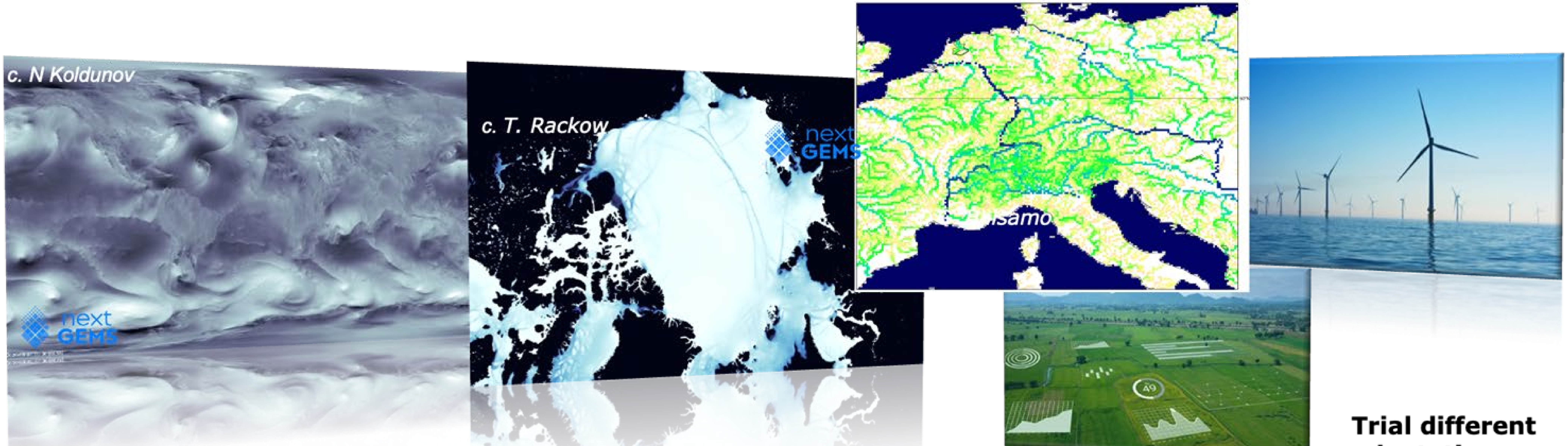
Climate Change Adaptation **Digital Twin**:
- capabilities and services in support of climate change **adaptation policies and mitigation scenario** testing **(multi-decadal)**

EuroHPC Joint Undertaking

Funded by the European Union

DestinE's Digital Twins: Quality + Impacts + Interaction

1. **Better simulations** based on **more realistic models**
2. **Better ways of combining all observed and simulated information** from entire Earth system = physical + food/water/energy/health **supporting action scenarios**
3. **Interactive and configurable access to all data, models and workflows**



More realistic at *global* scale

More realistic at *local* scale

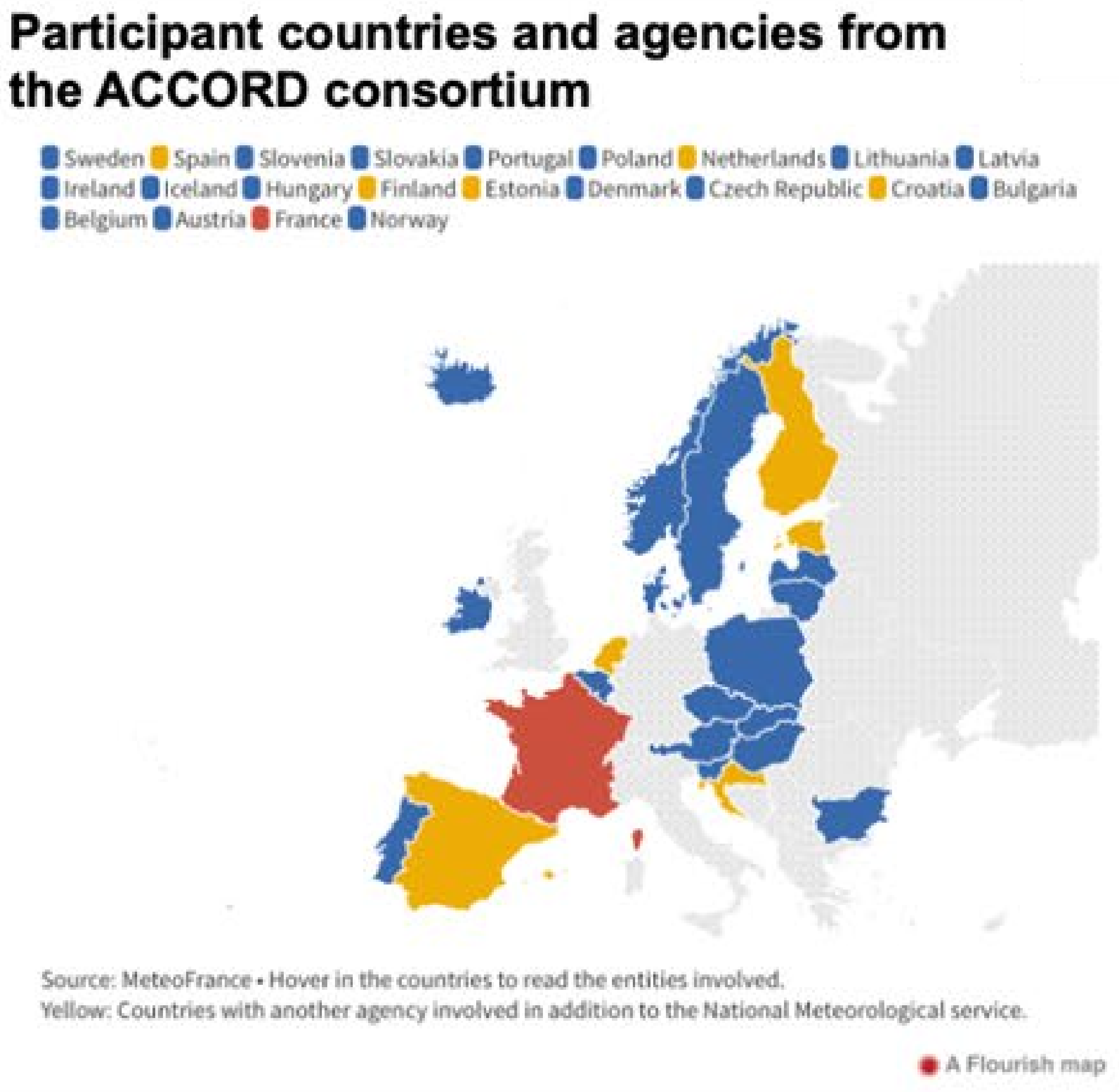
Include impacts where they matter

Trial different adaptation and mitigation scenarios

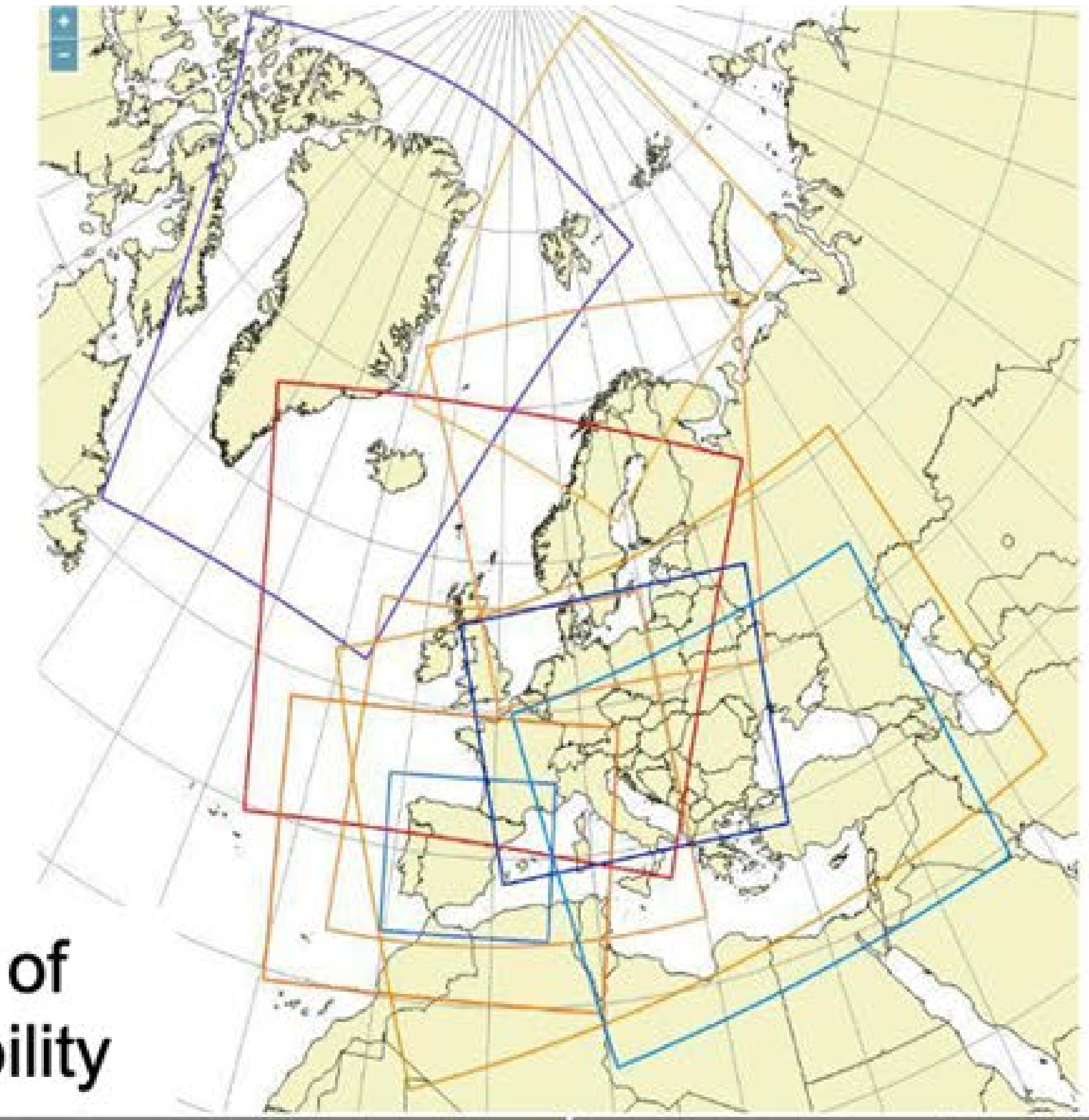
On-demand Extremes DT (procured)

Flexible and scalable workflows for the monitoring and short-range prediction of extremes at sub-km scales, that are configurable and operable on demand; builds on the ACCORD prediction system and selected impact models

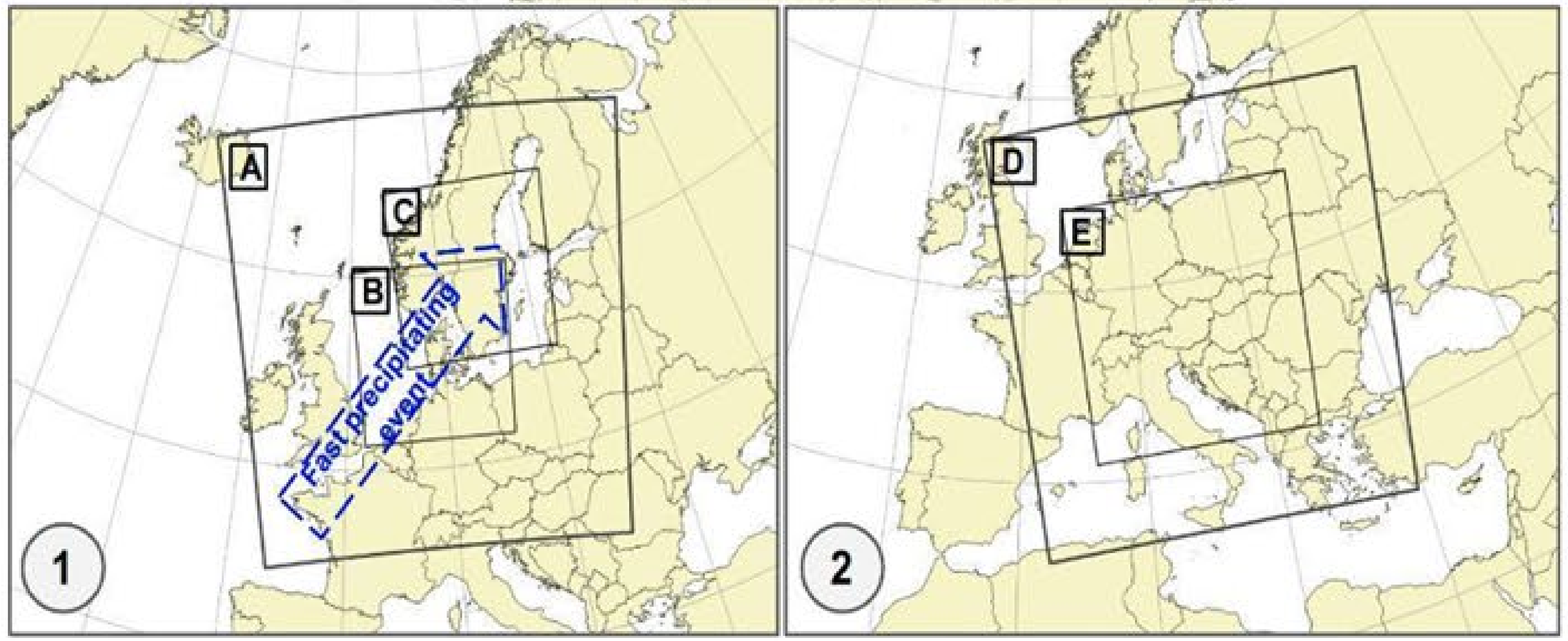
Meteo-France led consortium



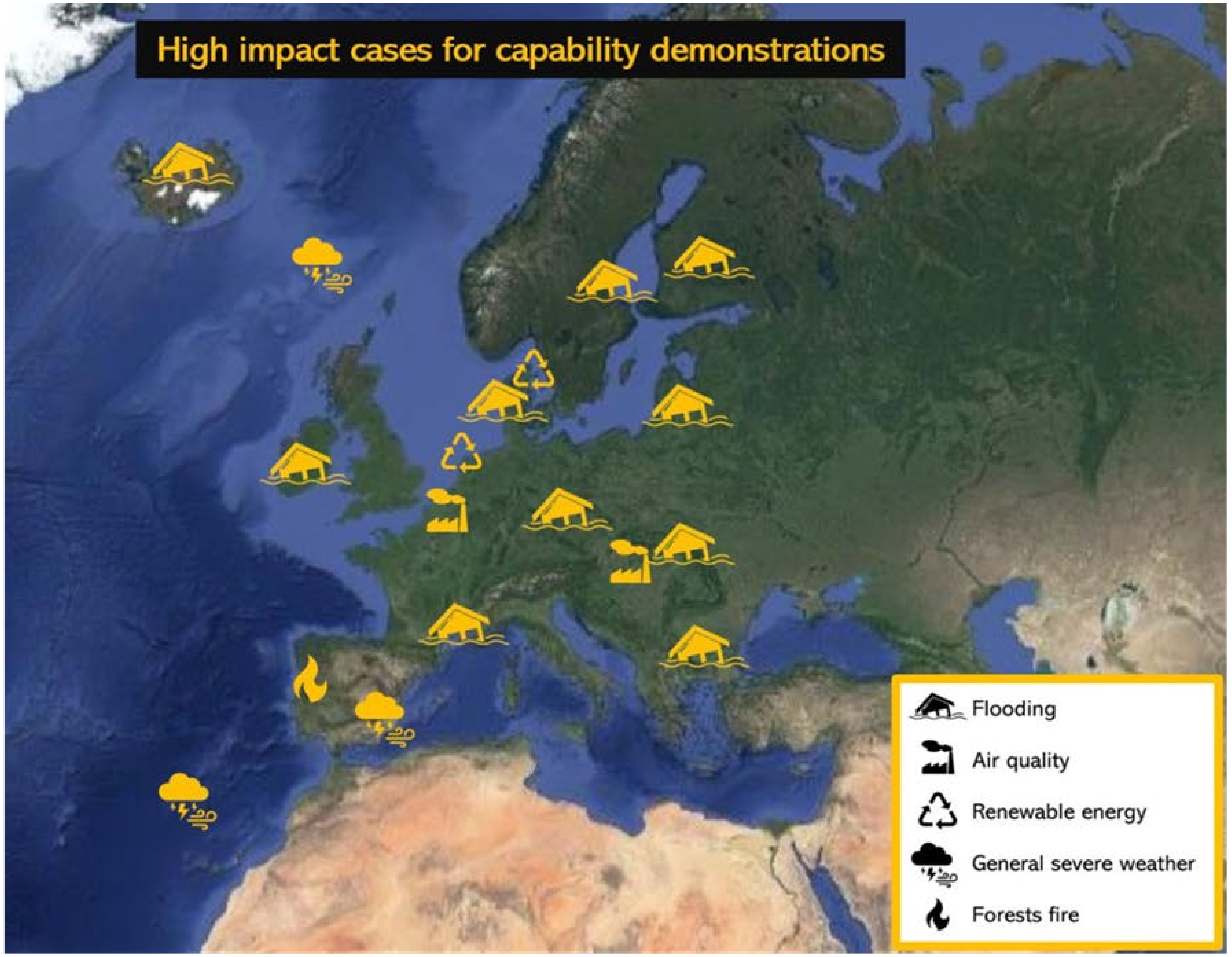
Today's prediction systems



Examples of configurability



Use cases in DT Extremes (on demand)



Hydrology / Extreme Flood Events

Workflows for flood modelling in BG, CZ, DK, FI, FR, IE, IS, SE, SK

SMHI

Air quality

Two air quality extremes:

- Cold inversion in Carpathian region, Jan 2017
- Ozone/heat in Benelux, Summer 2018

GeoSphere Austria

Renewable Energy

- North sea storms
- Ramping events (storms, fronts, …)
- Solar energy

KNMI

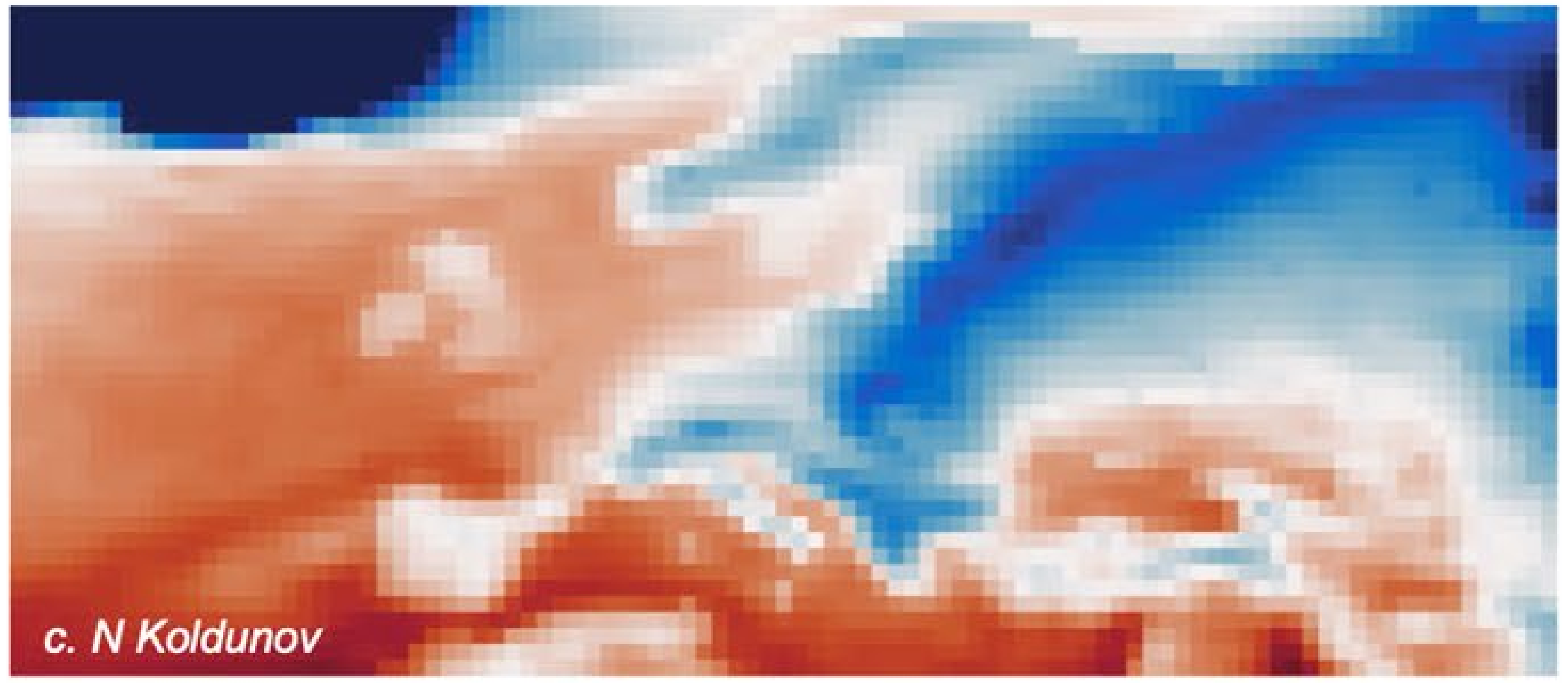
Climate DT

multi-decadal, global, storm/eddy-resolving numerical Earth-system simulation capability with the timely delivery of climate **information** for policy adaptation; observation based assessment framework; use cases for impact-sectors such as water, energy, food or health

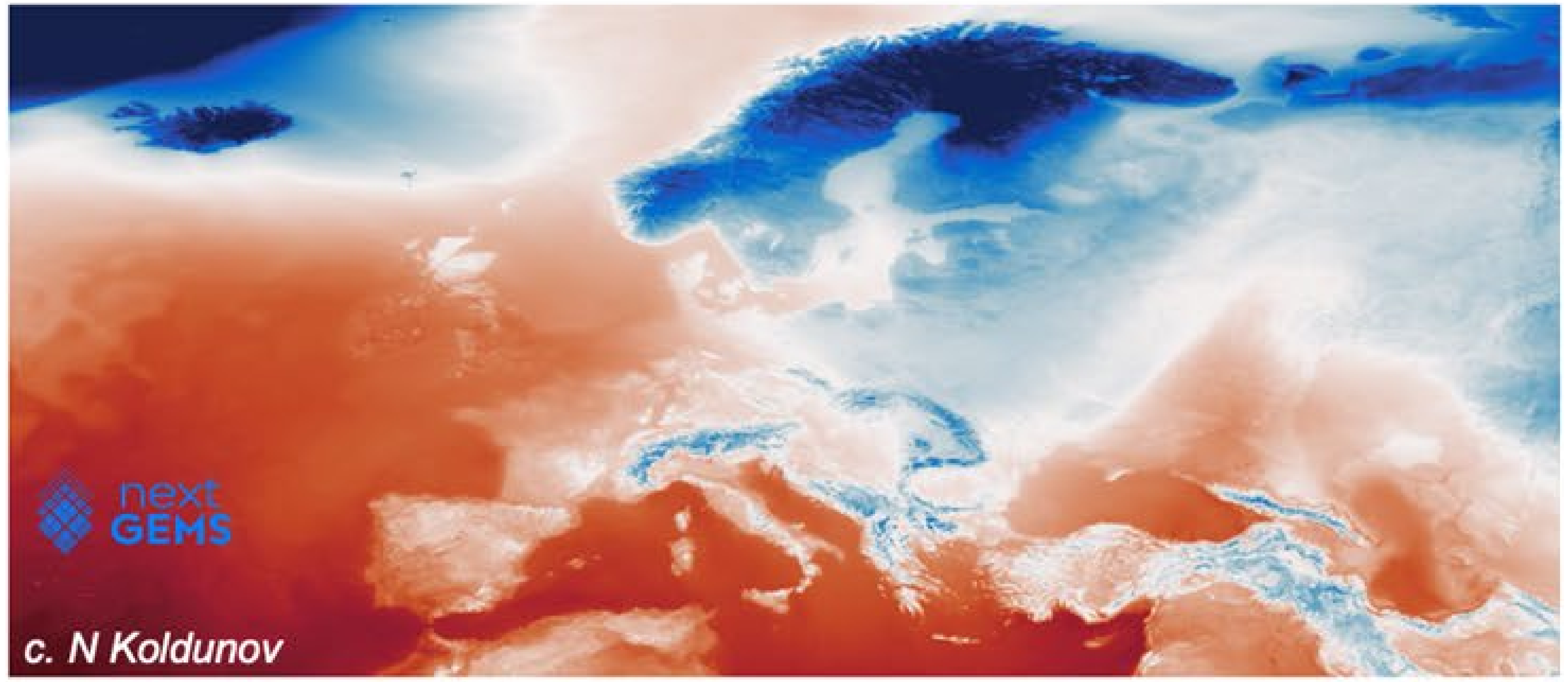
CSC led consortium

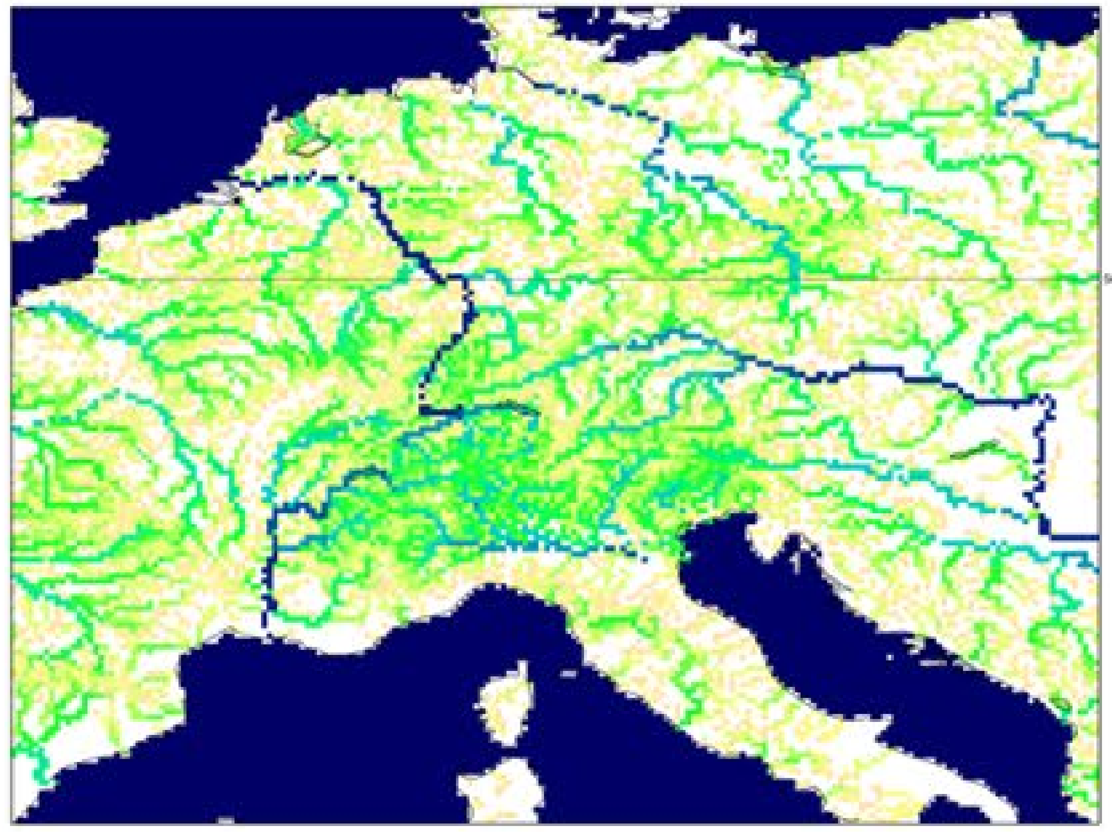
Today's global climate models

IPCC AR6 (2021)



Storm & eddy resolving simulations





Collocated weather, climate and impact-sector information on scales where impacts of climate change and extreme events are felt

Use cases in DT Climate

- Fire indices for Europe
- Fire spread models in Finland
- Burnt area, CO_2 emissions (Finland)

ILMATIETEEN LAITOS

- Future freshwater resources
- Future flood/drought
- Focus: Germany

UFZ HELMHOLTZ Centre for Environmental Research

- Extreme event statistics
- Event catalogue

Deutscher Wetterdienst
Wetter und Klima aus einer Hand
DWD

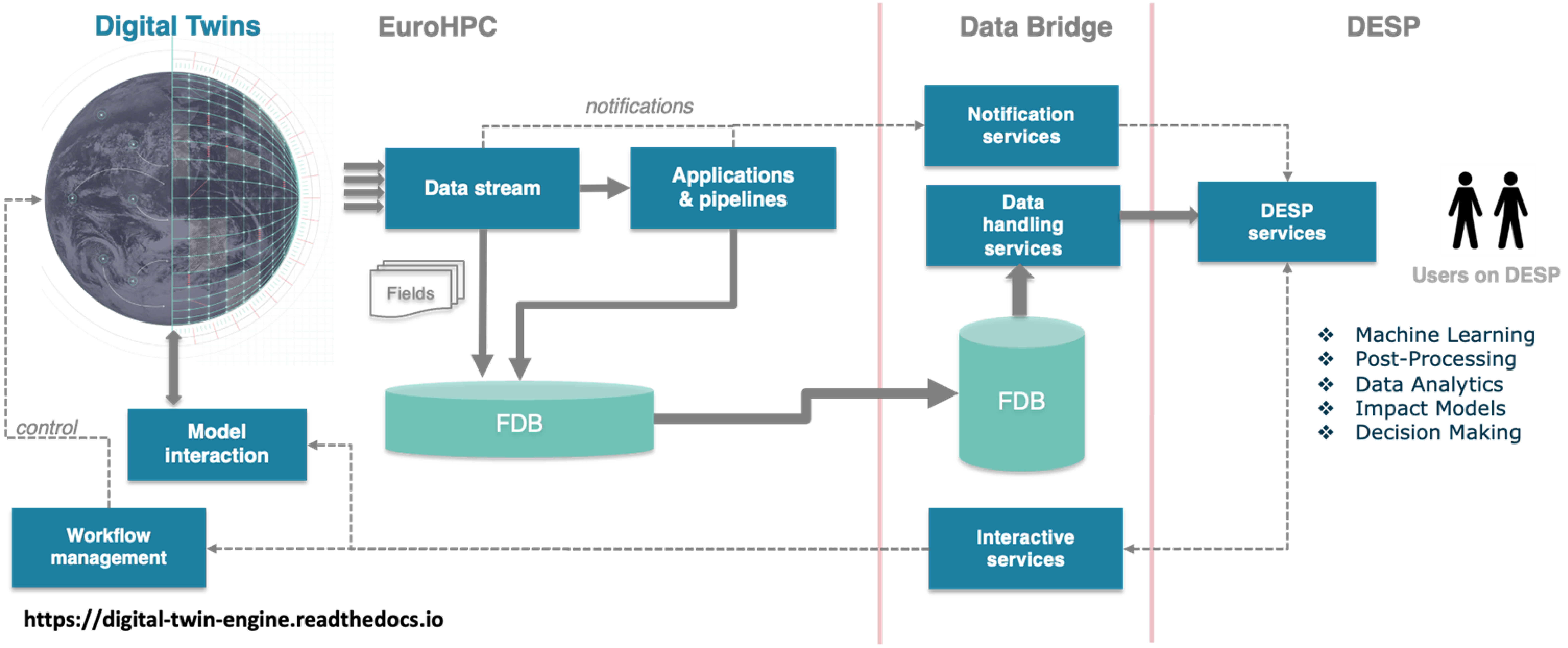
- Wind resources globally (onshore, offshore)
- Wind turbine vulnerability under extremes and icing

BSC Barcelona Supercomputing Center
Centro Nacional de Supercomputación

- Spatio-temporal variability of heat waves
- Human thermal comfort indicators

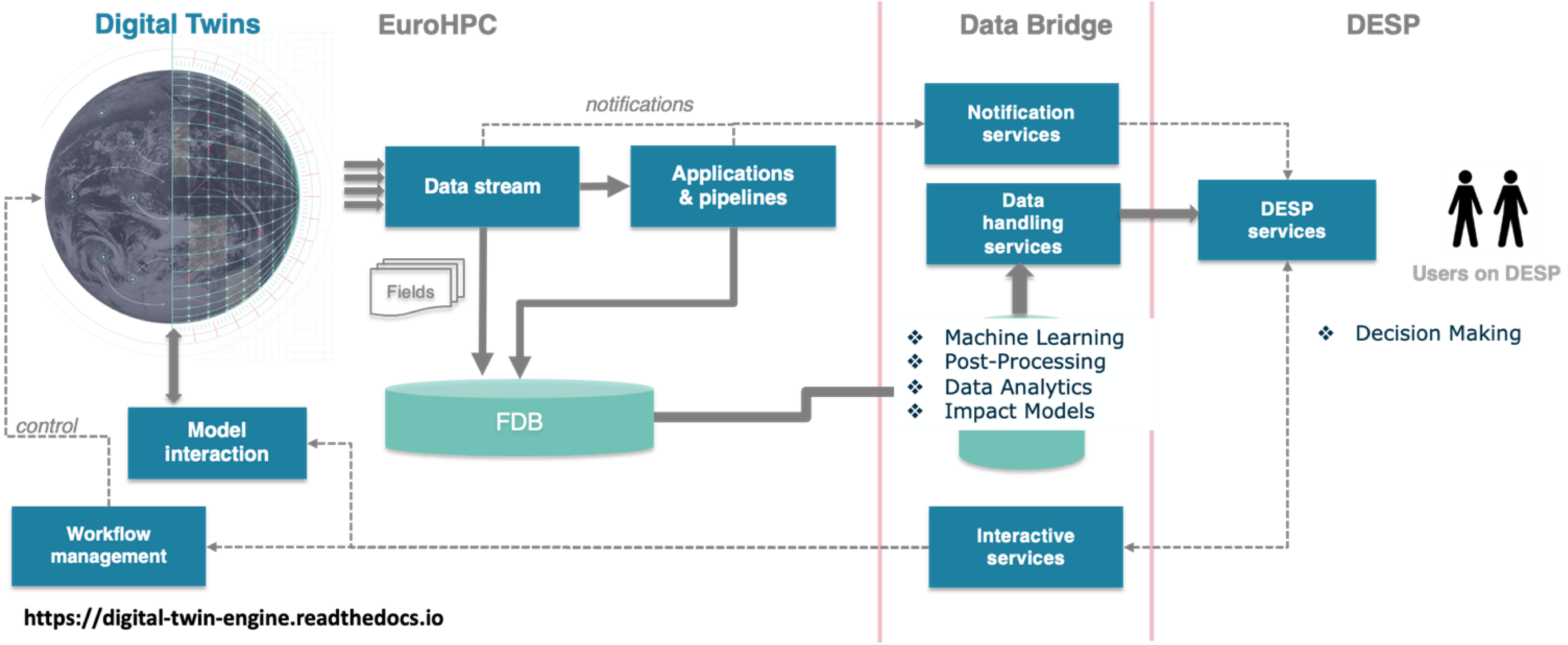
BSC Barcelona Supercomputing Center
Centro Nacional de Supercomputación

DTE components and objectives



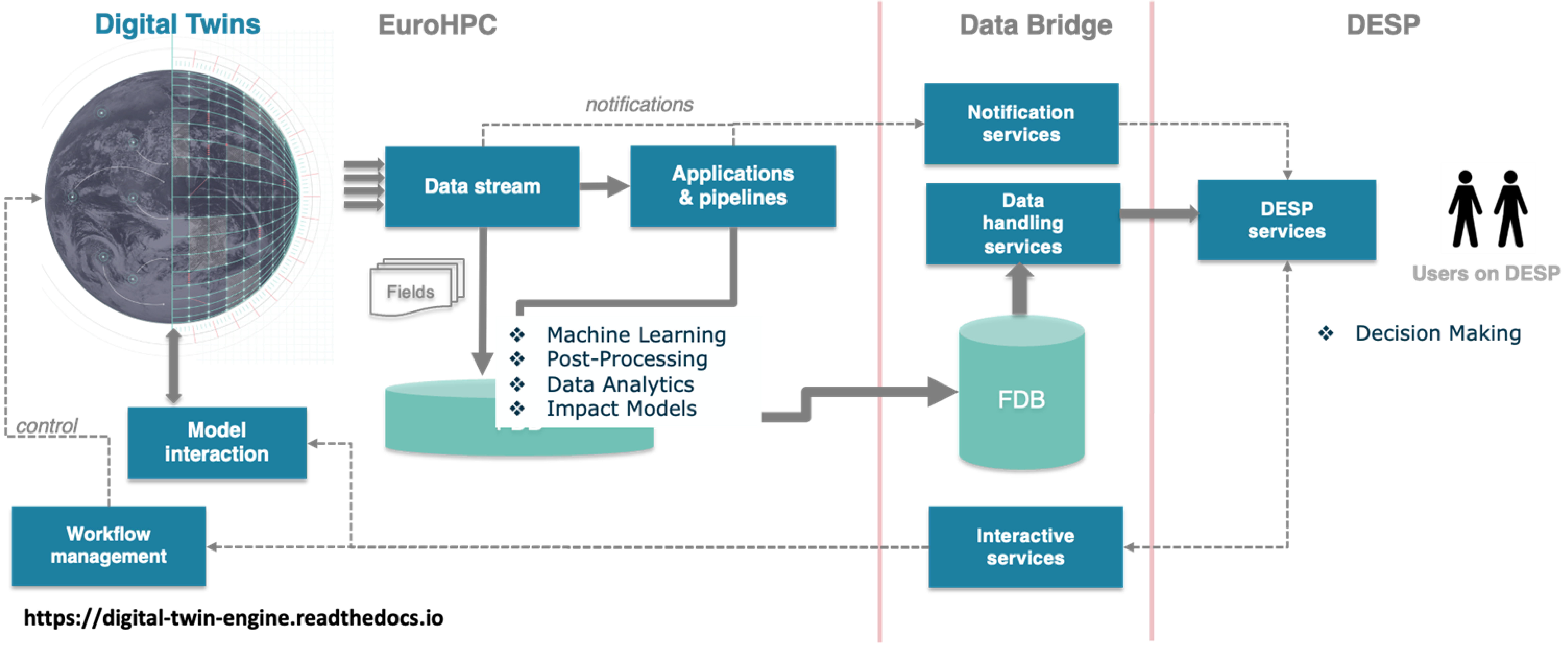
https://digital-twin-engine.readthedocs.io

DTE components and objectives



https://digital-twin-engine.readthedocs.io

DTE components and objectives



https://digital-twin-engine.readthedocs.io

Different types of Integration

Full Integration mode
Directly integrated in the DestinE simulation and data handling system

Coupling mode
Integrated in a workflow where Digital Twins have their own simulation and data fusion tasks interfacing with DestinE

Post-processing mode
Integrated as data post-processing application without own Earth-system simulation

Integration continuum

Use DTE
Workflow management, HPC and data handling software infrastructures

Compatible with DTE
Workflow management, HPC and data handling software infrastructures

Weak DTE coupling
independent Workflow management, data management support

DTE in the background
implicit data handling software infrastructure use By the end user from the DESP

EuroHPC Summit

2023 Göteborg

Paving the Path for Digital Twins on HPC

Digital Twins for Biodiversity

BIODT
biodiversitydigitaltwin

Acknowledgement:
- Original slides from Marcella Orwick Rydmark (UIO)
- Further input from Franziska Taubert, Volker Grimm, Jürgen Groeneveld (UFZ)

Dirk Pleiter (KTH), 2023-03-21

Pollinators - Background

- Pollinators are omnipresent in ecosystems
- Critical for food security and plant biodiversity
- Climate and and environmental changes are accelerating the decline of pollinators
- The full risks associated to their decline are not fully understood
- Focus here: Honey bees

What are the main stressors of honeybees?

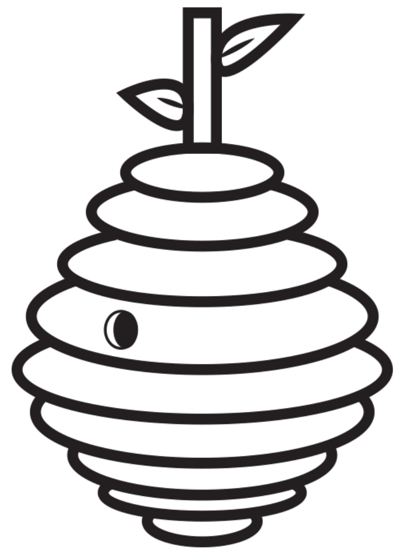
Varroa: http://www.bienenaktuell.com/
Pestizide: http://georgiaag.com/
Monokultur: http://www.taz.de/
Truck:http://georgiabees.blogspot.de/

- Varroa (mite)
- Diseases
- Pesticides
- Modern agricultural practices that lead to forage gaps
- Beekeeping practices

It is not practically possible to test multiple stressors with experiments

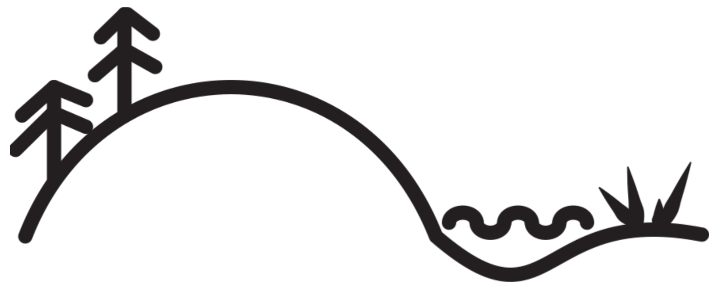
BEEHAVE simulator

- BEEHAVE is a computer model to simulate the development of a honeybee colony and its nectar and pollen foraging behavior in different landscapes
- The model continues being expanded by different modules



COLONY AND POPULATION DYNAMICS

FORAGING



LANDSCAPE AND FORAGE AVAILABILITY

VARROA AND BEEKEEPING

https://beehave-model.net/

BEEHAVE as part of a Digital Twin

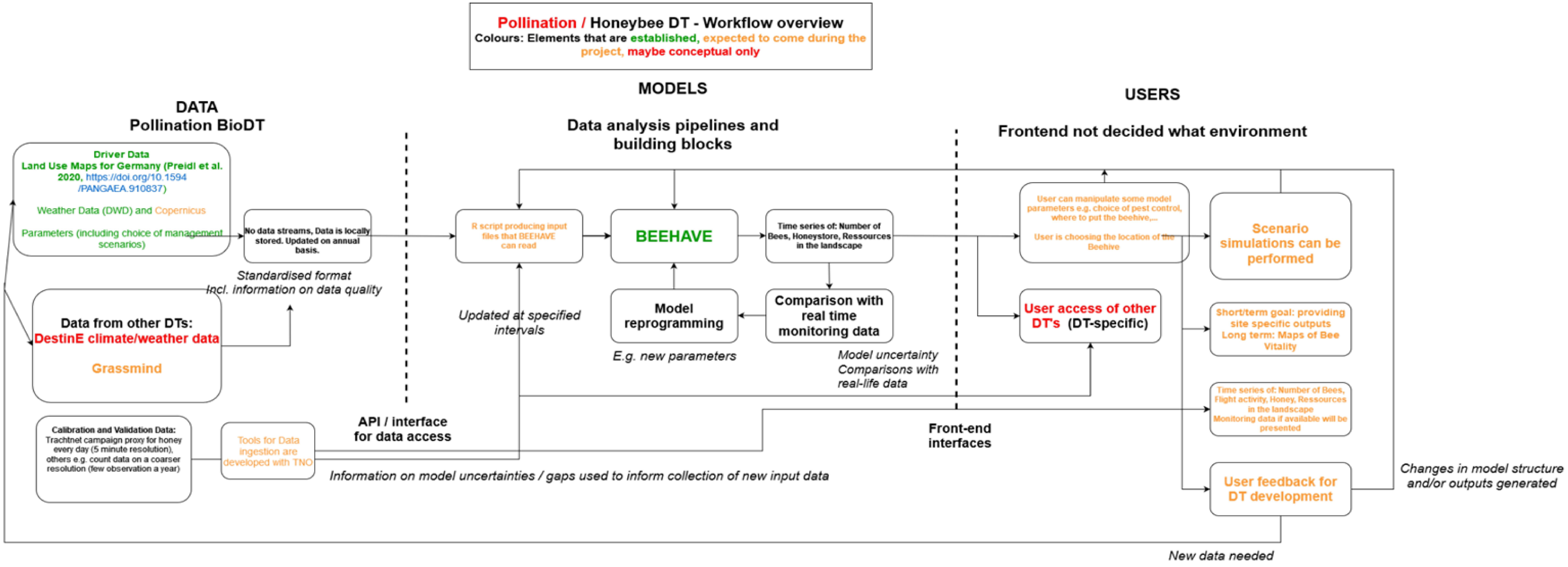
Why HPC?

- Access to fast computing and comprehensive data expertise is essential
- Increasing the model's spatial extent, while keeping the resolution (eg. running the model for the entirety of Germany)
- Comprehensive uncertainty and sensitivity analysis

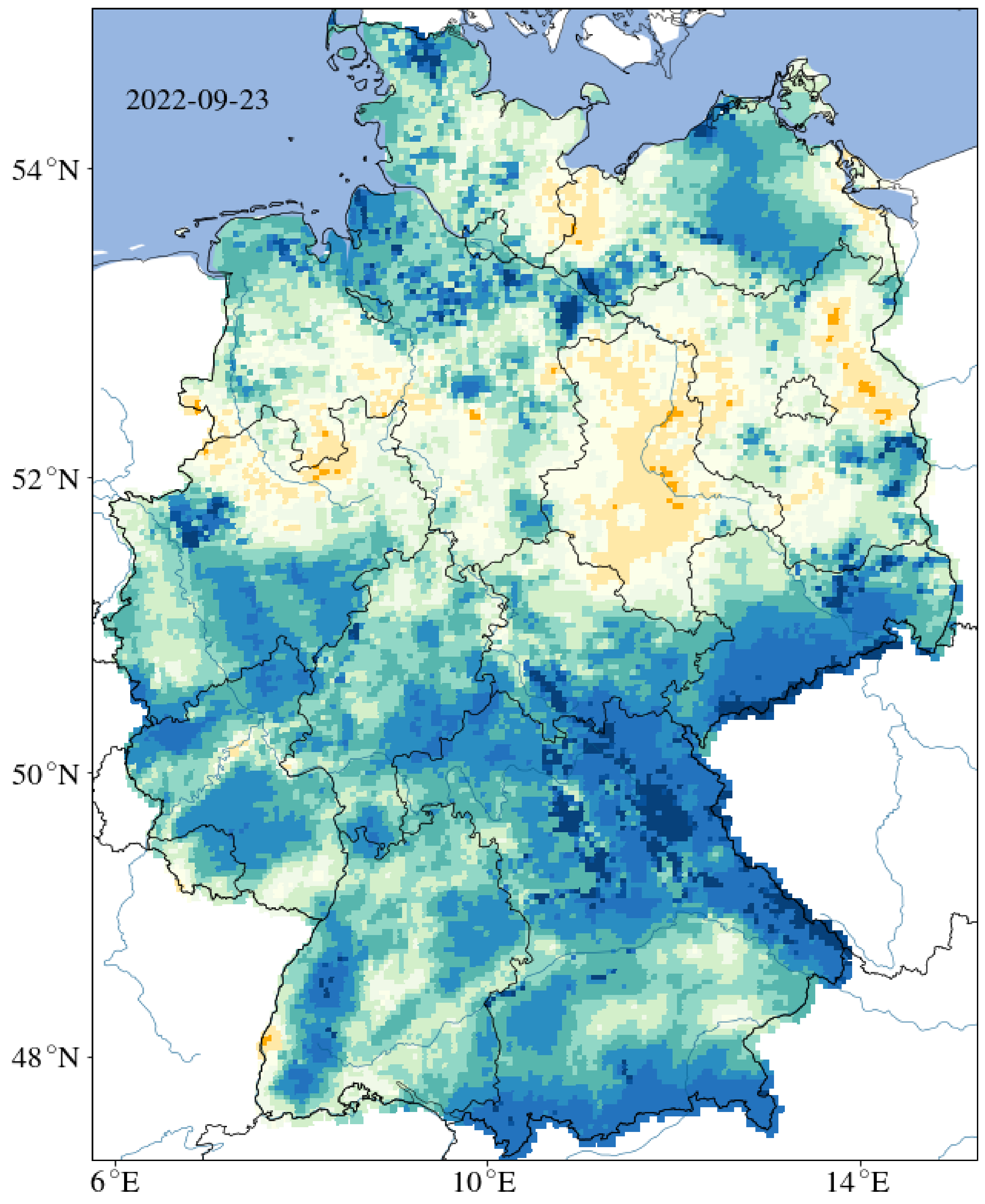
What turns BEEHAVE into a Digital Twin

- Automation of data flow
- Dynamic model updating (e.g. feeding in updated environmental data, followed by new model iteration)
- Automated model uncertainty analysis (comparisons with real-life data)

Tentative workflow



Envisaged outputs: risks maps



- Interactive and/or static maps where the color would code the risk of forage gaps and hence bee colony failure
- This will indicate where certain changes in land use could and should improve the forage supply situation for pollinators

Potential end-users

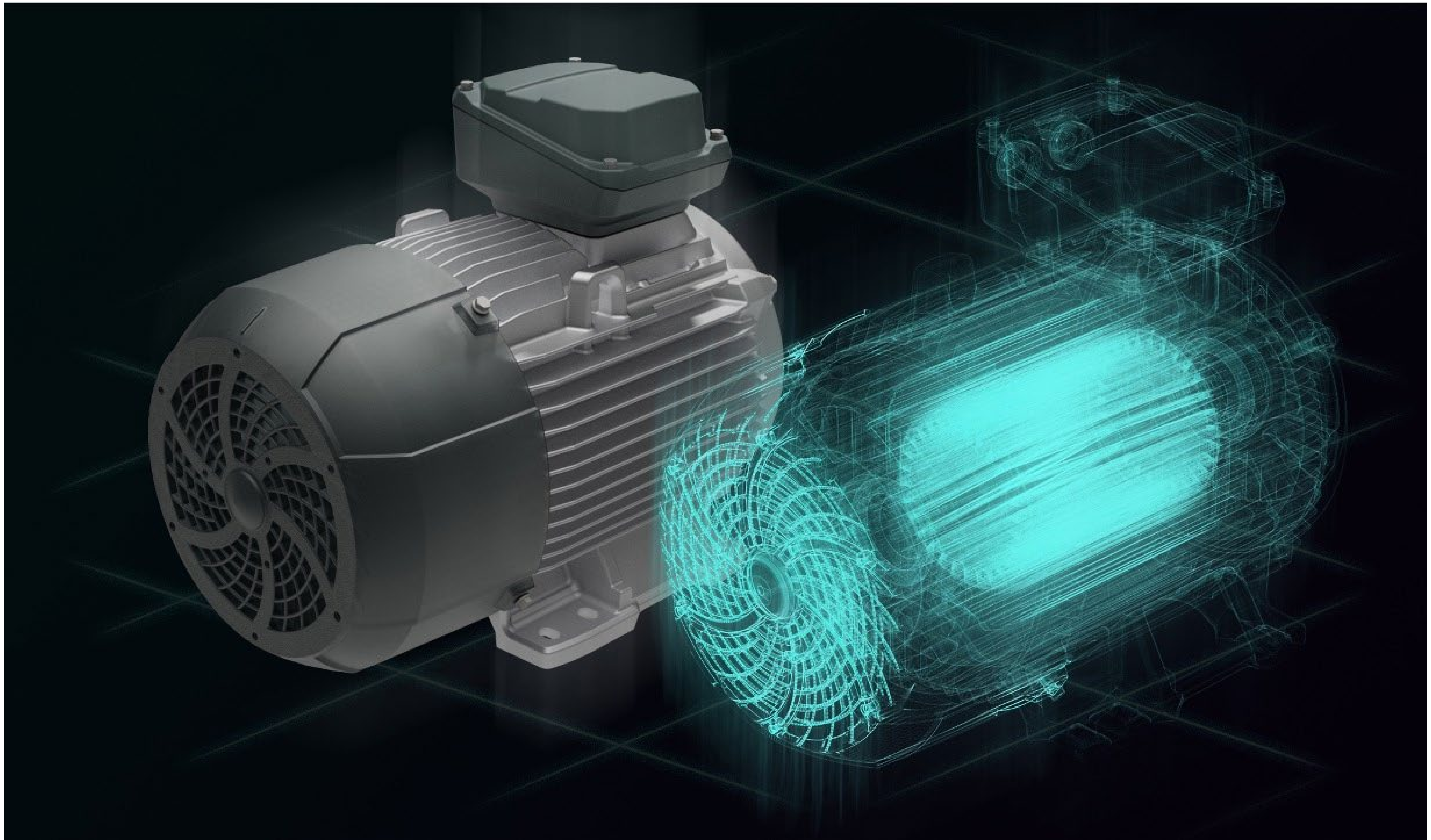
- Academia
- Beekeepers (institutes, associations)
- Farmers (land management)
- Policy developers (land use)

Paving the Path for Digital Twins on HPC

Product Digital Twin within Siemens Plants

Tomáš Karásek (IT4I), 2023-03-21

Digital Twin of the electric motor?



Complex nonlinear multiphysical problem – electric motor

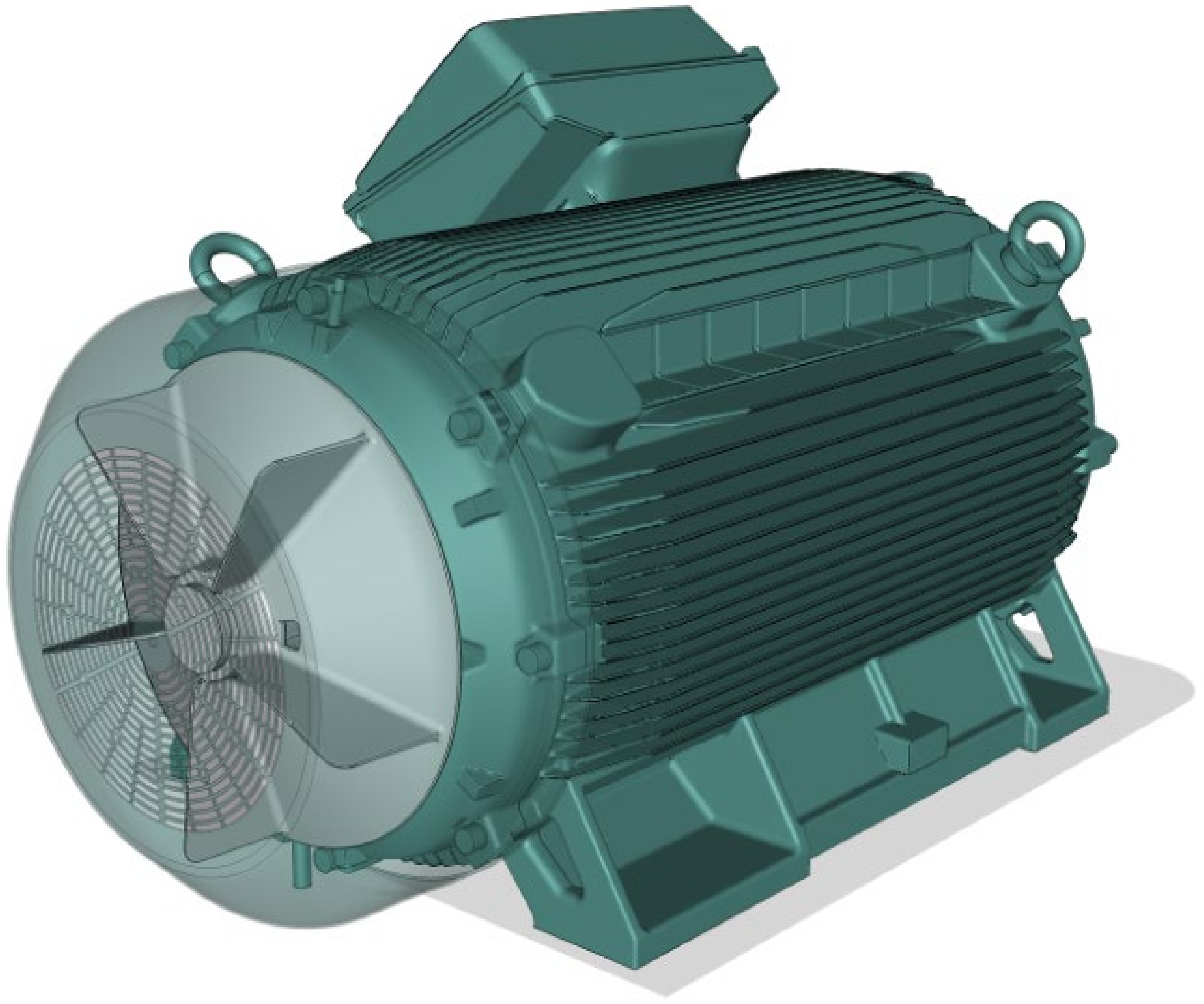
- Electric fields
- Electromagnetism
- Heat transfer
  - heat generated by magnetism
  - cooling system
- Structural Mechanics
  - structural integrity
  - vibration from motion
  - high speed motors
  - influenced by electromagnetism
- Active cooling system
  - fluid flow
- Acoustic
  - generated by fluid flow
  - generated by electromagnetism
  - generated by vibrations

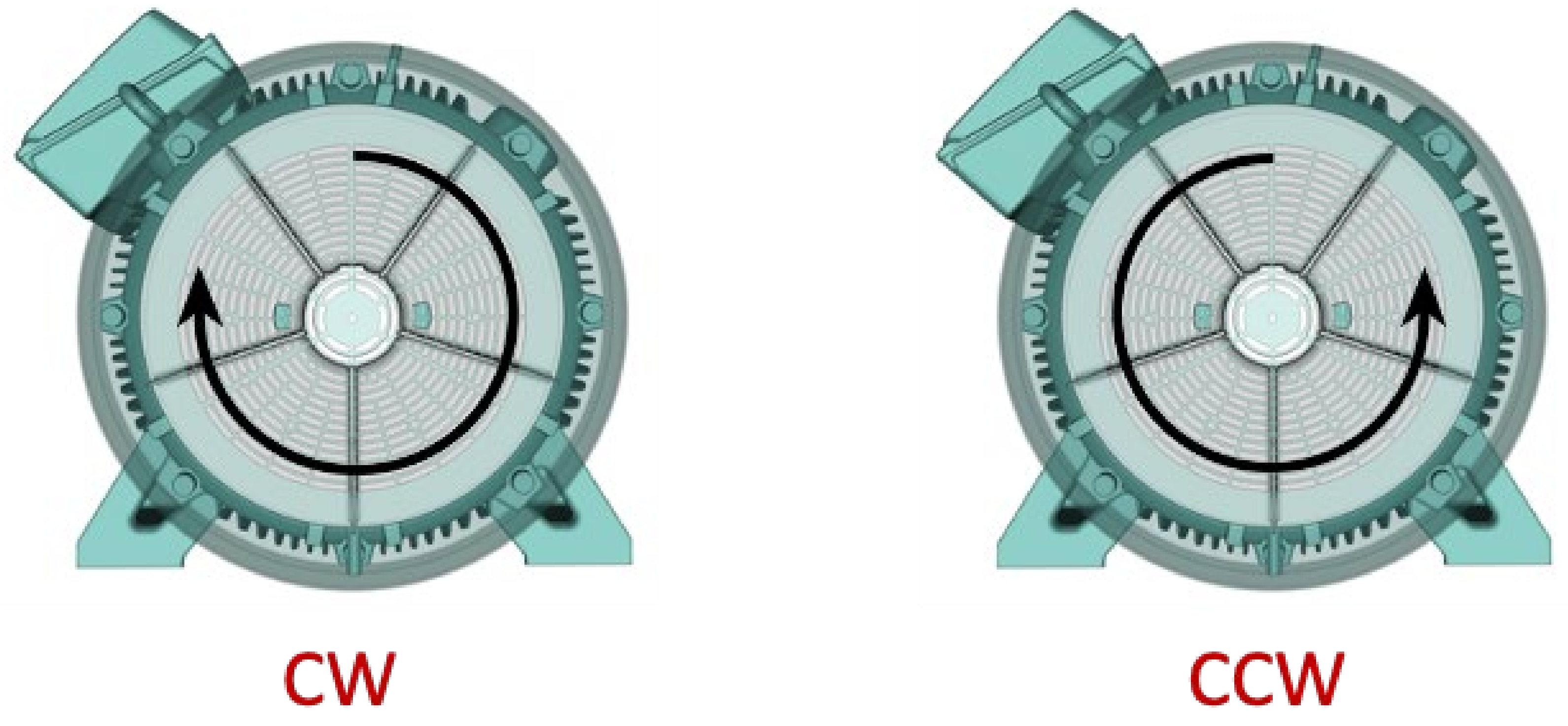
Settings for **Steady State** simulation

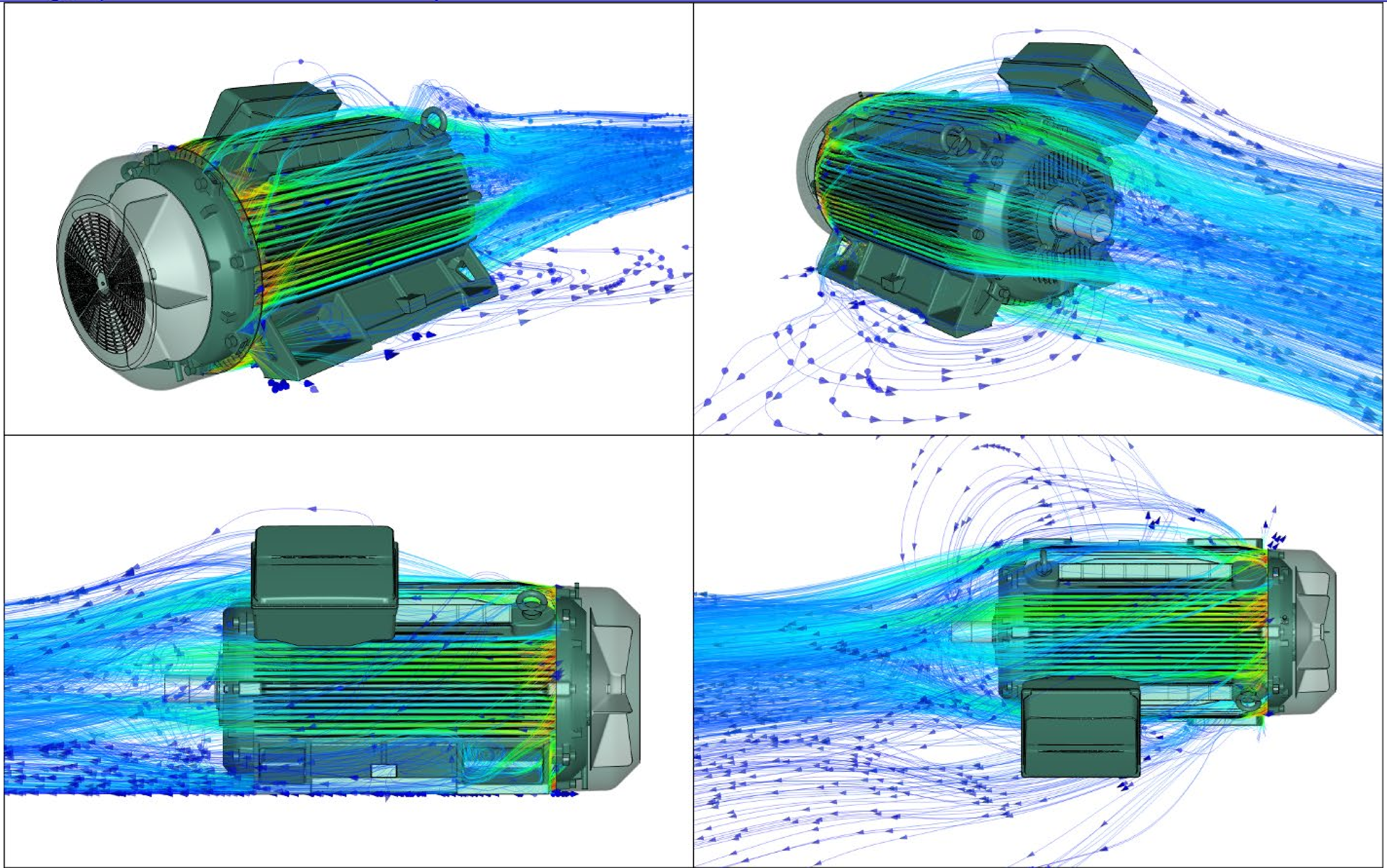
OpenFOAM solver:

- Incompressible simpleFoam with MRF Zone - Moving Reference Frame
- Simulation initialization by potentialFoam solver
- kOmega-SST turbulence model
- 2000 time step iterations to reach the convergence
- Solved for CW and CCW directions

- Solution time for one solver run on IT4I Salomon supercomputer:
  - 960 cores - 2 hours (price - 90 €)
  - 1200 cores - 1,6 hour (price - 90 €)
- **Standard workstation with 30 Cores ~ 64 hours**





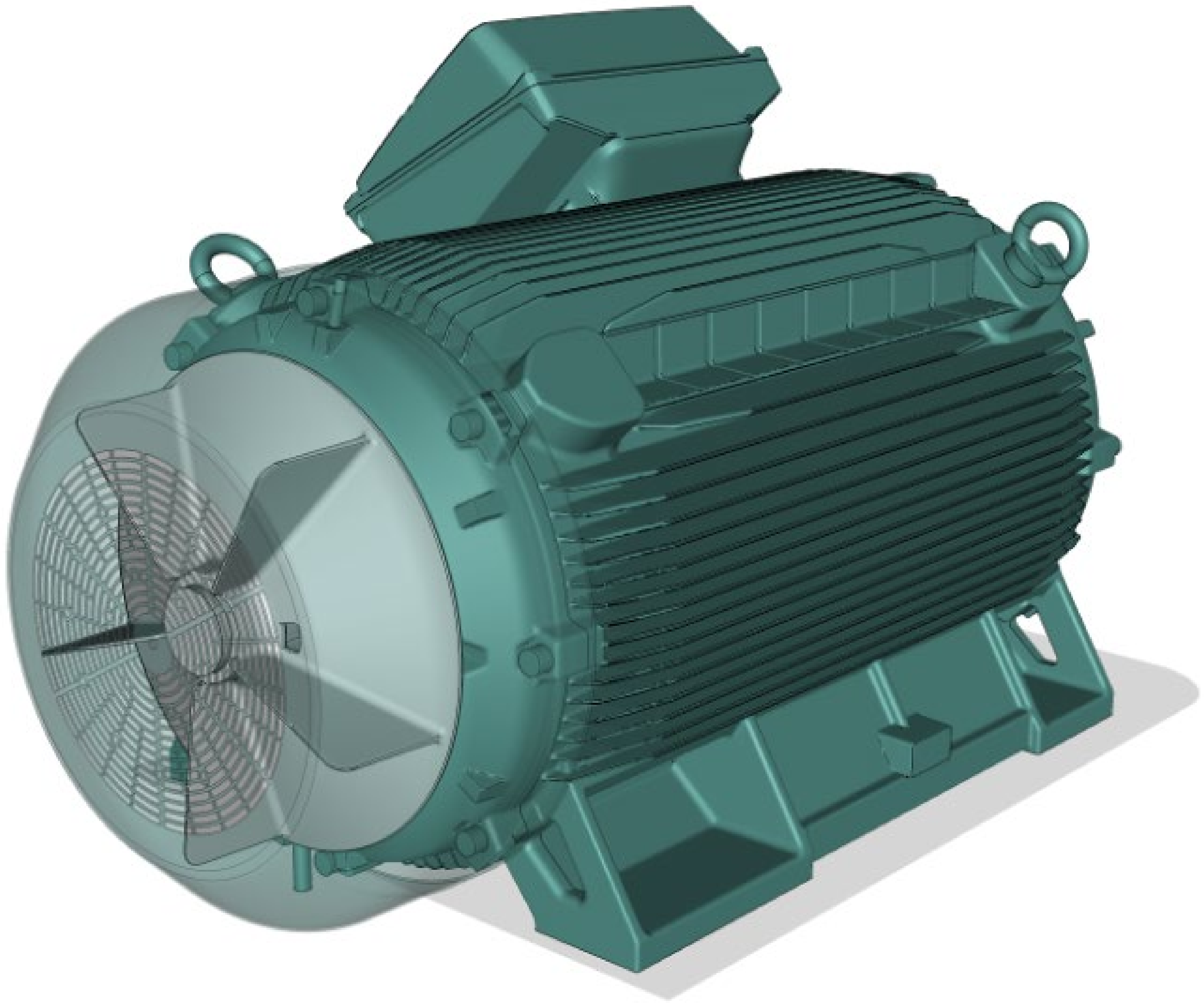


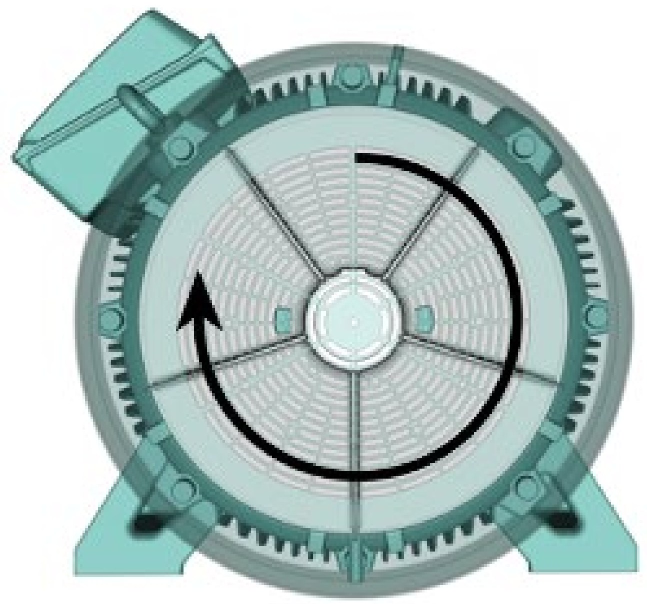
Settings for **<u>Transient</u>** simulation

OpenFOAM solver:

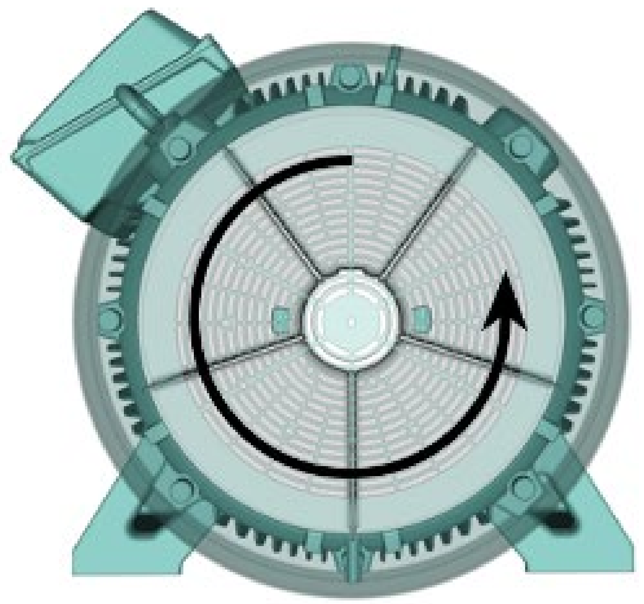
- Incompressible pimpleDyMFoam with dynamic solid mesh motion
- Simulation initialization by steady-state results
- Solid mesh motion - fan rotation with 994 RPM
- kOmega-SST turbulence model
- Constant time step - 2° per time step -> 3.353 E-04 [sec]
- 8 full fan rotations were calculated

- Solution time for one solver run on IT4I Salomon supercomputer:
  - 960 cores - 43 hours (price - 1920 €)
  - 1200 cores - 34 hour (price - 1920 €)
- **Standard workstation with 30 Cores ~ 1500 hours (2 months)**





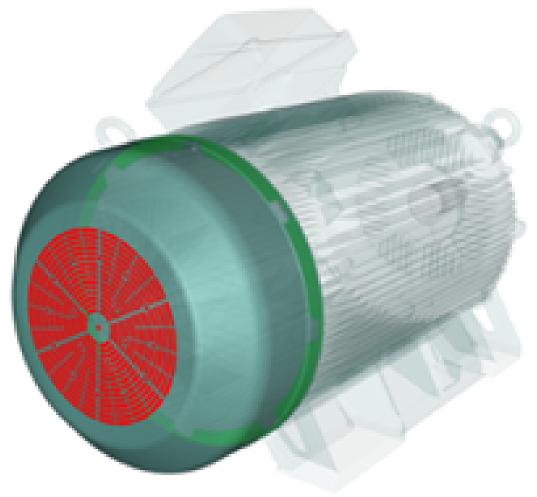
CW



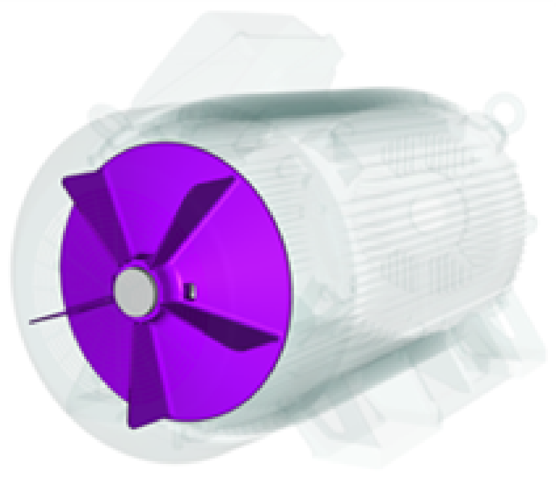
CCW

Verification by measurements

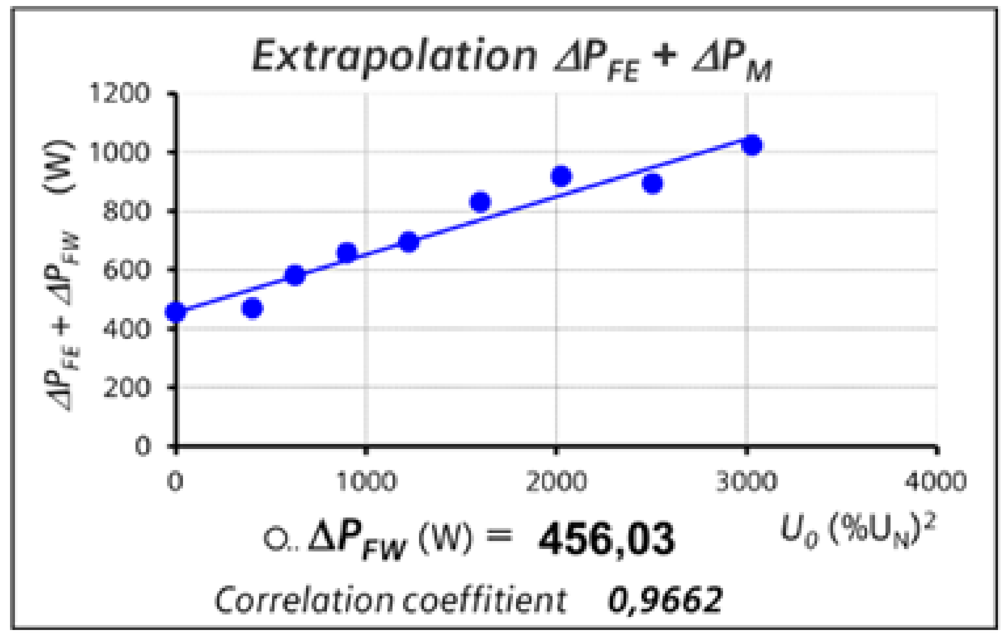
Flow Rate [m³/min]



Measurement	CW		CCW	
	CFD Transient	CFD STEADY	CFD Transient	CFD STEADY
46.90	47.58	40.70	46.40	40.00



Ventilation losses [W]

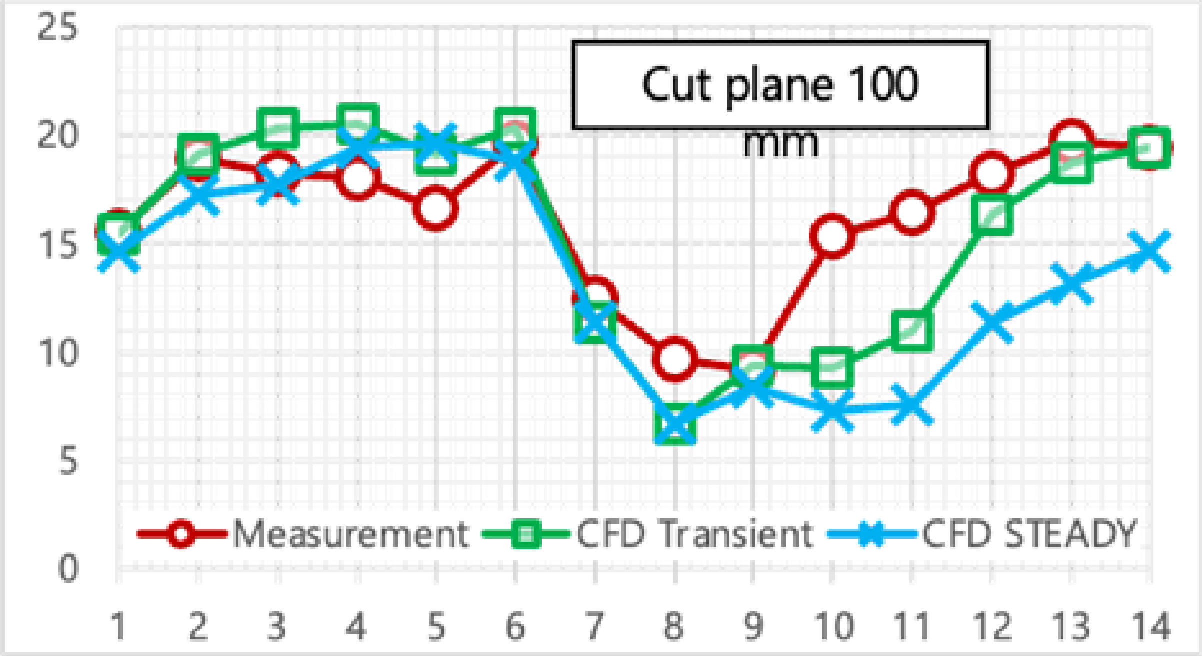


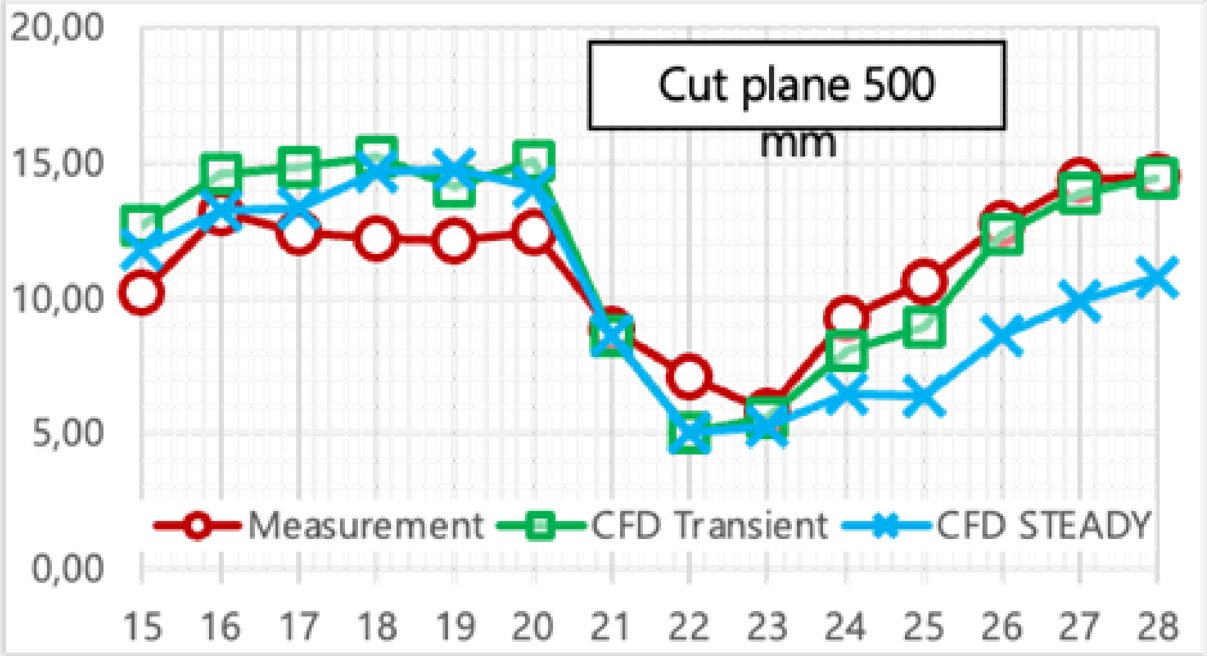
Extrapolation of the measured data

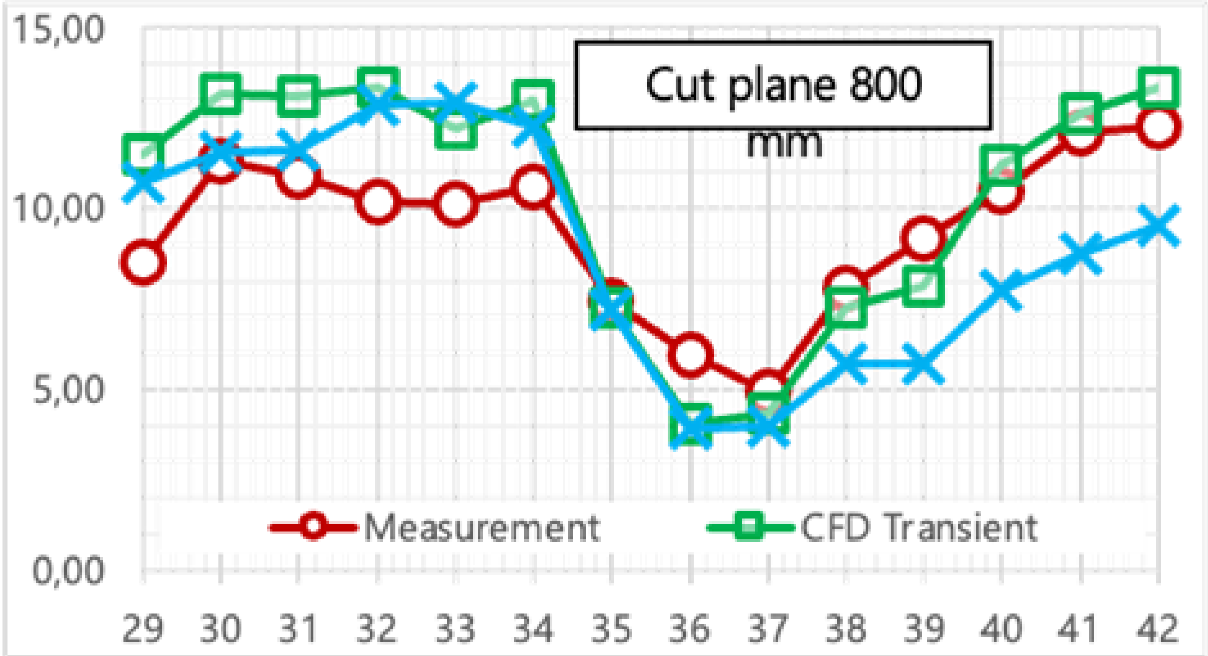
	CW				CCW			
Measurement	CFD Transient		CFD STEADY		CFD Transient		CFD STEADY	
560	**578**	625	**477.3**	518	**566**	619.3	**471.8**	510
Density	1.127	1.225	1.127	1.225	1.127	1.225	1.127	1.225

results depend on the density 1.127 [kg/m³] -> smaller density -> smaller torque moment

Verification by measurements





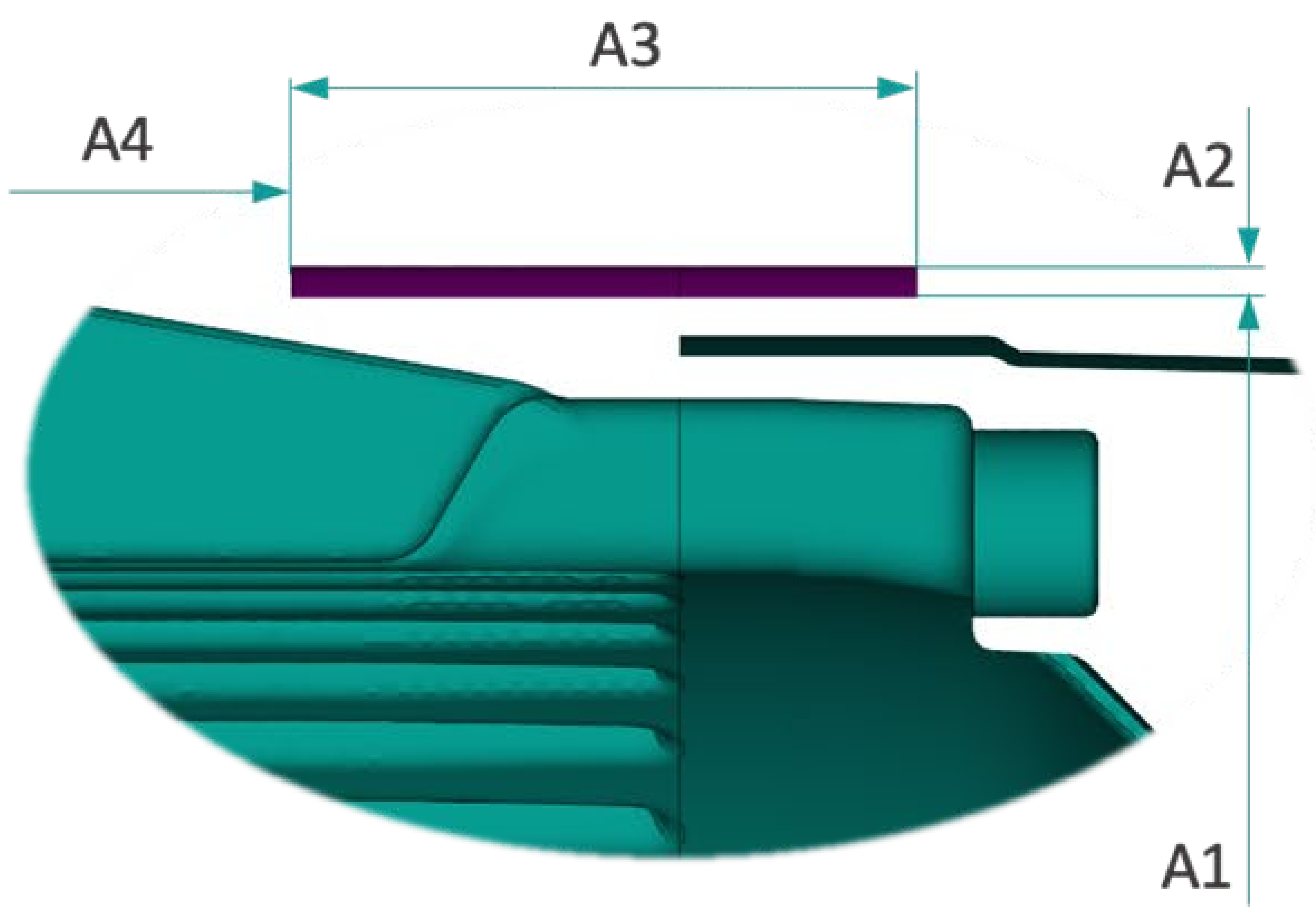


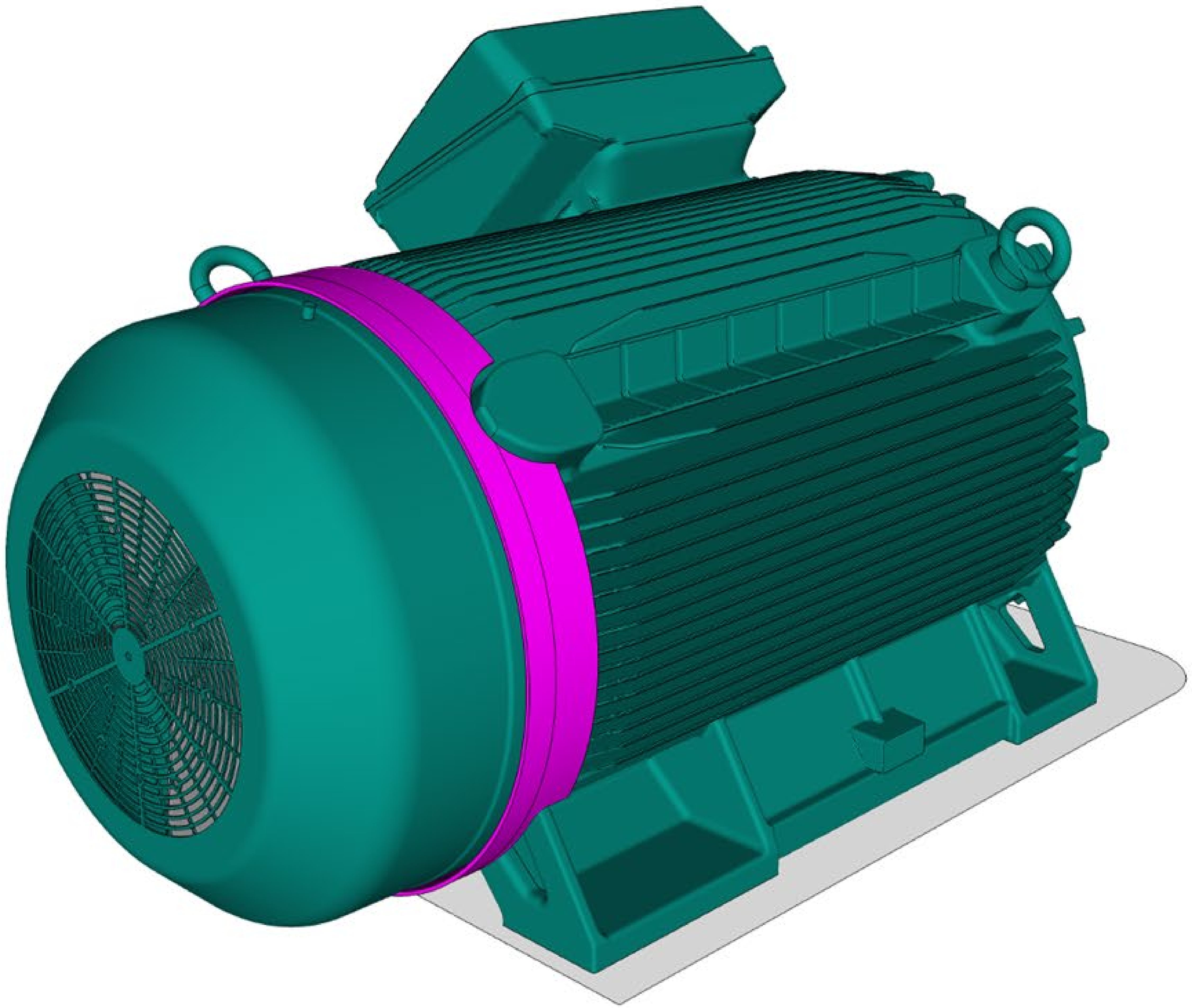
			CW		CCW				CW		CCW				CW		CCW	
	position	Measurement	CFD Transient	CFD STEADY	CFD Transient	CFD STEADY	position	Measurement	CFD Transient	CFD STEADY	CFD Transient	CFD STEADY	position	Measurement	CFD Transient	CFD STEADY	CFD Transient	CFD STEADY
TOP SIDE	1	15.53	15.45	14.64	19.04	14.04	15	10.23	12.70	11.79	14.63	10.46	29	8.51	11.48	10.75	13.42	9.07
	2	18.91	19.13	17.20	17.13	12.73	16	13.18	14.60	13.23	12.71	9.57	30	11.33	13.18	11.59	11.28	8.18
	3	18.21	20.29	17.78	15.33	12.46	17	12.46	14.83	13.32	11.31	9.42	31	10.88	13.14	11.61	10.07	8.25
	4	17.99	20.54	19.42	13.67	11.14	18	12.23	15.21	14.63	10.88	8.57	32	10.19	13.36	12.90	9.58	7.50
	5	16.65	19.18	19.58	10.33	8.27	19	12.11	14.15	14.77	8.17	5.65	33	10.12	12.24	12.92	7.16	4.48
	6	19.61	20.28	18.87	4.79	2.82	20	12.45	15.07	14.14	4.23	1.85	34	10.63	12.98	12.26	3.95	1.38
	7	12.47	11.40	11.37	6.01	5.72	21	8.85	8.57	8.64	5.14	4.75	35	7.44	7.24	7.19	4.01	3.75
	8	9.68	6.68	6.72	11.71	11.54	22	7.08	5.05	5.04	8.95	8.81	36	5.93	4.02	3.90	7.30	7.29
	9	9.18	9.40	8.37	21.33	20.52	23	5.82	5.58	5.25	15.94	15.31	37	4.91	4.36	4.00	13.83	13.27
	10	15.39	9.23	7.31	20.03	19.95	24	9.27	8.06	6.43	14.75	14.92	38	7.82	7.28	5.70	12.91	13.04
	11	16.49	10.96	7.56	20.63	19.33	25	10.58	8.90	6.36	15.27	14.71	39	9.18	7.86	5.72	13.58	13.04
	12	18.22	16.33	11.37	20.21	17.98	26	12.75	12.37	8.63	14.71	13.64	40	10.48	11.20	7.72	13.19	11.97
	13	19.77	18.76	13.12	18.86	17.85	27	14.35	13.90	9.86	14.23	13.83	41	12.11	12.66	8.77	12.88	12.23
	14	19.42	19.39	14.64	11.47	12.85	28	14.52	14.42	10.78	9.51	10.59	42	12.28	13.36	9.56	8.49	9.64
Averege		**16.25**	**15.50**	**13.42**	**15.04**	**13.37**		**11.13**	**11.67**	**10.20**	**11.46**	**10.15**		**9.42**	**10.31**	**8.90**	**10.12**	**8.79**

Use of virtual model: design modifications

RING Geometry modifications

	RING 01	RING 02	RING 03	RING 04
A1	0.361	0.361	0.365	0.359
A2	0.005	0.005	0.005	0.005
A3	0.1	0.075	0.1	0.1
A4	0.99	0.99	0.99	0.99





EuroHPC Summit

2023 Göteborg

Paving the Path for Digital Twins on HPC

Discussion and Q&A

Additional panel member:

- Pekka Manninen (CSC)
- Thomas Eickermann (JSC)

Dirk Pleiter, 2023-03-21