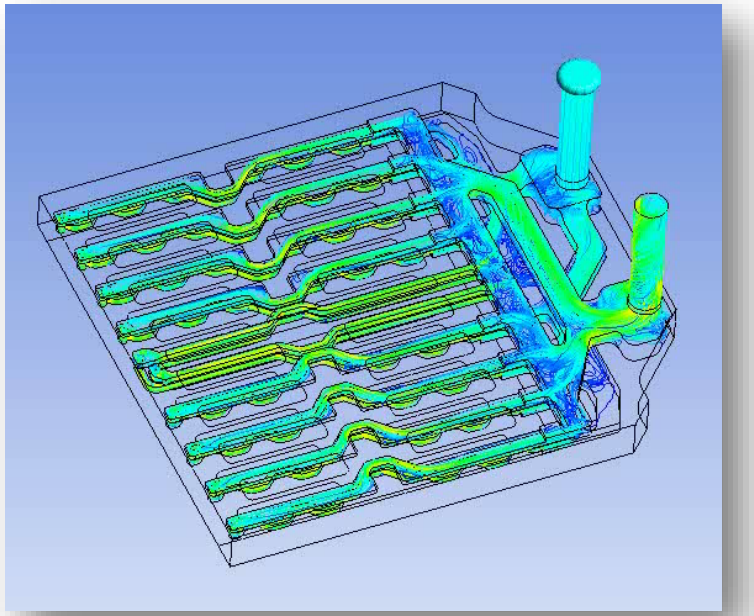
Advancing Simulation Capabilities at European XFEL: a Multidisciplinary Approach

F. Yang, D. La Civita, S. Goede, D. Loureiro, M. Rehwald, T. Stoye, L. Samoylova, M. Planas, M. Wuenschel, B. Friedrich, N. Kohlstrunk, M. Di Felice, H. Sinn

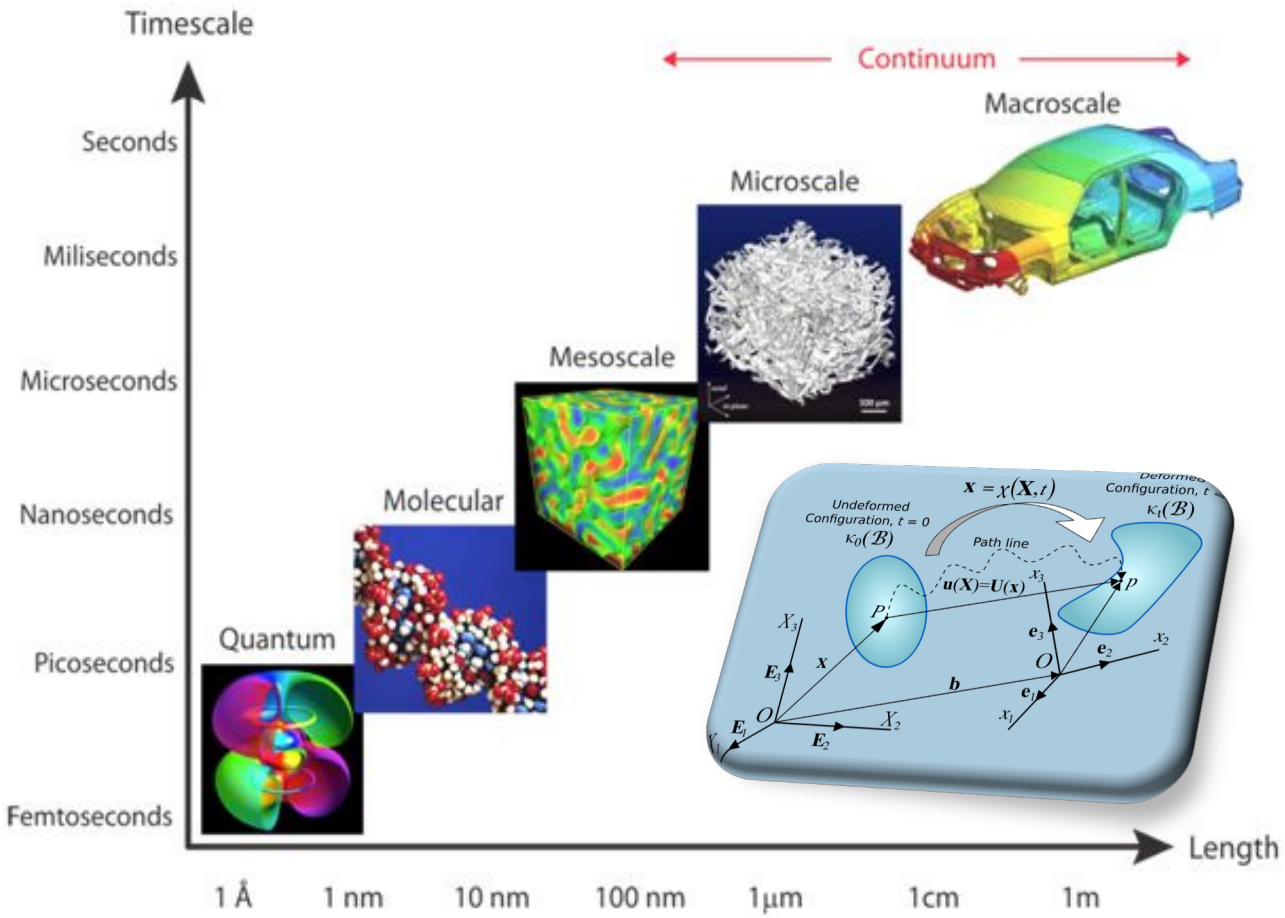
November 6-10, 2023
MEDSI 2023 in Beijing

Outline

- Overview of numerical simulation
- Verification, Validation and Uncertainty Quantification
- Simulation data management system
- Machine learning and AI powered numerical simulation
- Summary and outlook



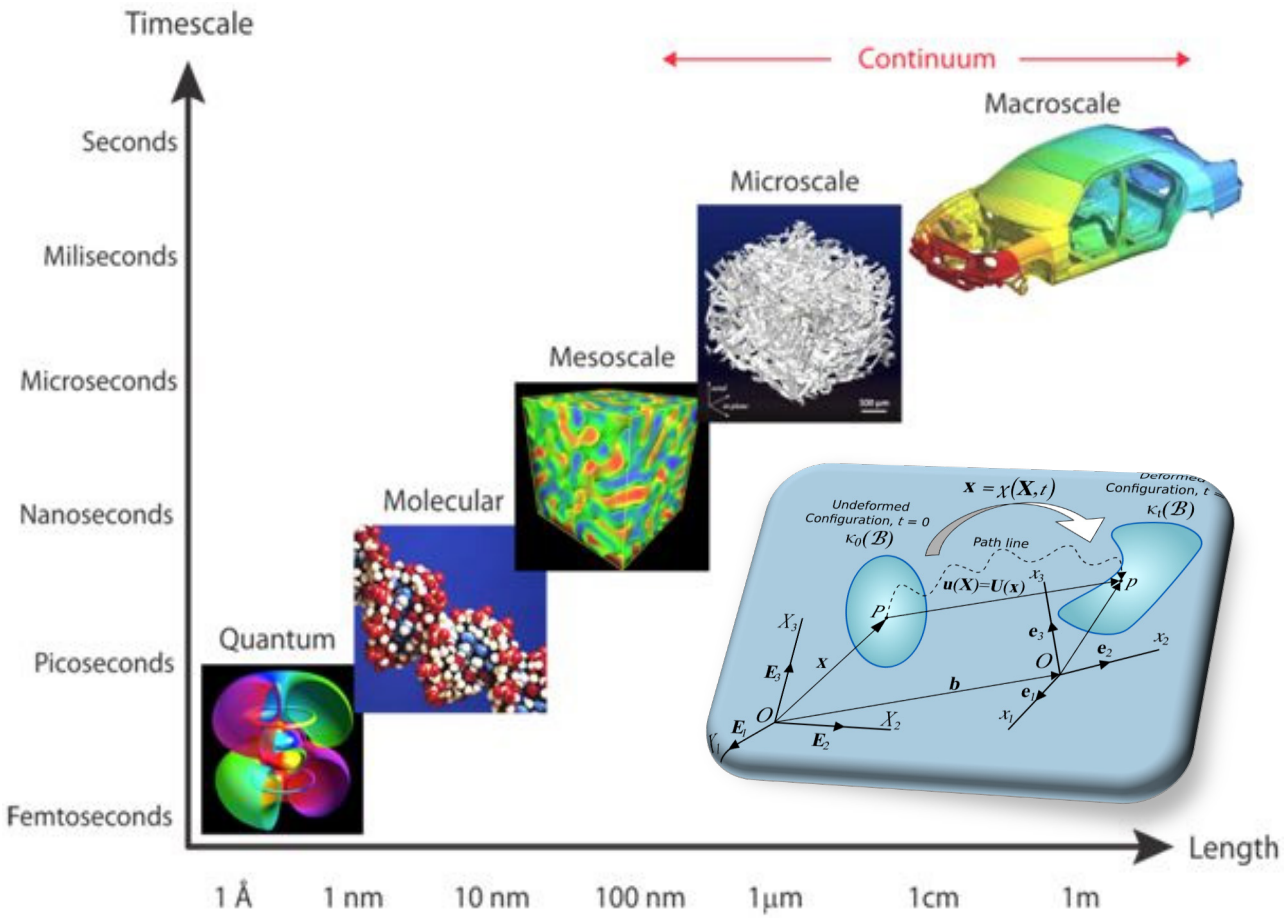
Overview of numerical simulation



- Numerical methods to solve PDEs

FEM, FVM, BEM, FDM, DEM, etc.

Overview of numerical simulation



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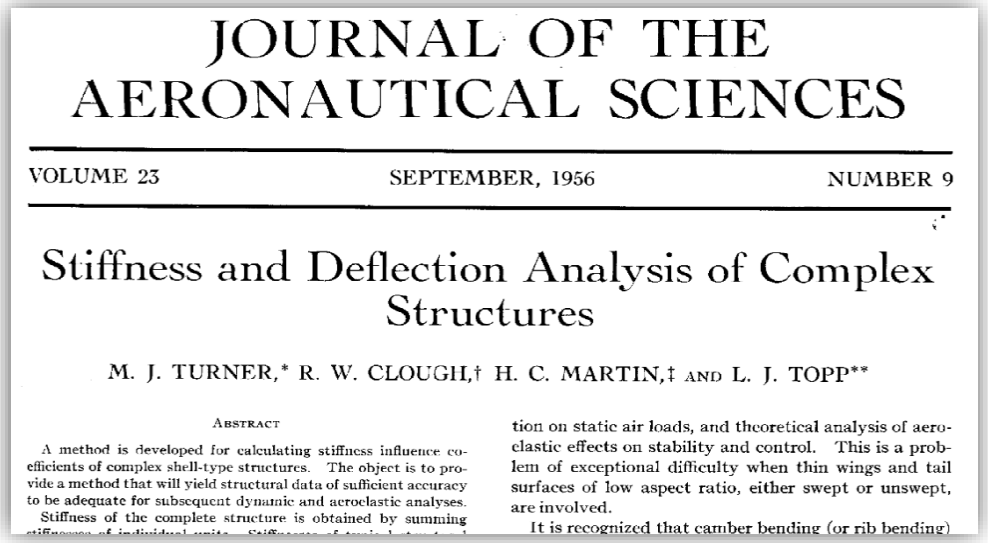

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Stiffness and Deflection Analysis of Complex Structures

M. J. TURNER,* R. W. CLOUGH,† H. C. MARTIN,‡ AND L. J. TOPP**

ABSTRACT

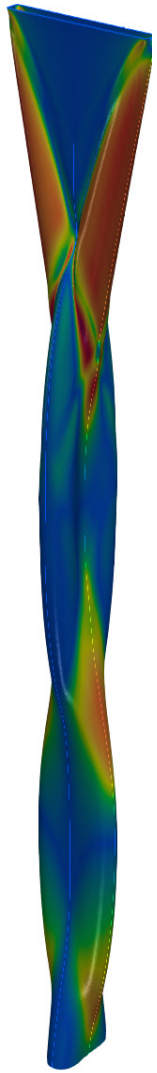
A method is developed for calculating stiffness influence coefficients of complex shell-type structures. The object is to provide a method that will yield structural data of sufficient accuracy to be adequate for subsequent dynamic and aeroelastic analyses. Stiffness of the complete structure is obtained by summing

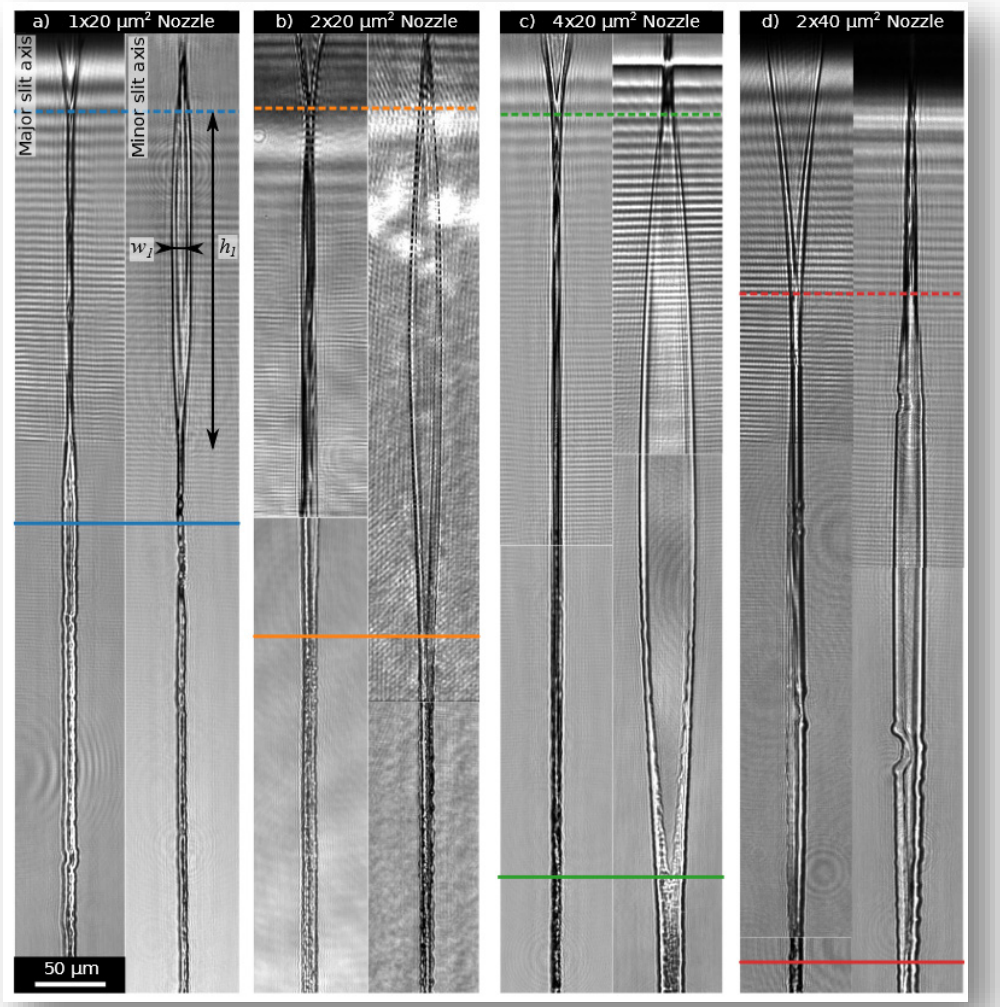
tion on static air loads, and theoretical analysis of aeroelastic effects on stability and control. This is a problem of exceptional difficulty when thin wings and tail surfaces of low aspect ratio, either swept or unswept, are involved.

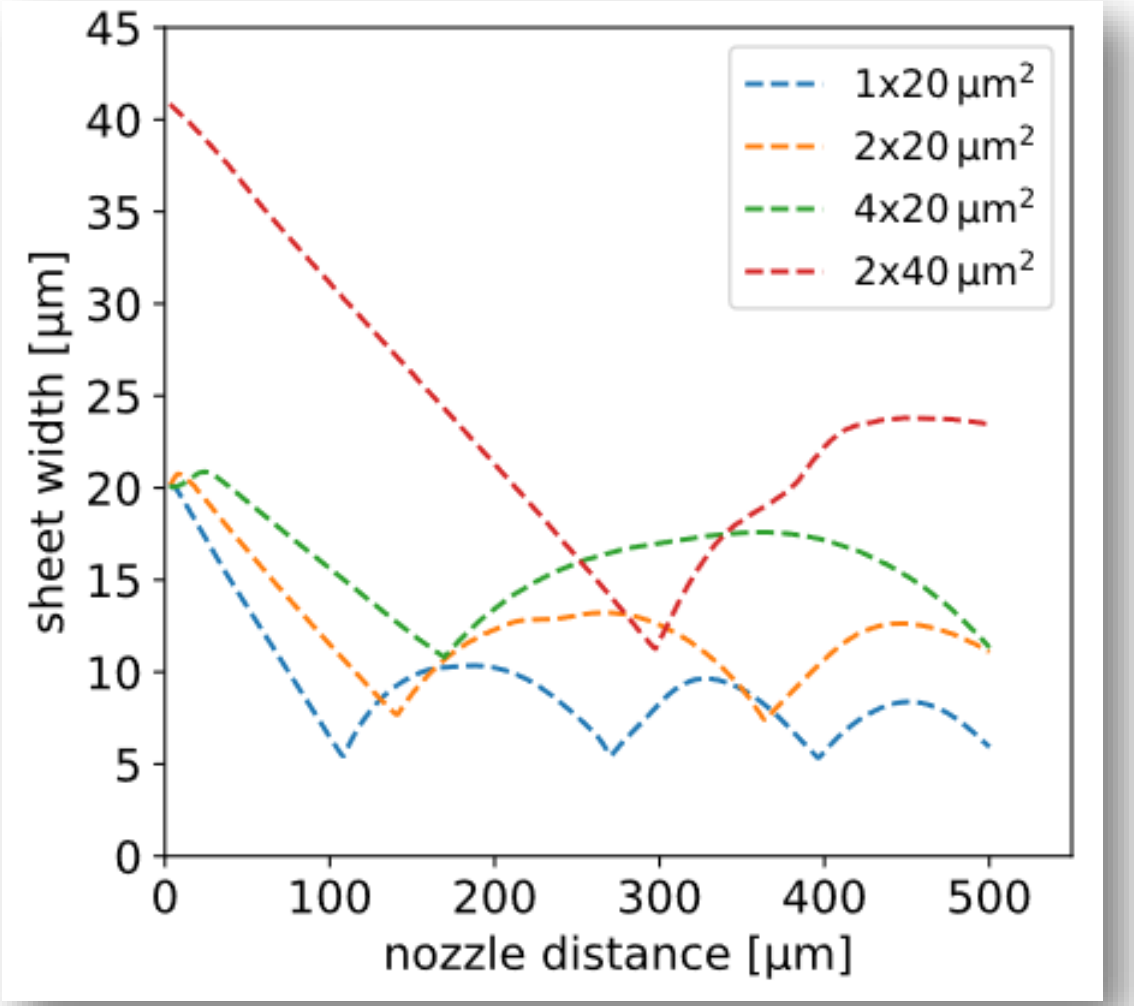
It is recognized that camber bending (or rib bending)

- State of the art
  - Multiphysics, multiscale, multibody problems
  - HPC for real time simulation
  - Cloud-based ROM simulation
  - ML and AI implemented SDM
  - Generative design and digital twin

Cryogenic liquid sheet jet

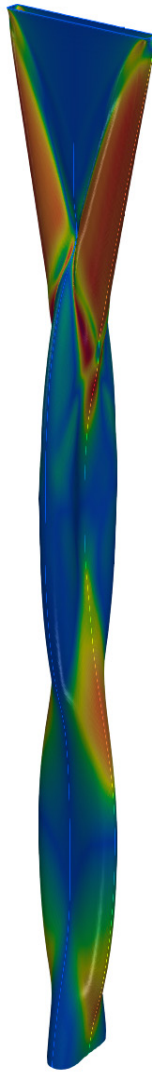


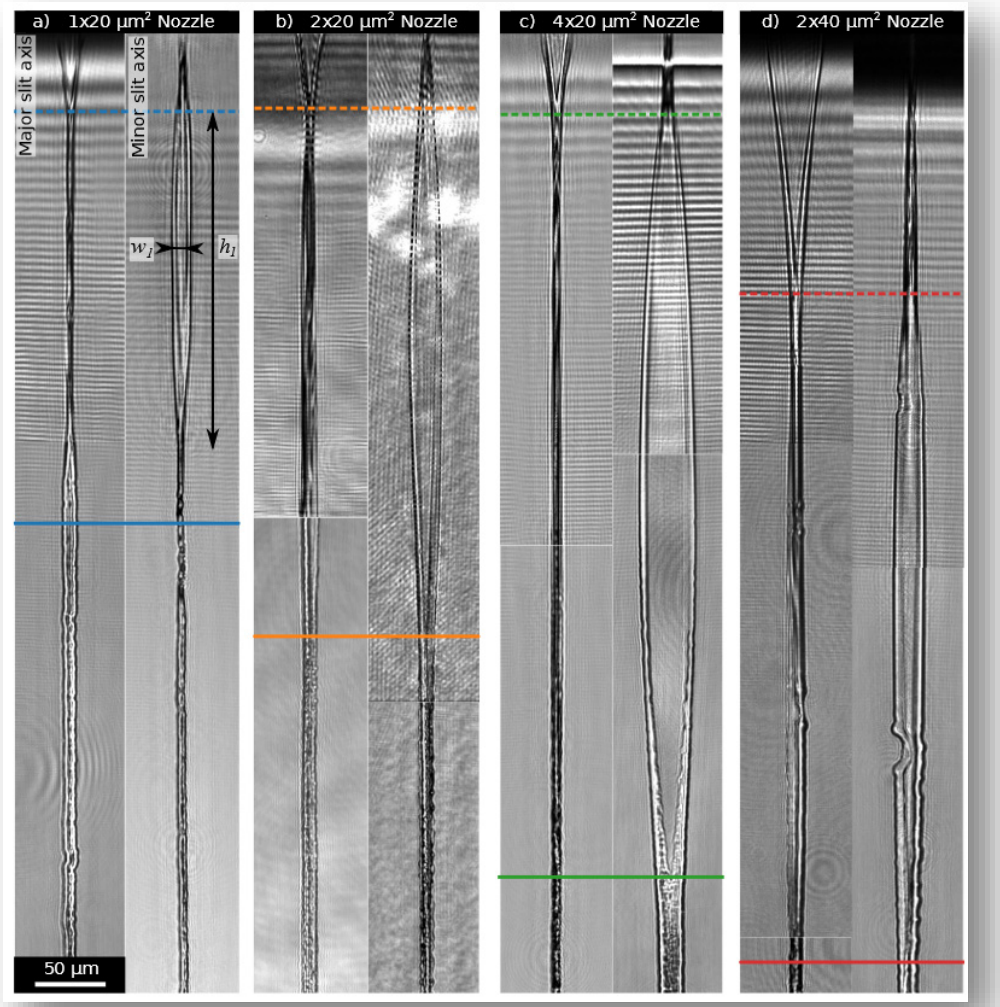


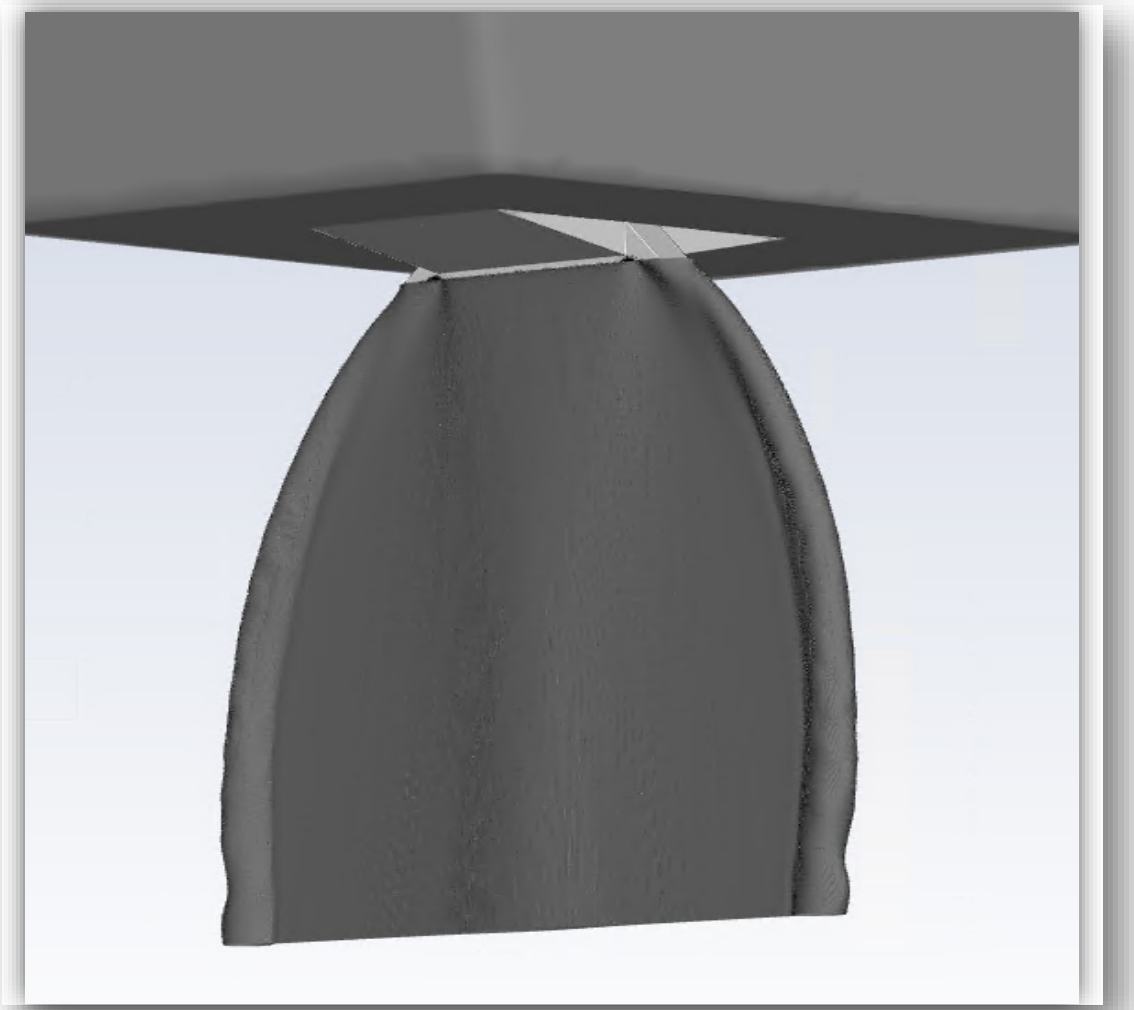


- parameters for sensitivity study: surface tension, viscosity, inlet pressure, etc.

Cryogenic liquid sheet jet







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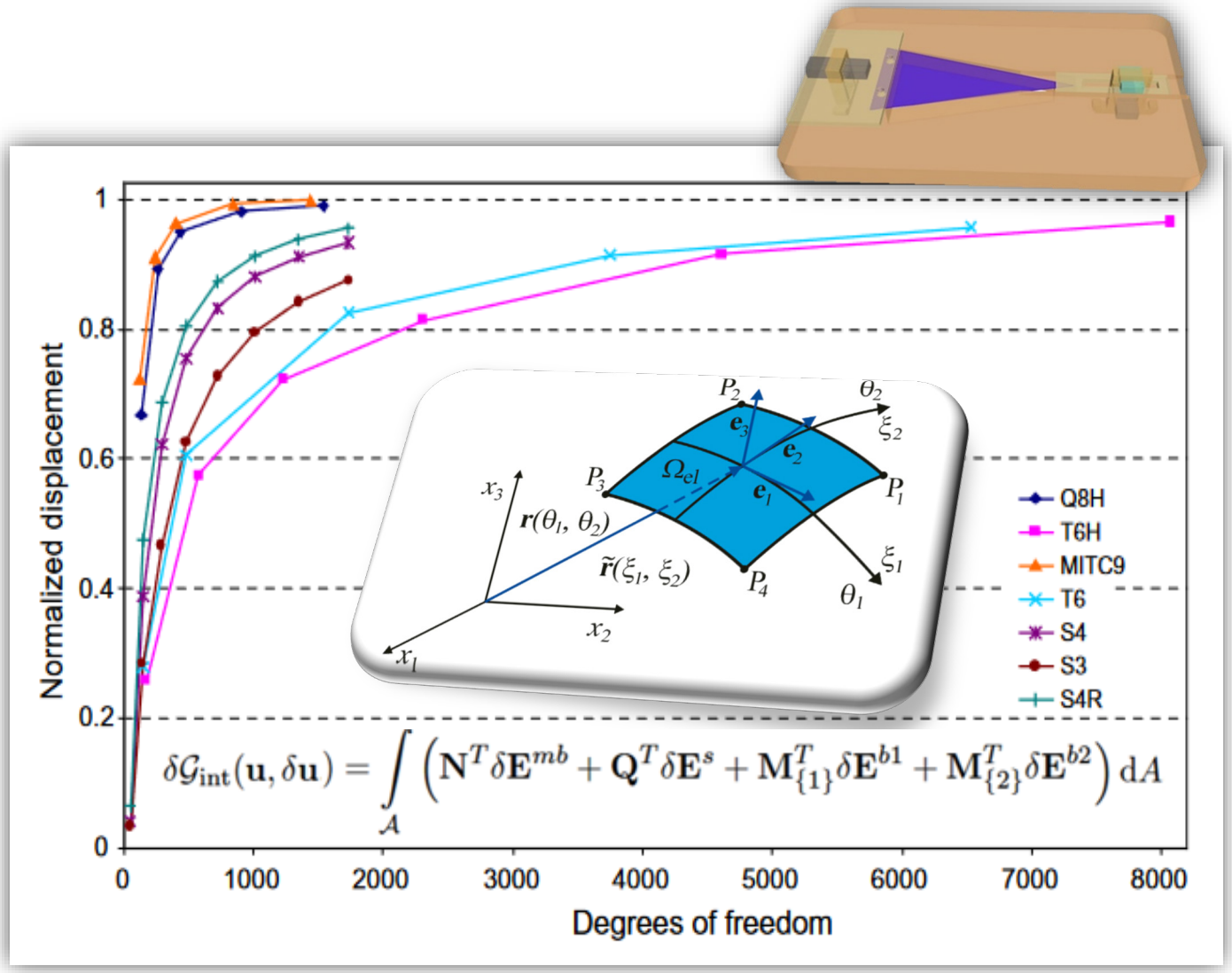
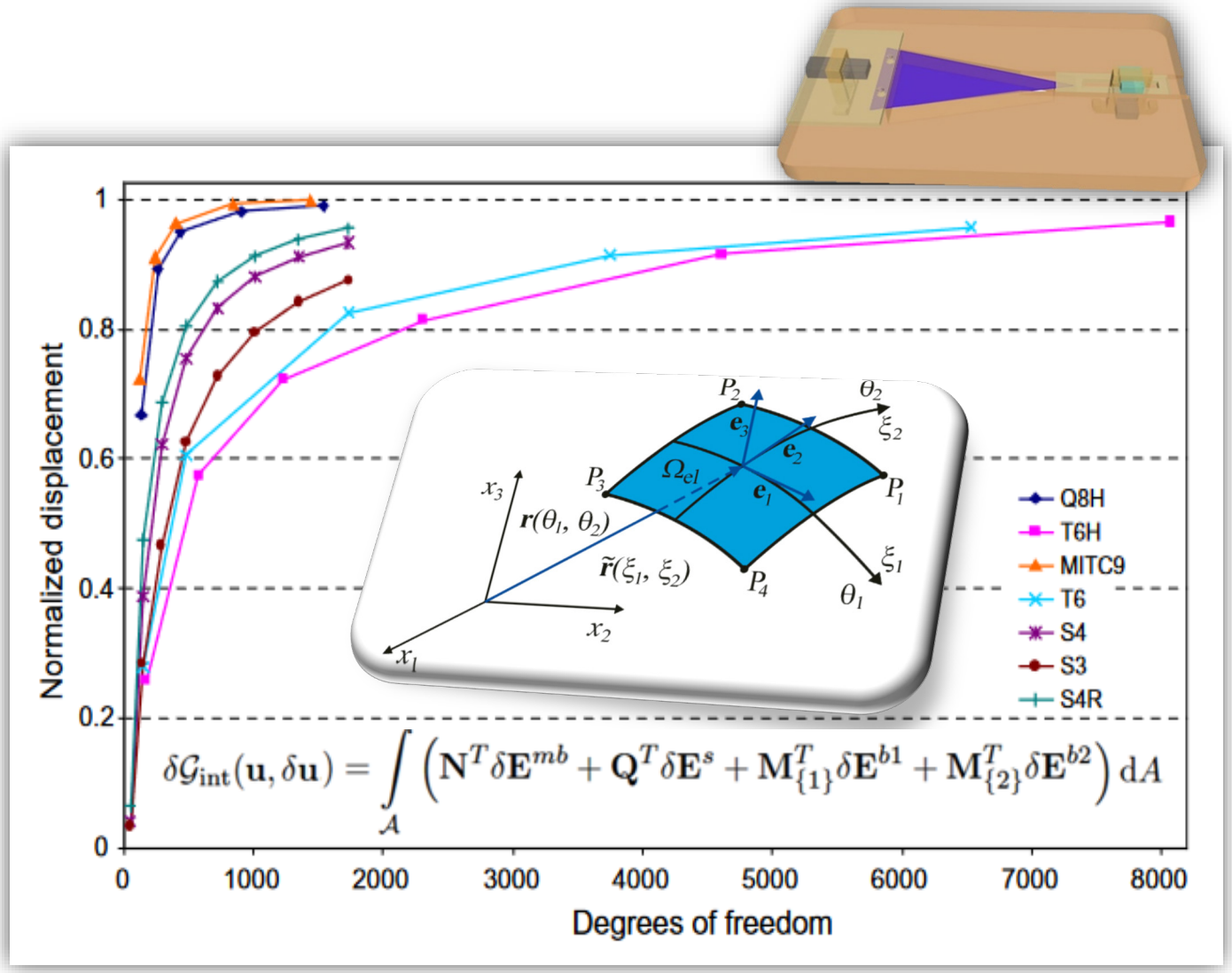
Verification &Validation, uncertainty quantification (VVUQ)



Shell element to avoid shear locking phenomena

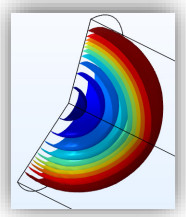
Verification &Validation, uncertainty quantification (VVUQ)

- **Verification** is performed to determine if the computational model fits the mathematical description.
- **Validation** is implemented to determine if the model accurately represents the real world application.
- **Uncertainty quantification** is conducted to determine how variations in the numerical and physical parameters affect simulation outcomes.

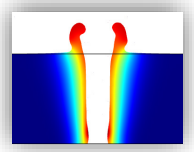


Shell element to avoid shear locking phenomena

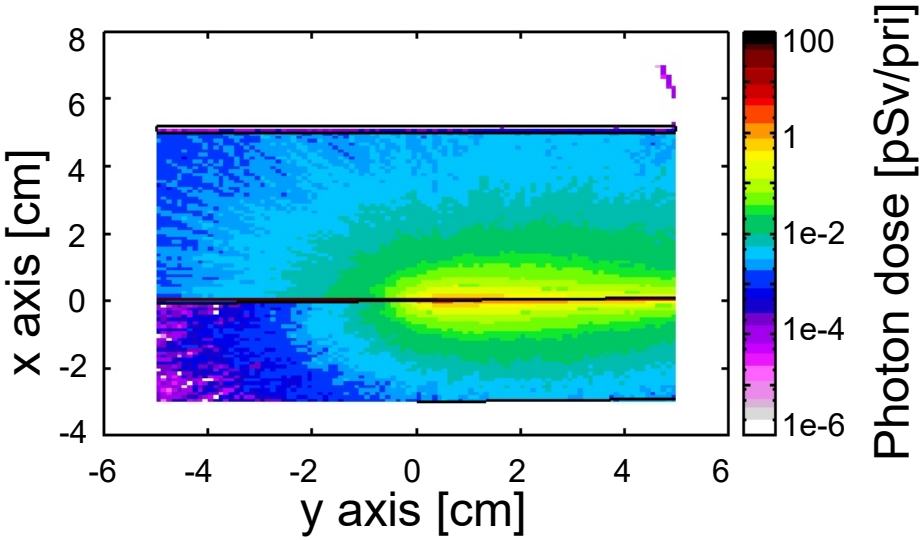
Simulation data management system



GasAttenuator_20221001_v1



Drilling_alum_202001010_9KeV_v2



radiation_tungsten2mm_ODLmirror_20230310_200KeV

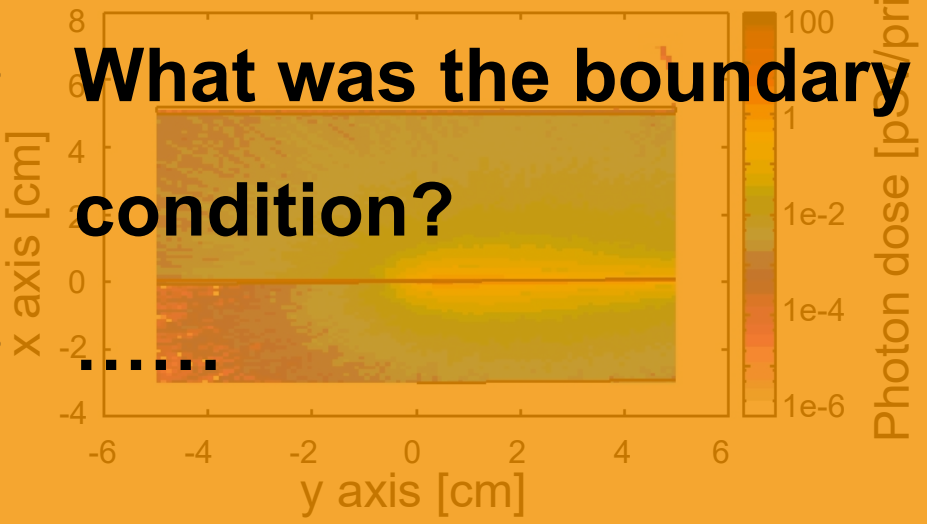
Simulation data management system

GasAttenuator_20221001_v1

- **Who did the job?**

Drilling_alum_202001010_9KeV_v2

- **Where was the simulation saved?**



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- **……**

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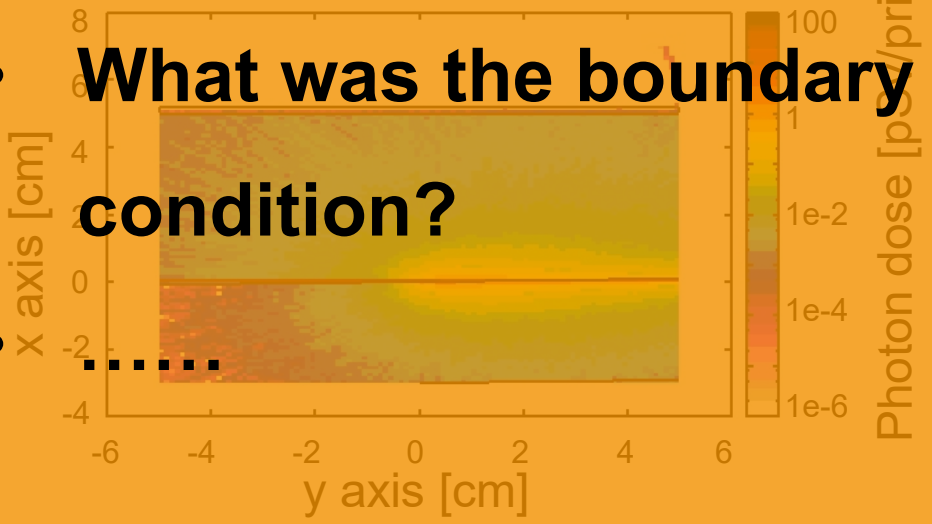

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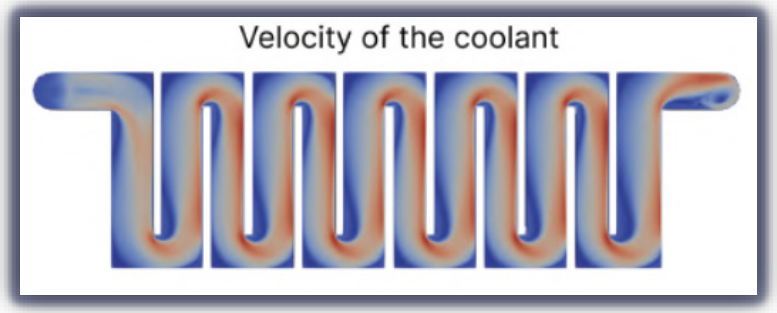
Models	Results
• Structured model setup • Central storage • Smart data management	• Results analysis • Sensitivity study • Visualization • Outlier detection • AI/ML implied for data scanning

AI and ML powered numerical simulation

Design challenge → (re)create CAD model → Setup numerical model → Post process → Data analysis → (re)create CAD model → A solution

Conventional Design



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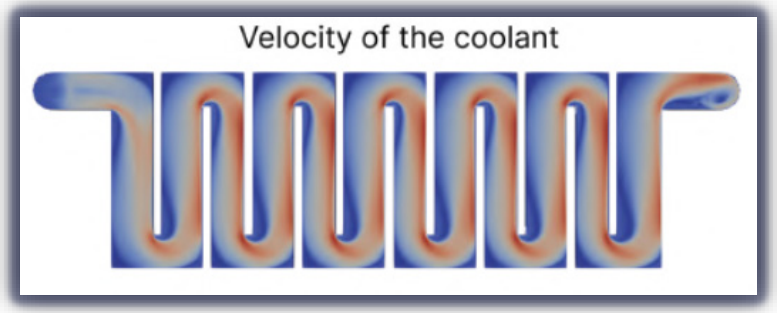
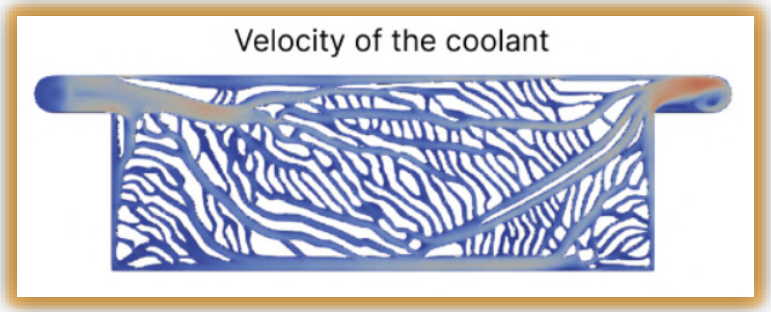


Generative Design



Design challenge → Input data → AI driven design → Optimal solution

AI and ML powered numerical simulation

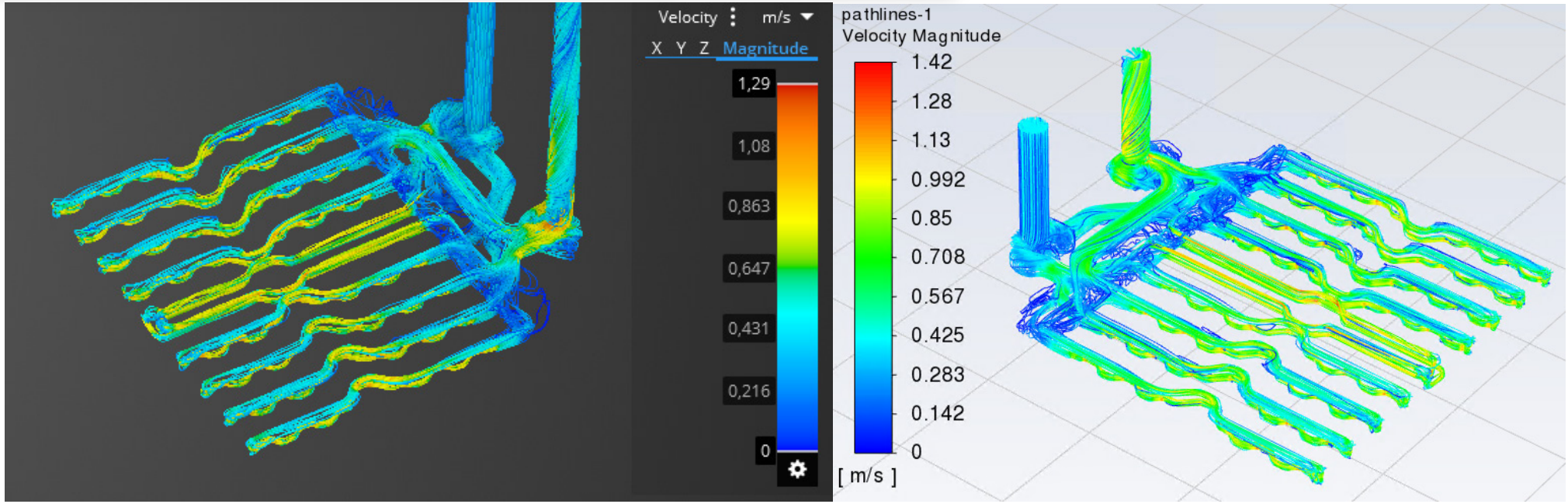
Machine Learning tools for instant predictions and data insights

Pulse energy [mJ]	Photon Energy [keV]	power [W]	FWHM [mm]	simulation results [°C]	AI predicted [°C]
1.87	10	5.05	0.2	29.34	30.77
1.56	12	4.21	0.19	26.23	27.94
1.34	14	3.61	0.18	24.90	24.99
1.17	16	3.16	0.17	24.13	23.46
1.04	18	2.81	0.17	23.60	23.04
0.94	20	2.53	0.16	23.41	22.63

Batch training of ML model predicting thermal behavior of optical components

AI and ML powered numerical simulation

Reduced Order Modeling with ML-augmented solvers



$$\rho \frac{D\vec{V}}{Dt} = -\nabla p + \mu \Delta \vec{V} + NN(\vec{V}, \omega_i)$$

$$\nabla \cdot \vec{V} = 0$$

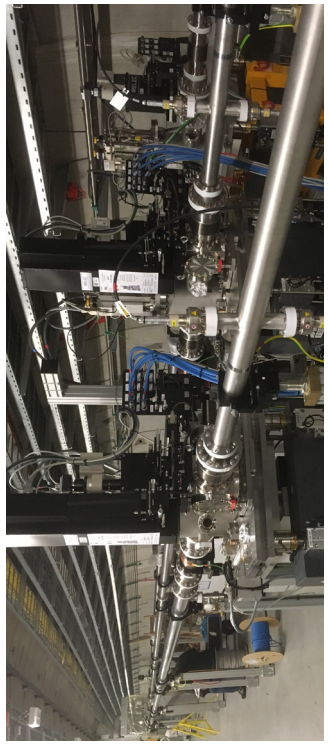
ROM solver	CFD solver
5 s	4 h
low fidelity +ML	high fidelity

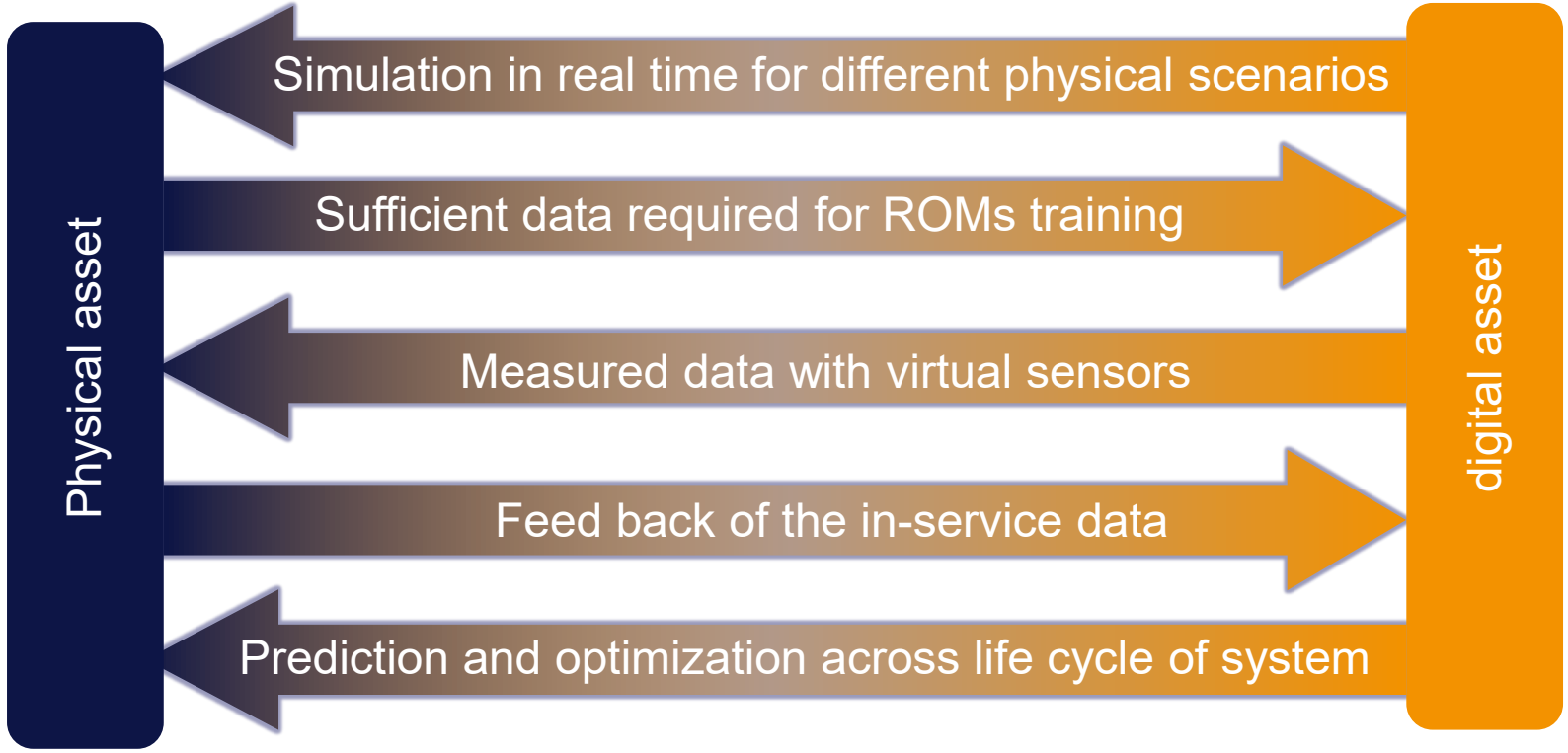
$$\rho \frac{D\vec{V}}{Dt} = -\nabla p + \mu \Delta \vec{V}$$

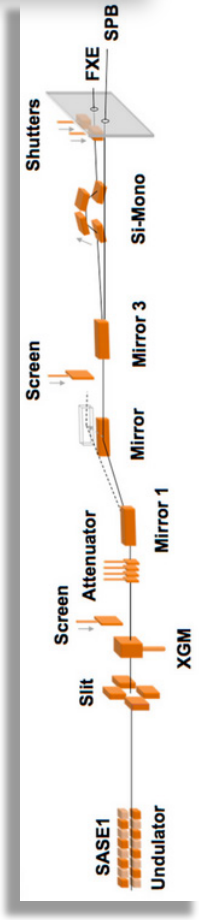
$$\nabla \cdot \vec{V} = 0$$

AI and ML powered numerical simulation

An analytics-driven, simulation-based digital twin is a connected, virtual replica of an in-service physical asset







Summary and Outlook

- Multi-physics simulation: ODL mirror and CFD analysis of liquid sheet jet
- Sensitivity study, VVUQ and simulation data management system for credibility of simulation results
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Foundation model will reshape the world of simulation

- User interface using natural language model
- Surrogate model driven decision making
- AI tools enhanced simulation data management system and workflow automation
- LLM for simulation results inspection and generative design
- Digital twin: improving operational efficiency, enhancing predictive maintenance and troubleshooting, and enabling predictive analytics for system performance.