Workflow Development in the EXCELLERAT Project

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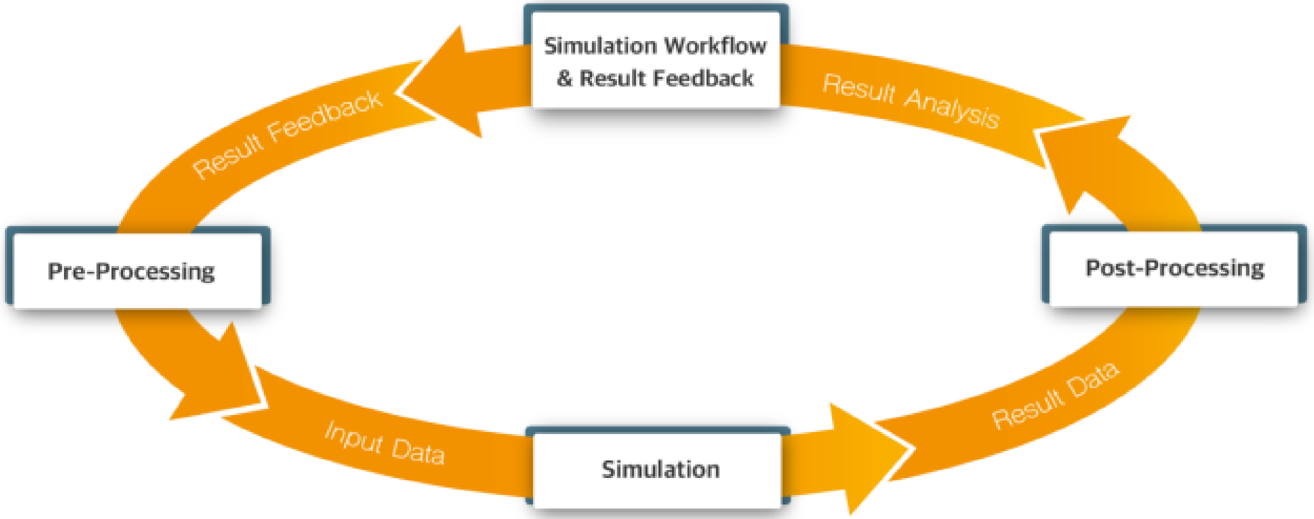
Overview

- The EXCELLERAT Project
- In Situ Visualisation
  - Vistle with Nek5000
  - Vistle with Alya
- In Situ Data Analytics
  - Uncertainty Quantification UQit
- Standardisation of HPC Workflows
  - Lemmings
  - Scales
- Automatic Static Mesh Refinement

EXCELLERAT P1: the foundation

- Duration: 1st Dec. 2018 – 31st May 2022
- Paving the way for engineering applications for evolution towards exascale.
- Two basic principles:
  1. Alignment of all developments along the four phases and activities of the engineering workflow.
  2. The provision of services based on the perspective of the identified user groups of the CoE.



EXCELLERAT P2 : what we aim for

- **Call**: Centres of Excellence for HPC applications
- **Topic**: Centres of Excellence for supporting supercomputing applications for Science and Innovation
- *Exascale engineering applications as targeted by EXCELLERAT consider three types of use case scenarios:*
  1. **Hero runs:** targeting maximum accuracy to gain detailed solutions that reveal an unprecedented level of details and generate scientific insight
  2. **Smaller scale, strong scaling production runs:** used in optimization and uncertainty quantification ensembles.
  3. **Large scale, strong scaling applications:** facilitate even larger parts of an Exascale system efficiently to shorten turnaround times in development

EXCELLERAT P2 : Project Partners

EXCELLERAT P2

ARCTUR

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

CERFACS

CINECA

Deutsches Zentrum für Luft- und Raumfahrt

E4 COMPUTER ENGINEERING

Fraunhofer SCAI

HLRS

KTH VETENSKAP OCH KONST

RWTH RHEINISCH-WESTFÄLISCHE TECHNISCHE HOCHSCHULE AACHEN

SICOS

SIPEARL

SSC

Teratec

University of Ljubljana

SAPIENZA UNIVERSITÀ DI ROMA

EXCELLERAT P2 : the Use Cases

UC-1: ***External aircraft aerodynamics*** (DLR, *CODA*)

UC-2: ***Hydrogen combustion for propulsion*** (CERFACS, *AVBP*)

UC-3: ***Migration of aeroacoustics noise*** (RWTH, *m-AIA*)

UC-4: ***Fully integrated aircraft simulation with emissions models*** (BSC, *Alya*)

UC-5: ***High-fidelity simulations of rotating parts*** (KTH, *Neko*)

UC-6: ***Active control for drag reduction of transonic airfoils*** (CINECA, *FLEW*)

FA-1: ***Engineering design and digital twin of the first wall of tokamak fusion reactor*** (Ljubljana University, *OpenFoam/Elmer*)

EXCELLERAT P2 : the Objectives

- Strengthen European competitiveness in HPC and HPDA-driven engineering
- Demonstrate the benefits of using large-scale HPC applications in solving engineering challenges
- Integrate the CoE users of all perspectives in the EXCELLERAT P2 evolution
- Further establish the EXCELLERAT brand to be the central entry point for all stakeholders of HPC in engineering across Europe
- Provide consultancy and support activities
- Provide mandatory economic and legal framework for a sustainable operation of EXCELLERAT

The Services

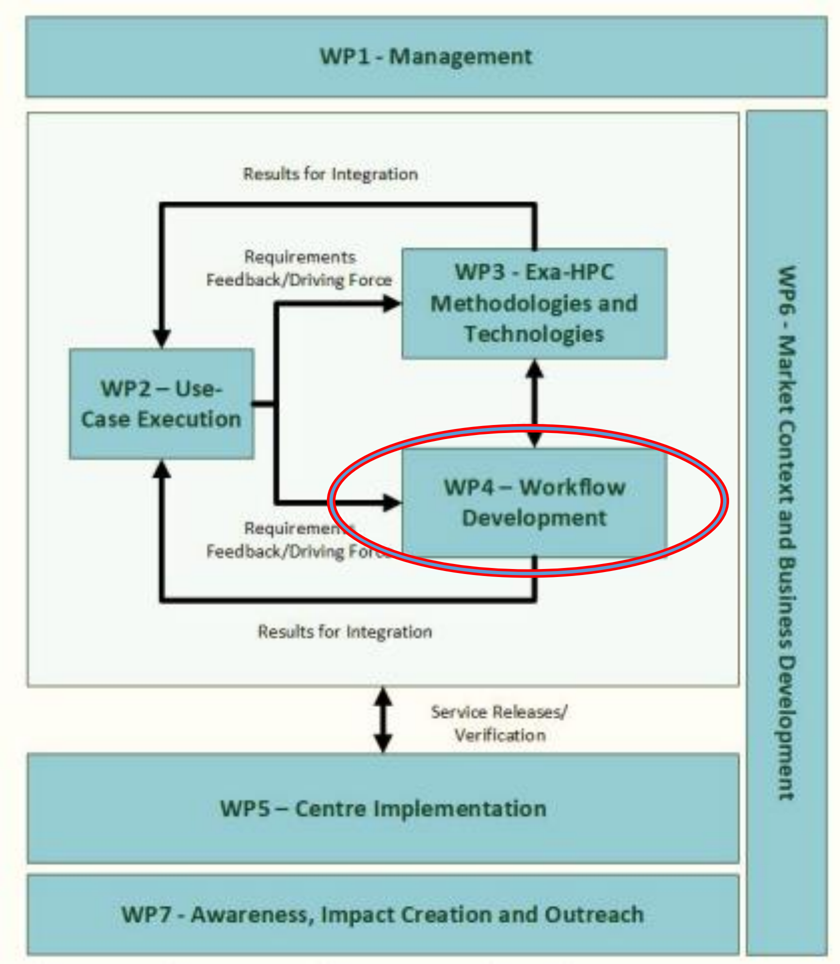
- Based on four service perspectives:
  - *Solution Evolution* (Perspective of the Application End-user)
  - *Code/Application Evolution* (Perspective of the Application Developer)
  - *System Evolution* (Perspective of the Vendor)
  - *Community Evolution* (Perspective of the Engineering Community)
- Training courses:
  - Regarded as 1-on-n consulting within the “Service-Perspectives” approach of EXCELLERAT
  - Objectives:
    - update the training overview developed with the support of the EuroCC National Competence Centres
    - promote their integration with complementary interdisciplinary aspects
    - Maintain an updated map of the existing initiatives in training and education and of the emerging needs
    - Expand collaboration with the NCCs and other EuroHPC initiatives like EuMaster4HPC

Industrial Impact

- Interest Groups consist of selected representatives of external companies
- Regular interaction with these entities and meetings (at least three F2F workshops per group)
- Feedback process & early adopter role
- Sharing of news from the CoE

EXCELLERAT P2 : the Structure

- Duration: 1st Jan. 2023 – 31st Dec 2026
- 7 Work Packages (WP)
- WP1 – Management and Technical Coordination
- Technical WPs
  - WP2: Use-cases Execution
  - WP3: Exa-HPC Methodologies and Technologies
  - WP4: Workflow Development
- Service-oriented WPs
  - WP5: Centre Implementation
  - WP6: Market Context and Business Development
  - WP7: Awareness, Impact Creation and Outreach



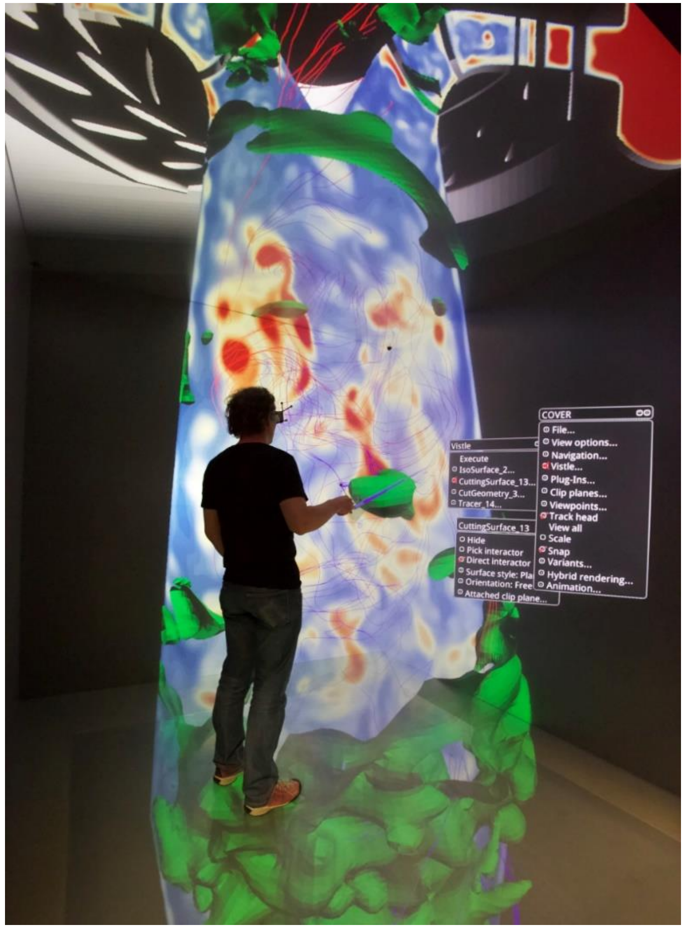
Workflow Development in EXCELLERAT

1. Workflow of individual simulation
   - In-situ analysis and visualisation
   - Automation and simplification of workflow
   - Automation of pre-processing
2. Workflow of an entire set (campaign) of simulations
   - Efficiency & Standardization

VISTLE

Visualization Testing Laboratory for Exascale Computing

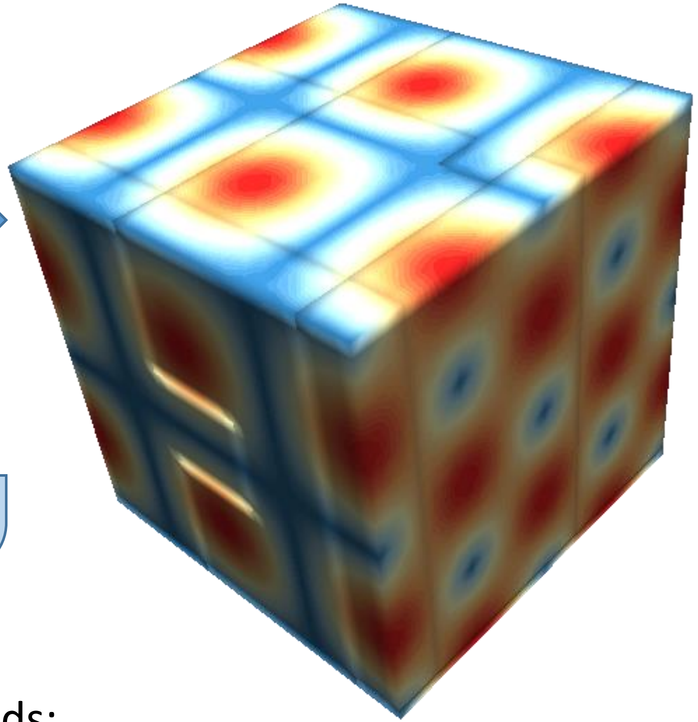
- Developed at HLRS since 2012.
- Software environment that integrates
  - simulations on supercomputers,
  - post-processing,
  - and parallel interactive visualization
  - in immersive virtual reality.
- Workflow consists of several processing modules distributed across several clusters.
- Configurable from Python or graphically.



In Situ Visualisation

SENSEI insitu defines interfaces for simulations and analysis tools to efficiently pass grid based data in both directions

VISTLE



Feed back commands:

- Pause
- Update frequency
- Bounding conditions
- Grid

VISTLE with Nek5000

EXCELLERAT P2

- Implement SENSEI analysis adaptor

Simulation: Nek5000
Language: Fortran
Build-Tool: make

Analysis-adaptor

SENSEI
Language: C++
Build-Tool: CMake

Data-adaptor

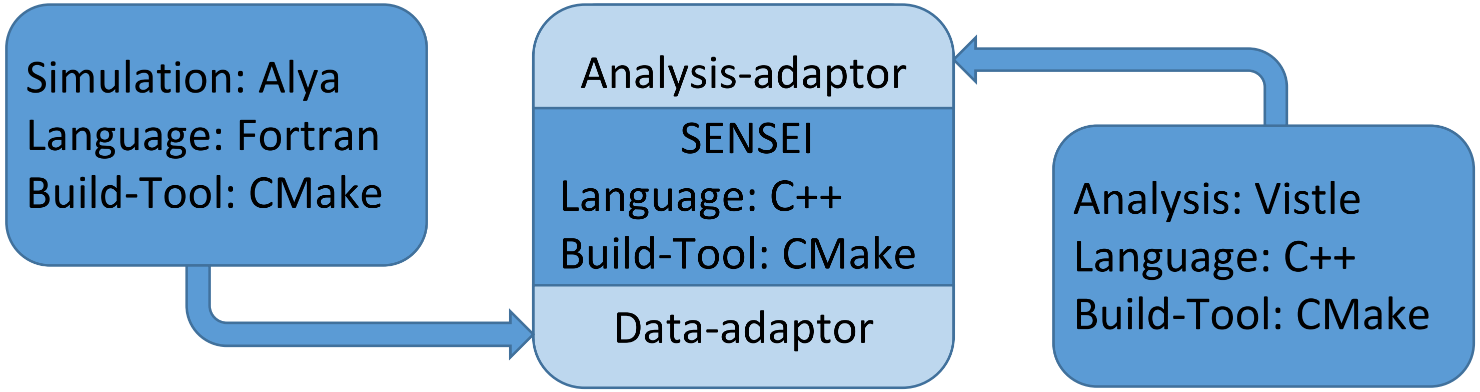
Analysis: Vistle
Language: C++
Build-Tool: CMake

- Implement SENSEI data adaptor
- Use C interface to access SENSEI's C++ classes from Fortran
- Port to CMake to automate linking

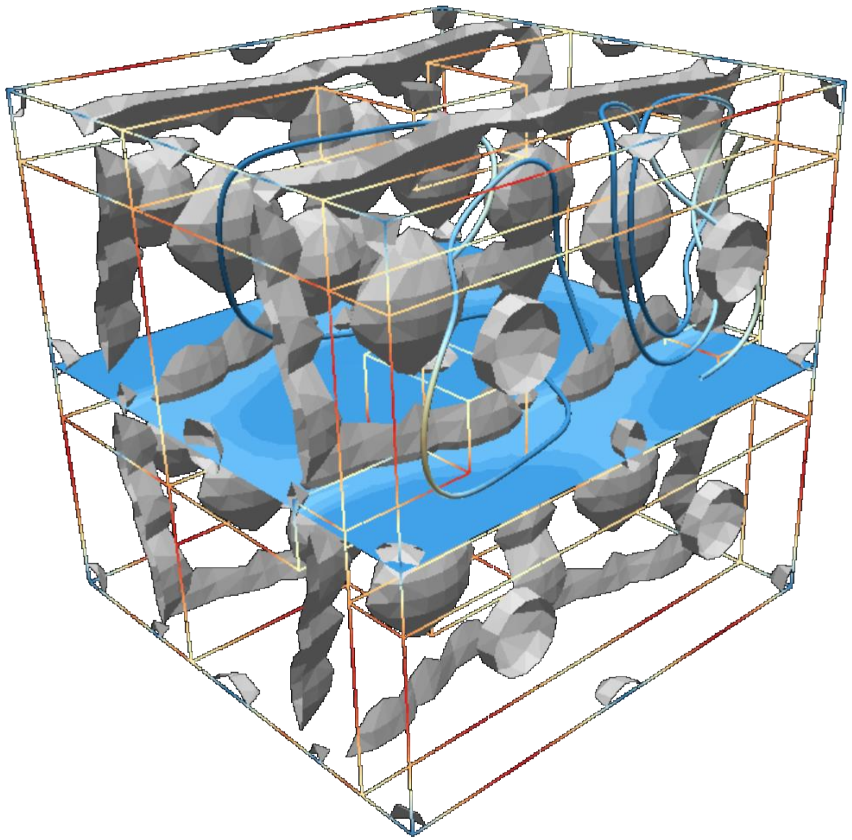
Nek 5000 rotor case simulated and rendered on Hawk,
Displayed in our CAVE @ HLRS

VISTLE with Alya

- Implement SENSEI analysis adaptor

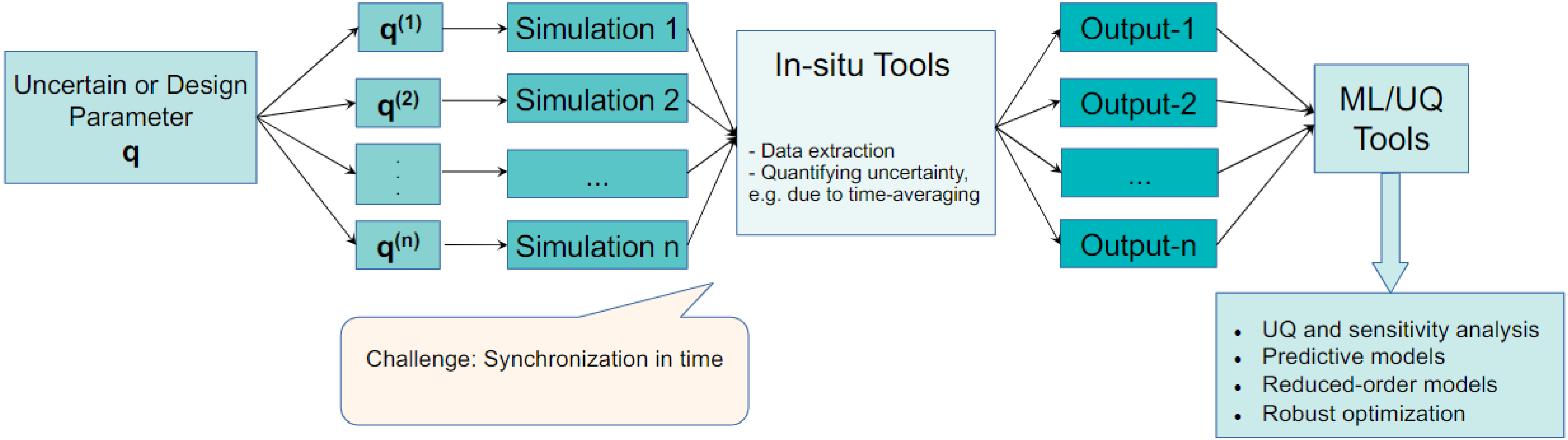


- Implement SENSEI data adaptor
- Implement C interface to access SENSEI's C++ classes from Fortran



Tracelines, iso- and cuttingsurface in Alya simulated test case

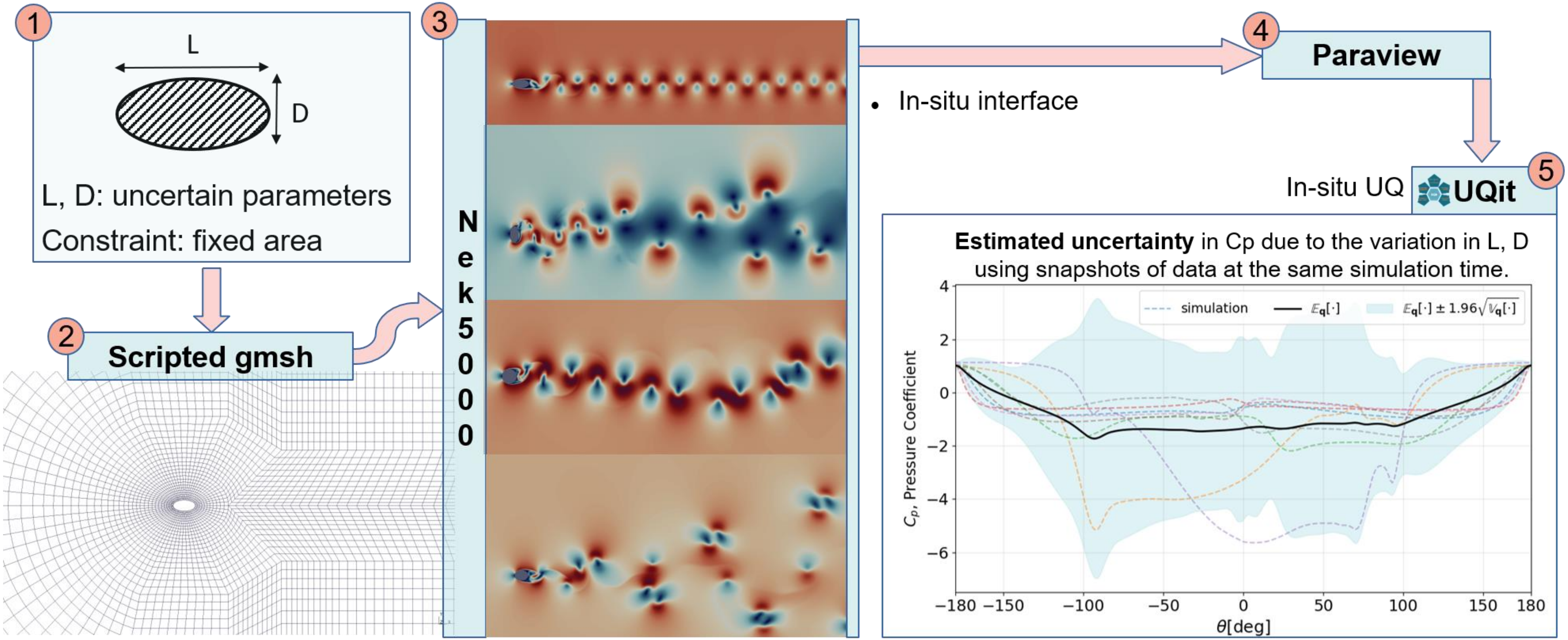
In Situ Uncertainty Quantification



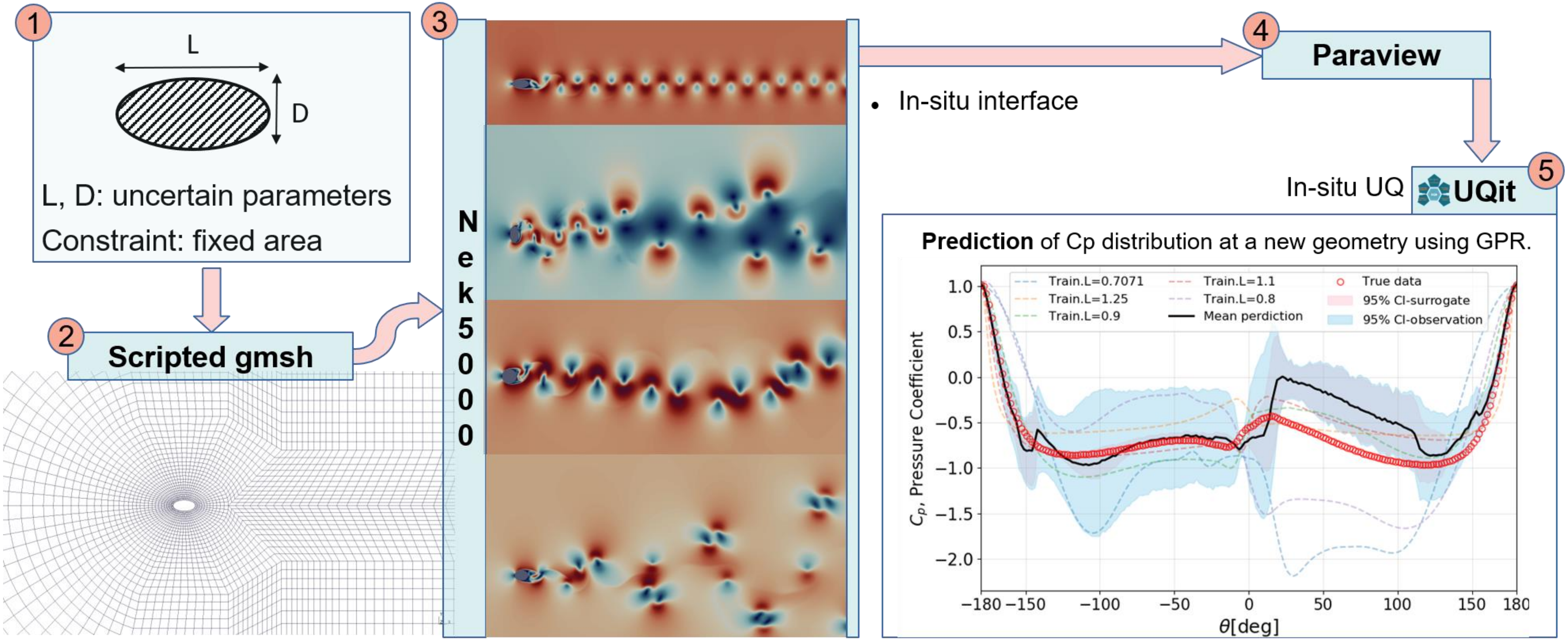
UQit developed in EXCELLERAT

- Different types of sampling
- Uncertainty propagation
- Global sensitivity analysis
- Surrogates

UQit Workflow

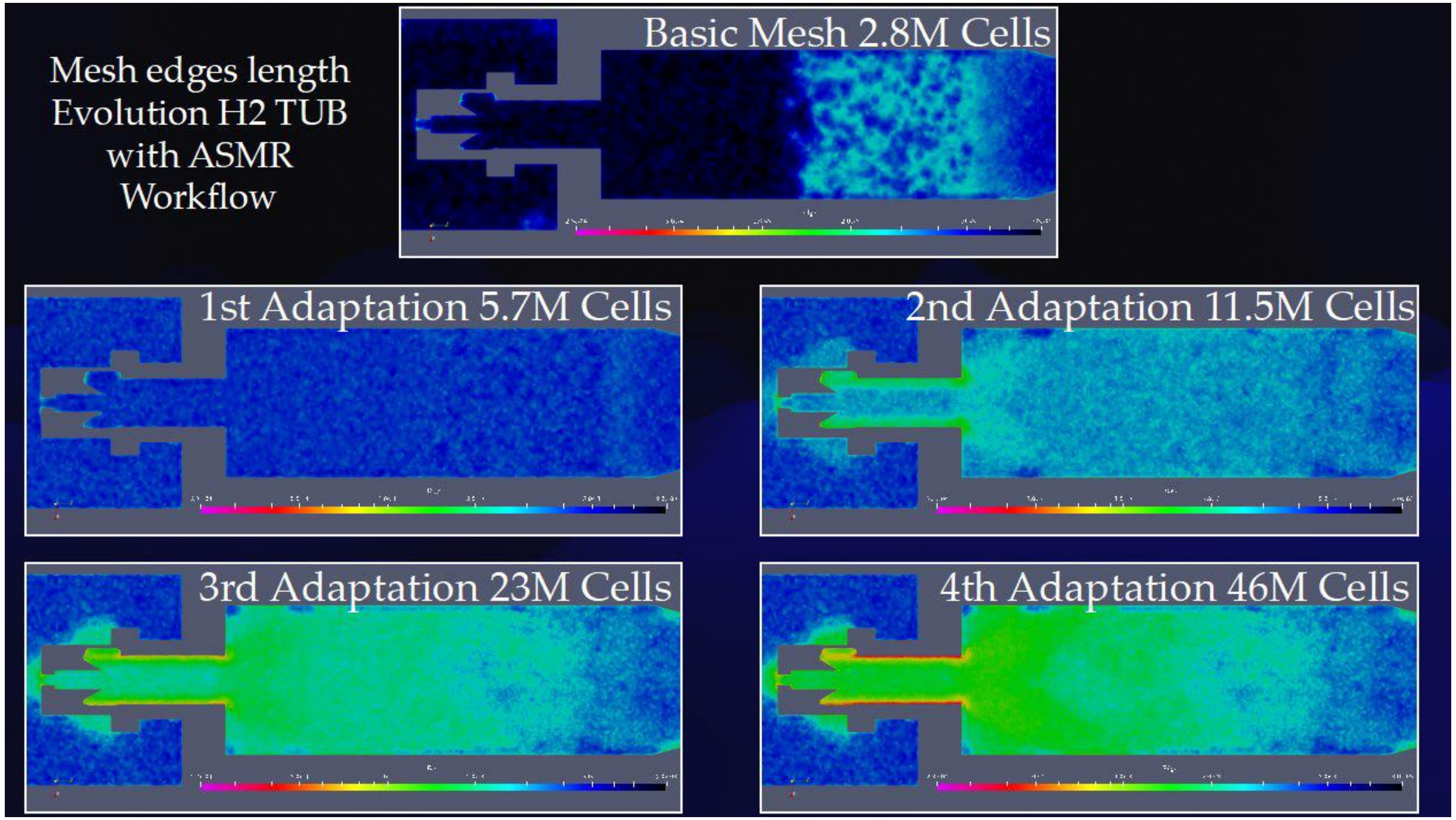


UQit Workflow

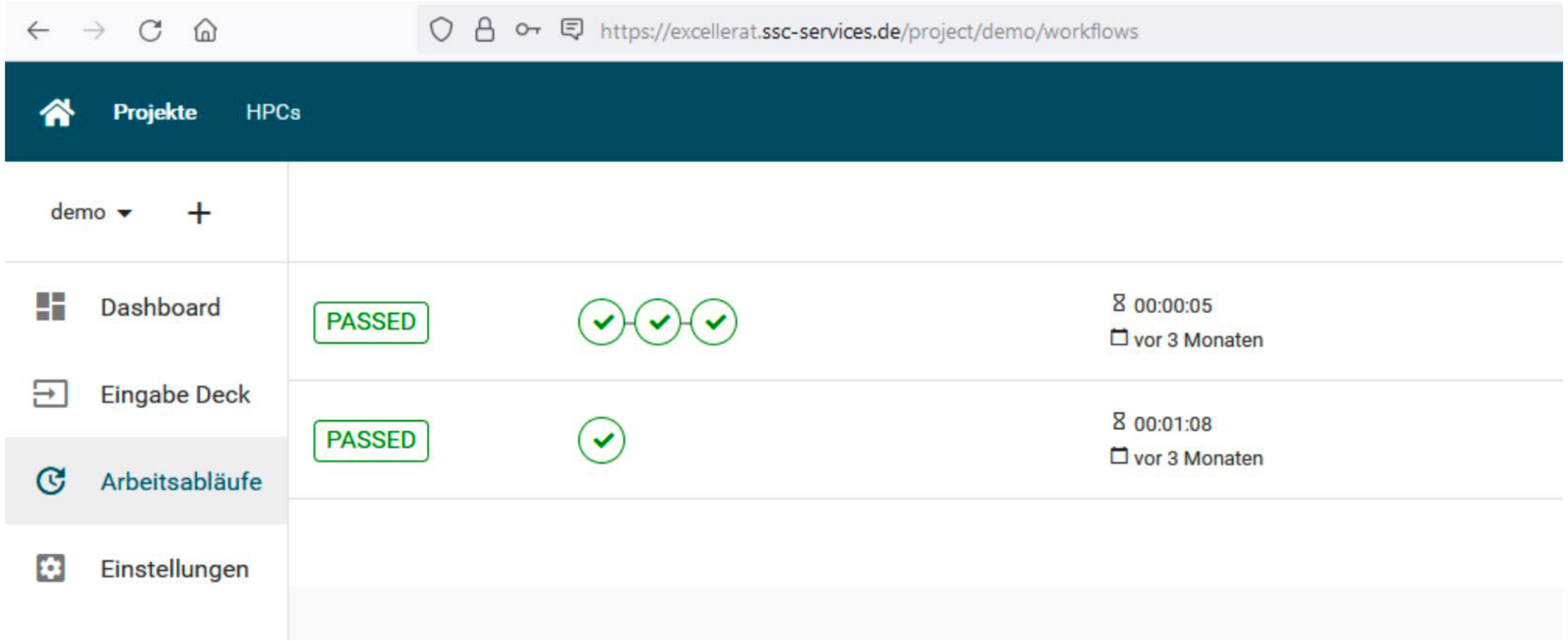


Automatic Static Mesh Refinement

- Implemented and tested in AVBP code
- Use case: hydrogen combustion for propulsion
- Simulations are conducted on increasingly refined meshes.
- Iterative workflow uses information from previous mesh and solution. (Discards simulation history.)
- WIP: parallel mesh development
- Targeting refinements on the order of a billion grid cells.



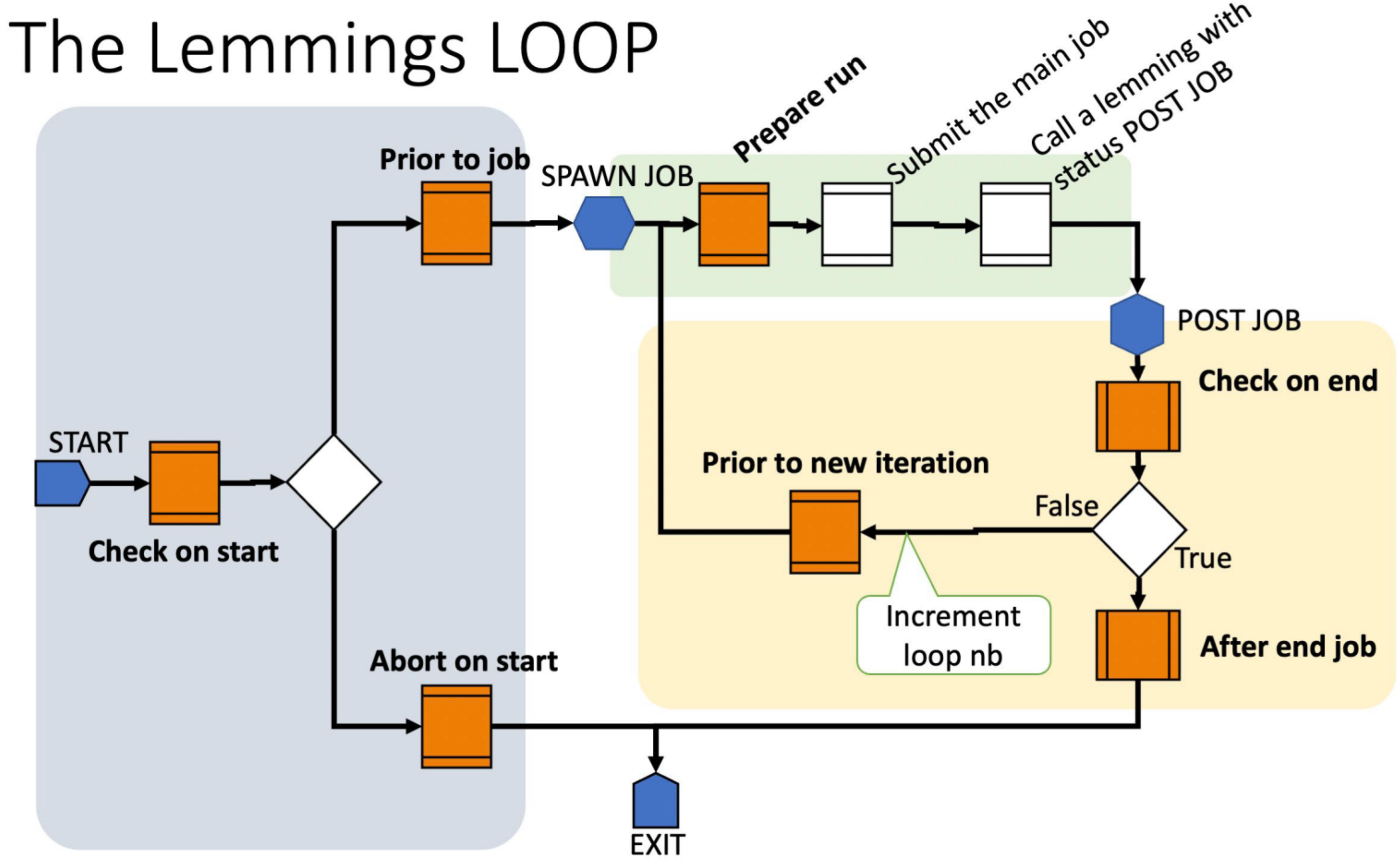
Scales



- Aimed at SMEs lacking HPC expertise.
- Integrates workflows into a web portal.
- UX resembles that of gitlab pipelines using YAML configuration files.
- Offers intuitive learning curve with reduced training time for new users of HPC.

Lemmings

- Ensemble of functionalities that facilitates interactions with a Job Scheduler
- Designed for large scale jobs on HPCs
- Interacts with either Slurm or PBS
- Developed for but not limited to CFD
- Python package



Conclusions

- In-situ visualization and data analysis required for exascale CFD
  - Reduce requirements for IO and storage resources
- Standardizing workflows is particularly important in simplifying workflows for new (industrial) users
- Or to solve complex engineering problems through standardized simulation campaigns
- Automatization workflows including feedback-driven pre-processing such as ASMR

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