EXCELLERAT: paving the way to the evolution towards Exascale

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Agenda

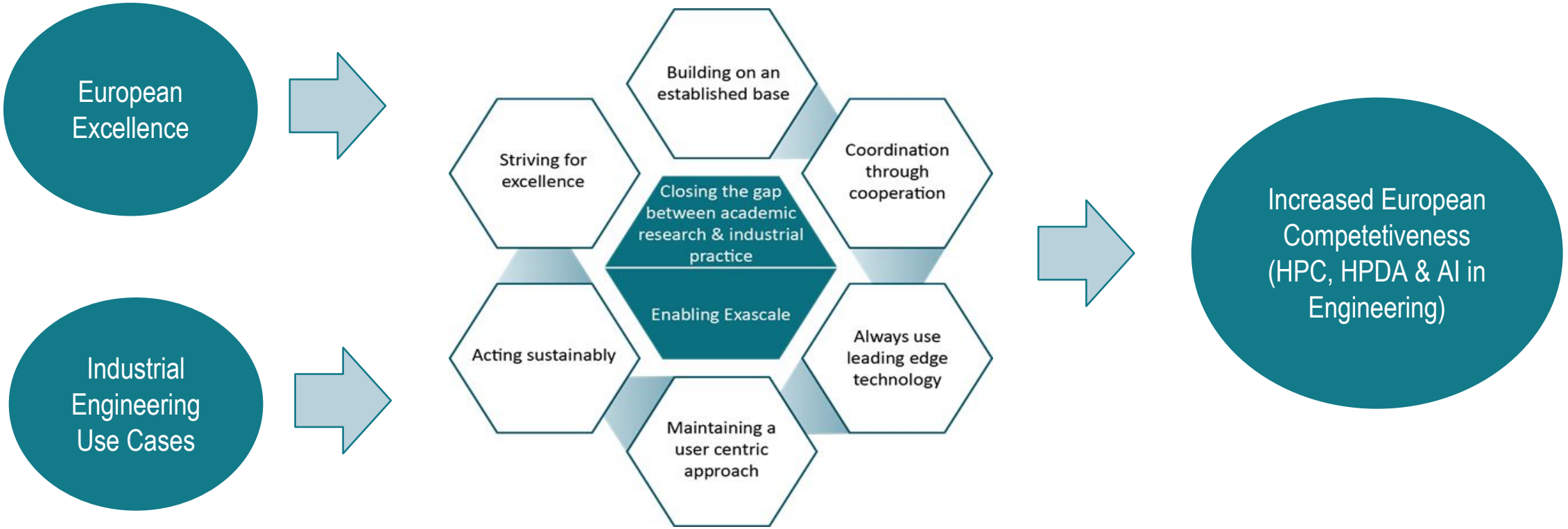
- Overview
- Objectives of EXCELLERAT
- EXCELLERAT approach
- EXCELLERAT use cases & requirements
- Samples of technical progress
- Service Portfolio – Service implementation
- Outlook

Overview

- EXCELLERAT - The European Centre of Excellence for Engineering Applications
- Horizon 2020 - The EU Framework Programme for Research and Innovation
- 13 partners
- Funding programme: H2020-EU.1.4.1.3. Development, deployment and operation ICT-based e-infrastructures
- Subject: H2020-INFRAEDI-2018-1 - Centres of Excellence on HPC
- Start: 01.12.2018
- Duration: 3 years

Objectives of EXCELLERAT

- What is EXCELLERAT and why do we need it?



EXCELLERAT Approach

- Using Reference Applications to setup the frame of the centre (and its services)
- Extension of the applications by integrating external entities through the concept of interest groups (leading to smaller satellite activities)

Reference Applications:

Alya

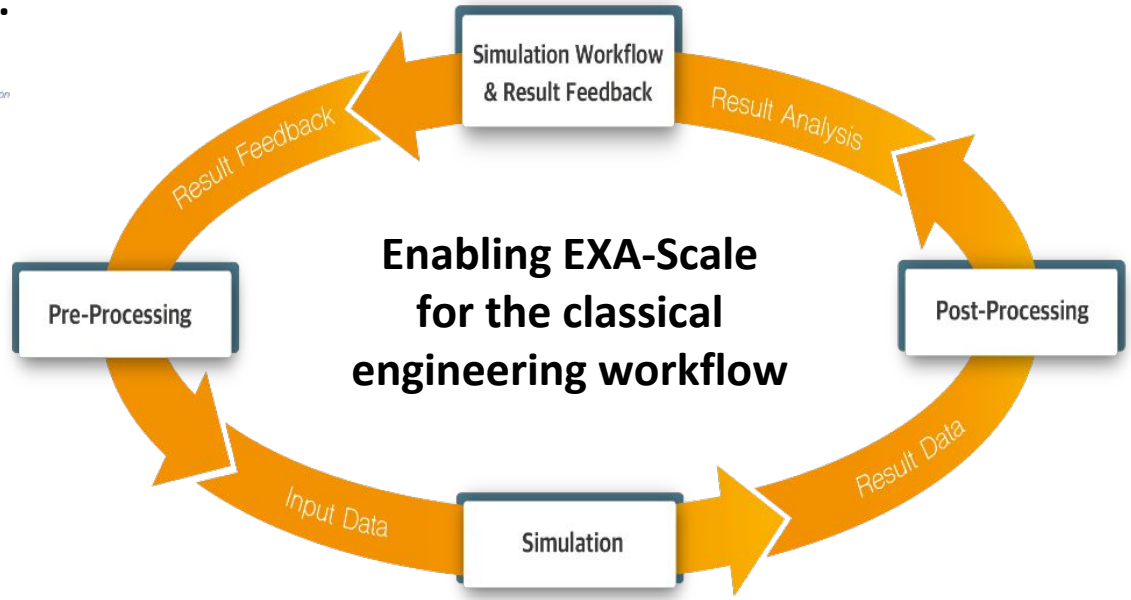
AVBP

TPLS

NEK5000

CODA/FLUCS

FeniCS



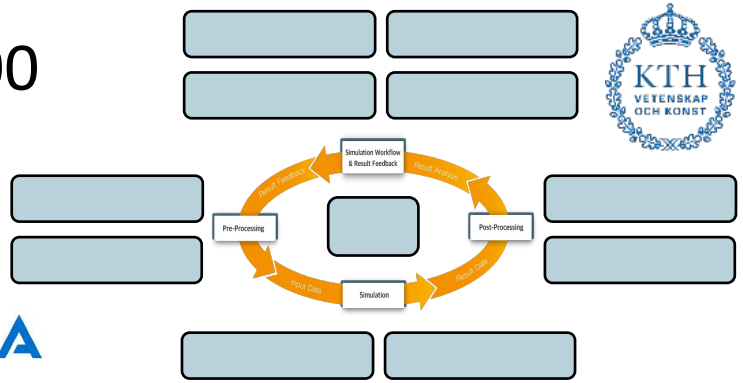
EXCELLERAT Interest Groups:

- Industrial End Users
- Code Developers/ISVs
- Scientific Experts
- Technology Providers

EXCELLERAT Use cases & requirements

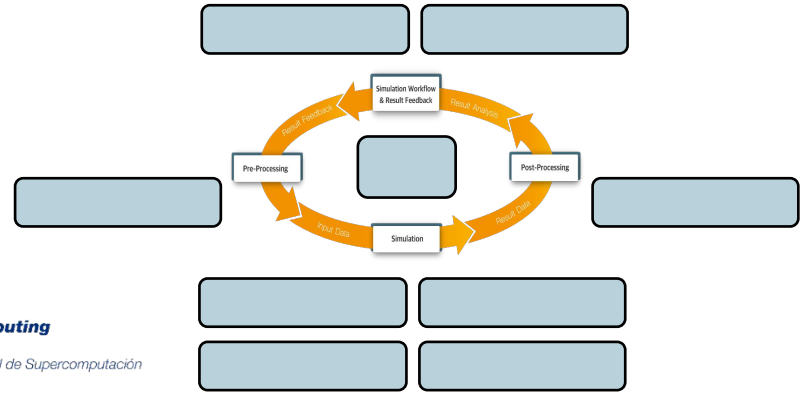
Nek5000 **Spectral element discretisation** **Suitable for direct numerical simulation (DNS)**	Aerospace - Flow around aerofoil with rounded wing tip
	Aerospace - High fidelity simulation of rotating parts
Alya **Finite Element Method (FEM)** **Multi-Physics**	Automotive/ Aerospace - Emission prediction of internal combustion and gas turbine engines
	Aerospace - Active flow control of aircraft aerodynamics including synthetic jet actuators
	Transport systems - Coupled simulation of fluid and structure mechanics for fatigue and fracture

Nek5000



CINECA

Alya

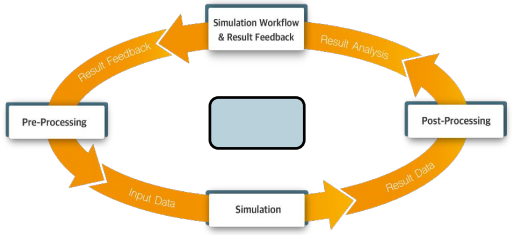


Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELLERAT Use cases & requirements

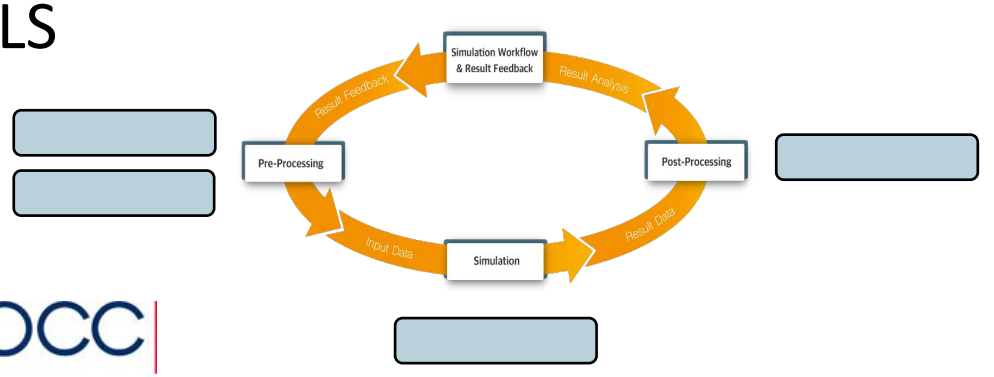
AVBP **FEM type low-dissipation Taylor-Galerkin** **Large Eddy Simulation (LES)**	Safety applications - Explosion in confined spaces Aerospace and energy - Combustion instabilities and emission prediction
TPLS **DNS Multiphase flows**	Chemicals and Energy - Two-Phase vertical pipe flow

AVBP



CERFACS
CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE

TPLS



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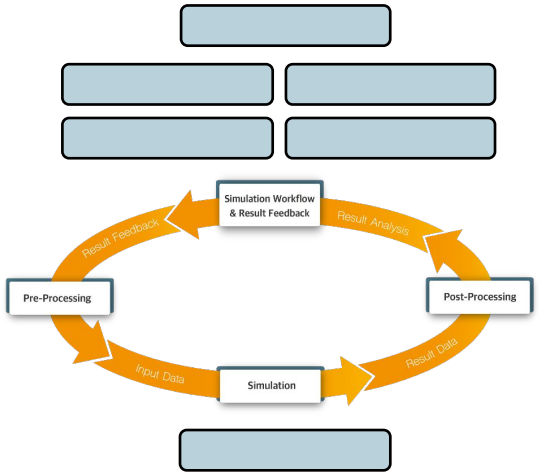
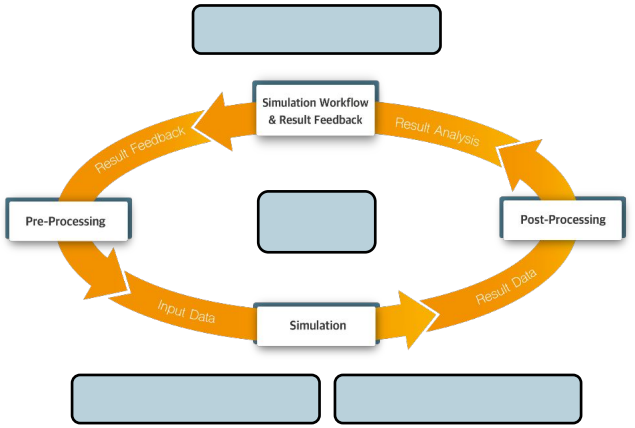
EXCELLERAT Use cases & requirements

FEniCS **Calculation platform for automatic solution of partial differential equations**	Aerospace and Automotive - Adjoint optimisation in external aerodynamics shape optimisation
CODA **Finite Volume Method (FV) Discontinuous Galerkin Method (DG)**	Aerospace - Design process and simulation of full equipped aero planes Aerospace – computational fluid dynamics (CFD) coupling with computational structural mechanics including elastic effects

FEniCS



CODA



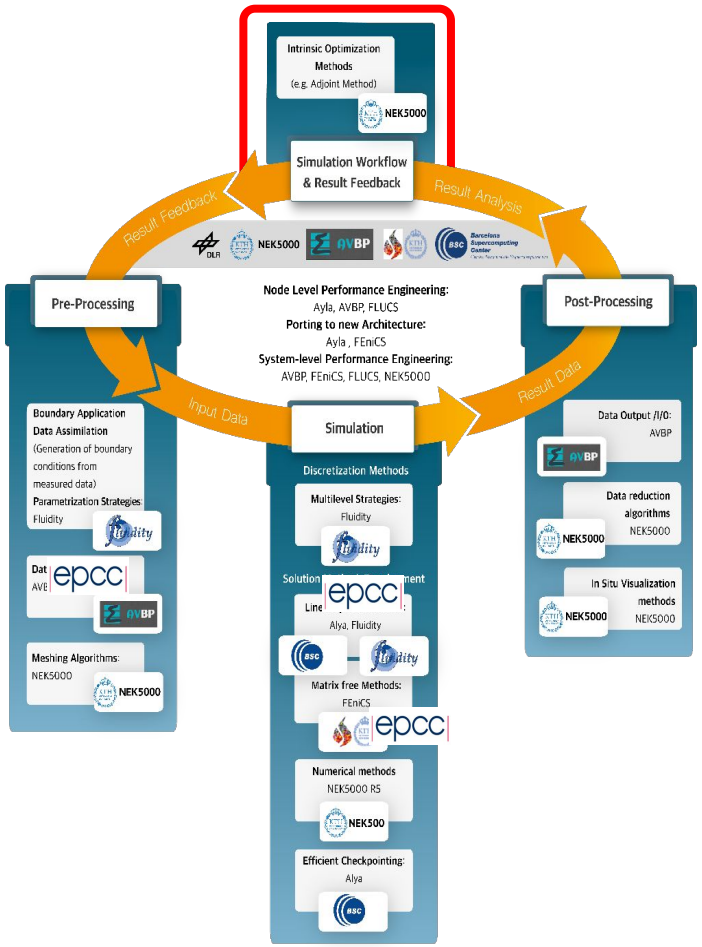
EXCELLERAT Use cases & requirements

Focus on Engineering Applications' Challenges

Numerical Simulation / Codes: Discretisation methods, Numerical methods, Parallel performance.

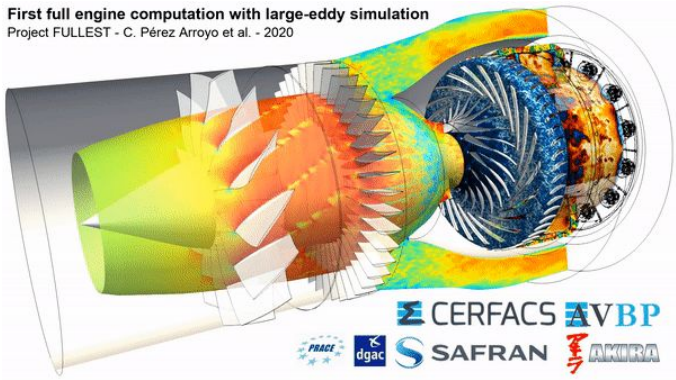
Pre- / Post-Processing: Meshing algorithms, Efficient input/output, In-Situ visualisation.

Simulation Workflow & Result Feedback: Data transfer, Data management, Usability, External optimisation processes.



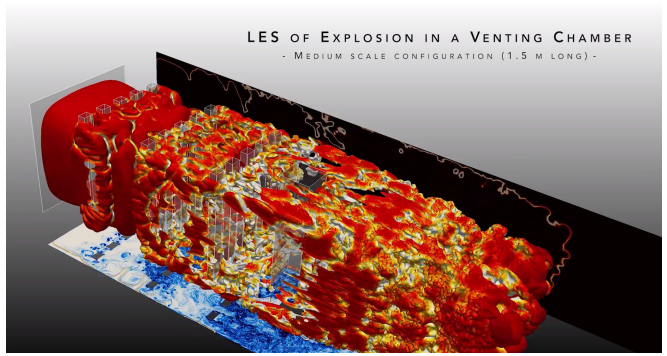
Samples of technical progress

AVBP

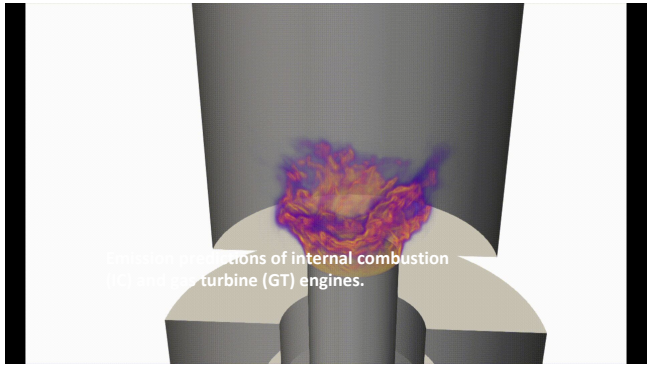


EXCELLERAT ported AVBP to AMD rome architecture evaluated up to **130k cores** with almost **90% ideal scaling**.

The CoE extended AVBP to use GPUs under OpenACC: **excellent strong scaling up to 32 GPUs** using a static mesh (new implementation).

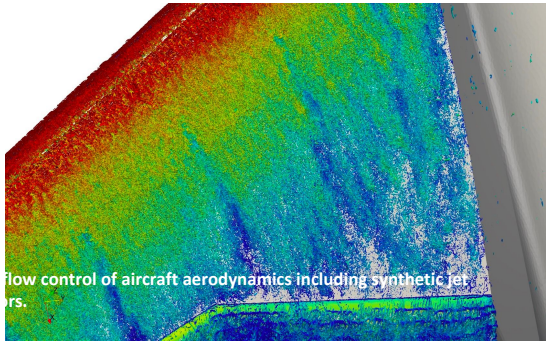


Alya



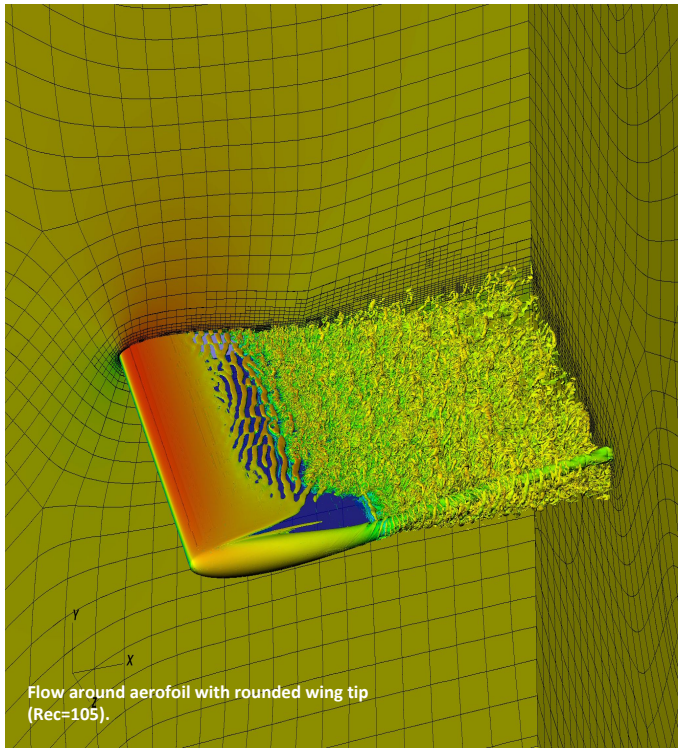
The project scaled Alya up to **96,000 cores** on **2 billion cells** compared to 25,000 core on 345 million cells before EXCELLERAT.

EXCELLERAT achieved a **well-balanced co-execution** of Alya using both the CPUs and GPUs simultaneously, **23% faster** than using only the GPUs (new implementation).



Samples of technical progress

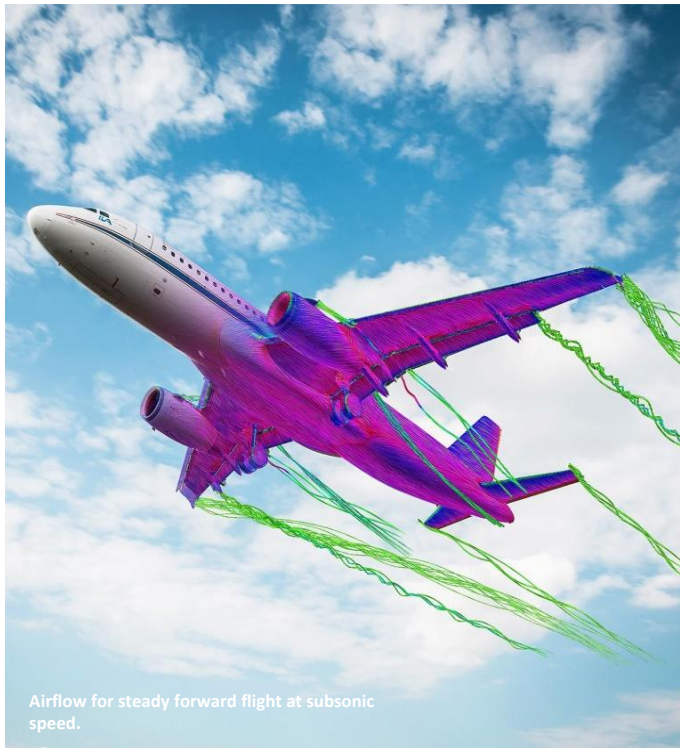
NEK5000



Flow around aerofoil with rounded wing tip (Rec=105).

Adaptive mesh refinement is implemented, which **improves computational efficiency** in rototcraft off body grid **by 50-70% of total cell** (new implementation).

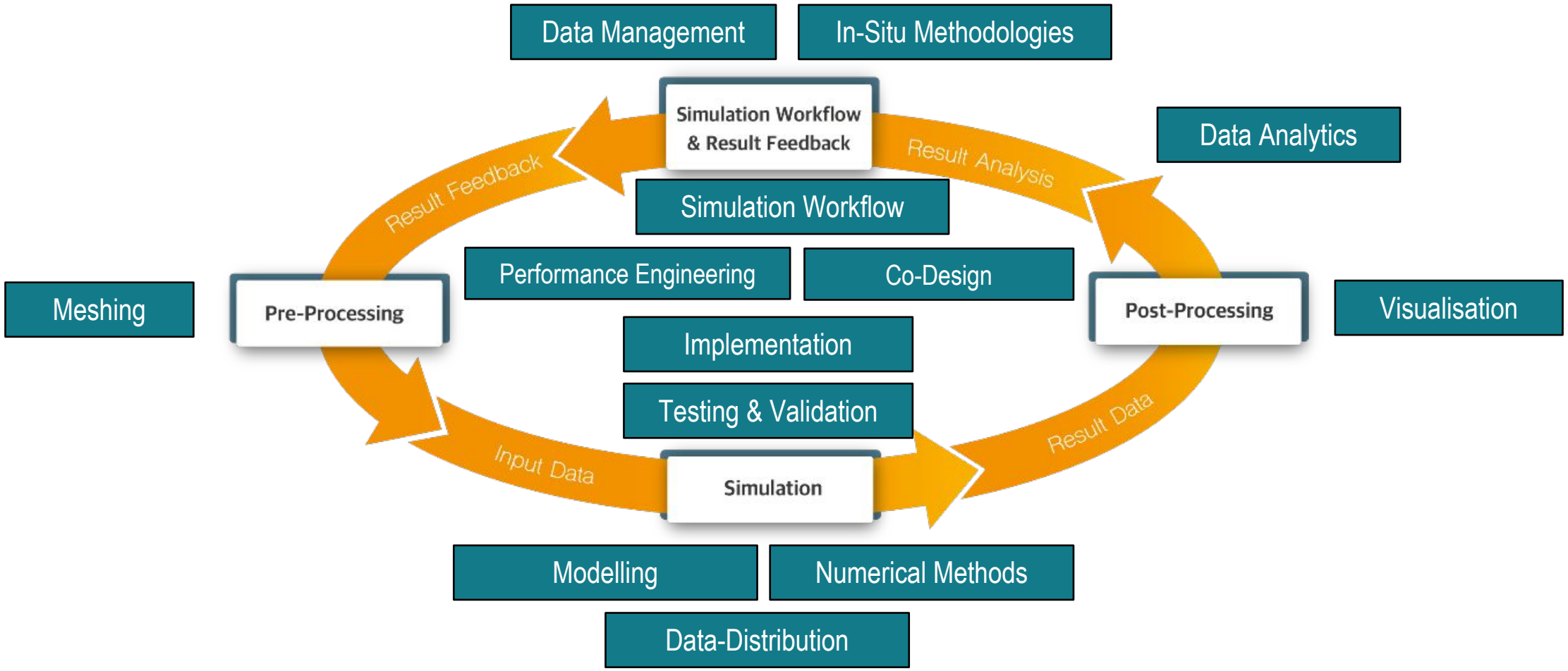
CODA


Airflow for steady forward flight at subsonic speed.

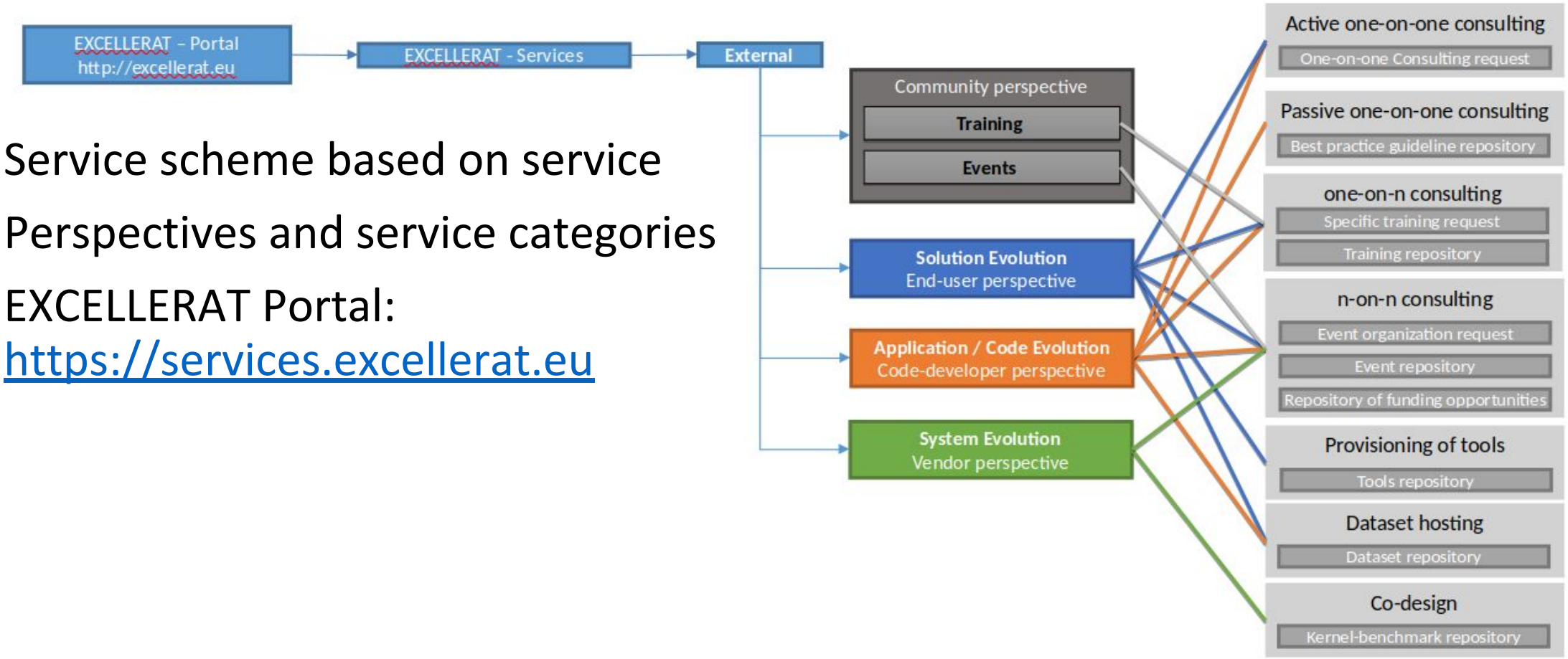
EXCELLERAT analysed the mesh partitioning of CODA, achieving up to **30% better load balance** and **55% faster runtime** with the appropriate mesh partitioning method (new implementation).

EXCELLERAT scaled efficient hybrid MPI+OpenMP to **32k cores** even for small meshes with **60% efficiency** (new implementation).

Service Portfolio – Service implementation



Service Portfolio – Service implementation



- Service scheme based on service
- Perspectives and service categories
- EXCELLERAT Portal: https://services.excellerat.eu

Outlook

- EXCELLERAT is the first Centre of Excellence in Engineering science simulations.
- EXCELLERAT has built from the need of having Exascale technology.
- In EXCELLERAT we strive to enable the Exascale for the full simulation workflow.
- Six reference applications were selected that are supported by the community.
- The services schemes are driven from the selected use-cases and the user requirements.
- Widen the aspect of the current service portfolio towards further Engineering applications which are not included in the use-cases.

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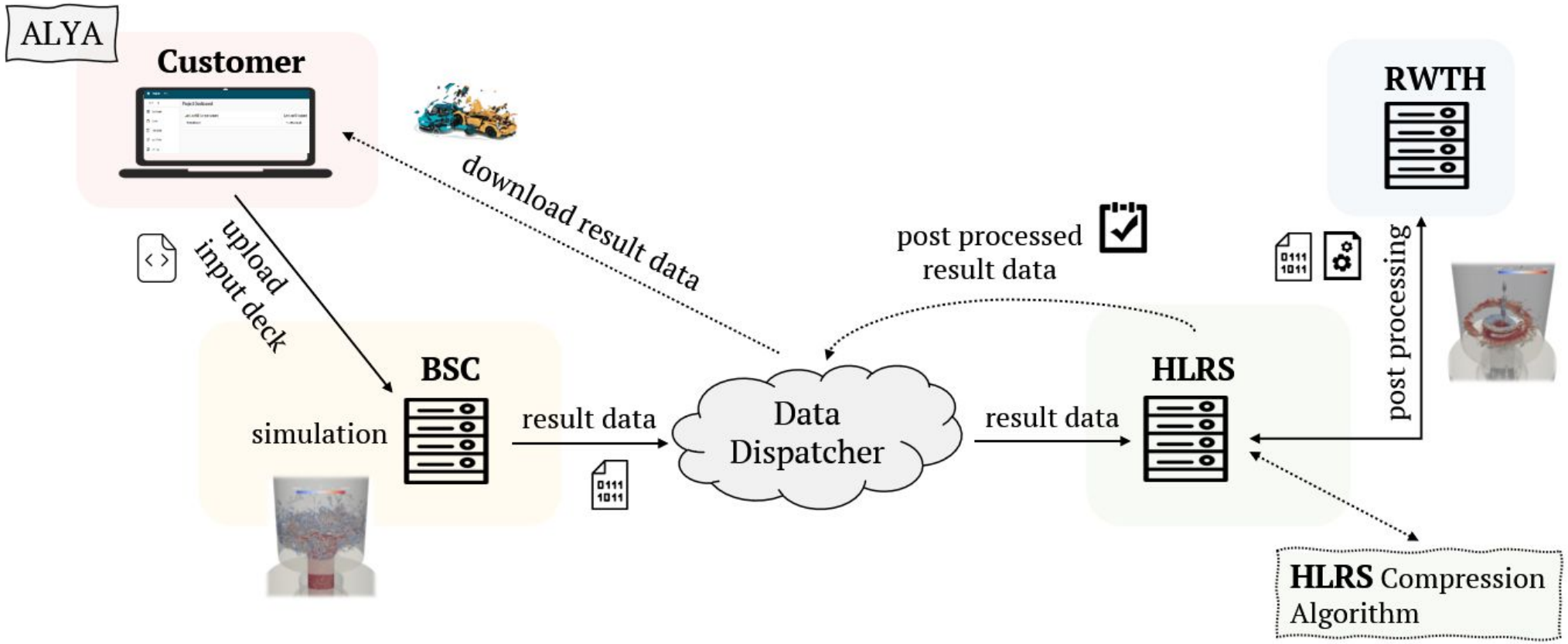
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simulation
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Data
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HLRS
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RWTH
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HLRS Compression
Algorithm