HPC Methods for Engineering Applications 19-21 June 2017 Milan

Pre and Post-processing on HPC platforms: tools and way of doing

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- CAE workflow bottlenecks
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Computer Aided Engineering

Computer-aided engineering (CAE) is the broad usage of computer software to aid in engineering analysis tasks. It includes:

- Finite Element Analysis (FEA)
- Computational Fluid Dynamics (CFD)
- Multi-body dynamics (MBD)
- Optimization

Computer Aided Engineering

CAE areas covered include:

- Stress analysis on components and assemblies using FEA (Finite Element Analysis);
- Thermal and fluid flow analysis Computational fluid dynamics (CFD);
- Multi-body Dynamics (MBD) & Kinematics;
- Optimization of the product or process

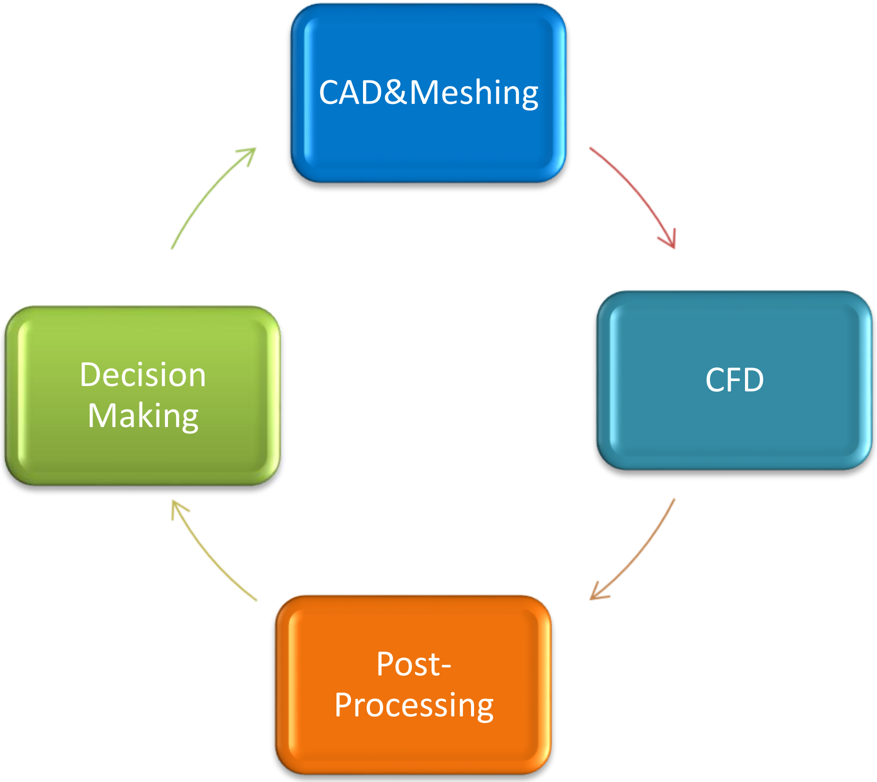
Computer Aided Engineering

In general, there are three phases in any computer-aided engineering task:

- Pre-processing – defining the geometry model, the physical model and the boundary conditions
- Computing (usually performed on high powered computers (HPC))
- Post-processing of results (using scientific visualization tools & techniques)

Computer Aided Engineering

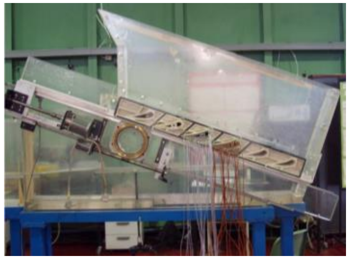
This cycle is iterated, often many times, either manually or with the use of automation techniques or using optimization software.



Computer Aided Engineering on HPC Platforms

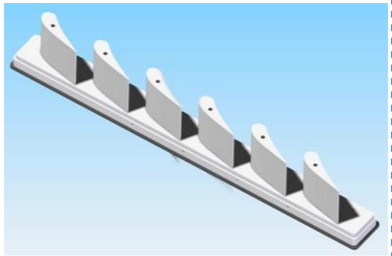
PRE-PROCESSING → **COMPUTATION** → **POST PROCESSING**

PHYSICAL



MODEL

COMPUTATIONAL

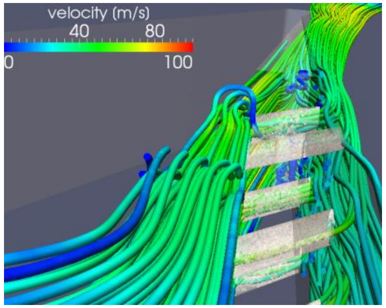


MODEL

SOLVING

HPC ENVIRONMENT

VISUALIZATION



RESULTS

CAD&Meshing

CFD/FEM/…

Post-Processing

CAE workflow bottlenecks

CAE applications involves a set of activities that can be automatized.
Nevertheless today this happens in a very limited cases.
The actual status of CAE applications standard activities time usage is as follows:

Activity	CAD Design	CAD Cleaning	Meshing	CFD modelling	Post Processing	Decision making
Human	100%	100%	80%	40%	80%	100%
Computing	0%	0%	20%	60%	20%	0%

There are at least three way of doing to manage standard CAE workflow on HPC platforms:

- Poor (and ineffective): move bites
- Average (and effective): use remote GUI
- Best (and highly productive): automatize

Way of doing: poor

A poor and ineffective way of doing on HPC platforms is to use the HPC platform merely to perform number crunching.

- Pre-processing is performed on desktop PC
- Input files are uploaded to the HPC infrastructure
- **Calculations are performed on the HPC system in batch**
- Output files are download to the desktop PC
- Post-processing is performed on desktop PC

Way of doing: average

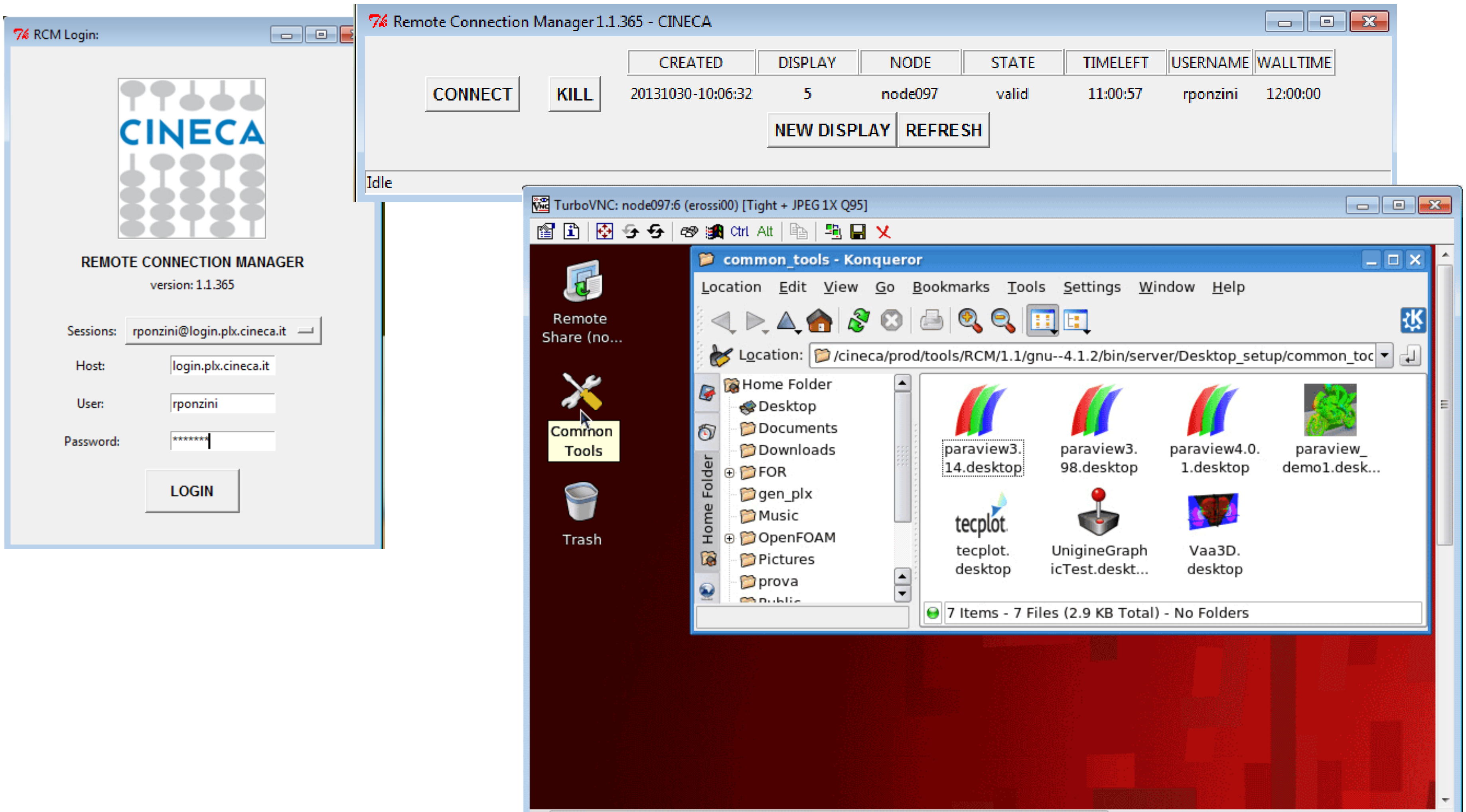
An average and more effective approach is to use remote Graphical User Interface (GUI) performing manually on the HPC platforms the whole CAE workflow.

- CAD input files are uploaded to the HPC infrastructure (light)
- **Pre-processing is performed on the HPC system manually**
- **Calculations are performed on the HPC system in batch**
- **Post-processing is performed on the HPC system manually**
- Synthetic results (figure, tables) are downloaded to desktop PC

Remote Connection Manager

http://www.hpc.cineca.it/content/remote-visualization

Remote Connection Manager



Engineframe webcompute

- Services are hosted at: https://webcompute.cineca.it/enginframe/runyourjob/
- Users can login using their LDAP credential (the same used to acess the HPC infrastructure)
- Users can ask for GUI sessions or use more vertical application interfaces

Way of doing: best

The best way of doing on HPC platforms is to automate the CAE workflow by means pof a-rpiroi knoldge of the problem we want to solve and by means pf standardization.

- CAD input files are uploaded to the HPC infrastructure (light)
- **Pre-processing is performed on the HPC system automatically**
- **Calculations are performed on the HPC system automatically**
- **Post-processing is performed on the HPC system manually**
- Synthetic results (figure, tables) are downloaded to desktop PC (light)

External CFD application automation

- The CFD aerodynamics workflow is well-defined.
- Inputs are the CAD provided by the designers and the velocity condition to be tested.
- Outputs are aerodynamics key parameters indices (KPI) usually used to rank a design a perform decision making
- The velocity conditions and the CAD design are changing usually in a well defined and quite limited range.
- A-priori knowledge can drive standardization of this workflow allowing for a strong automation process.

Standardization and a-priori knowledge are the main drivers for any automation activity

Implementation: the workflow

The software stack selected is all based on open-source applications.

This choice is strategic since once properly designed open source allows for unlimited concurrent runs (no licensing limits) that may be fully exploited by modern HPC infrastructures.

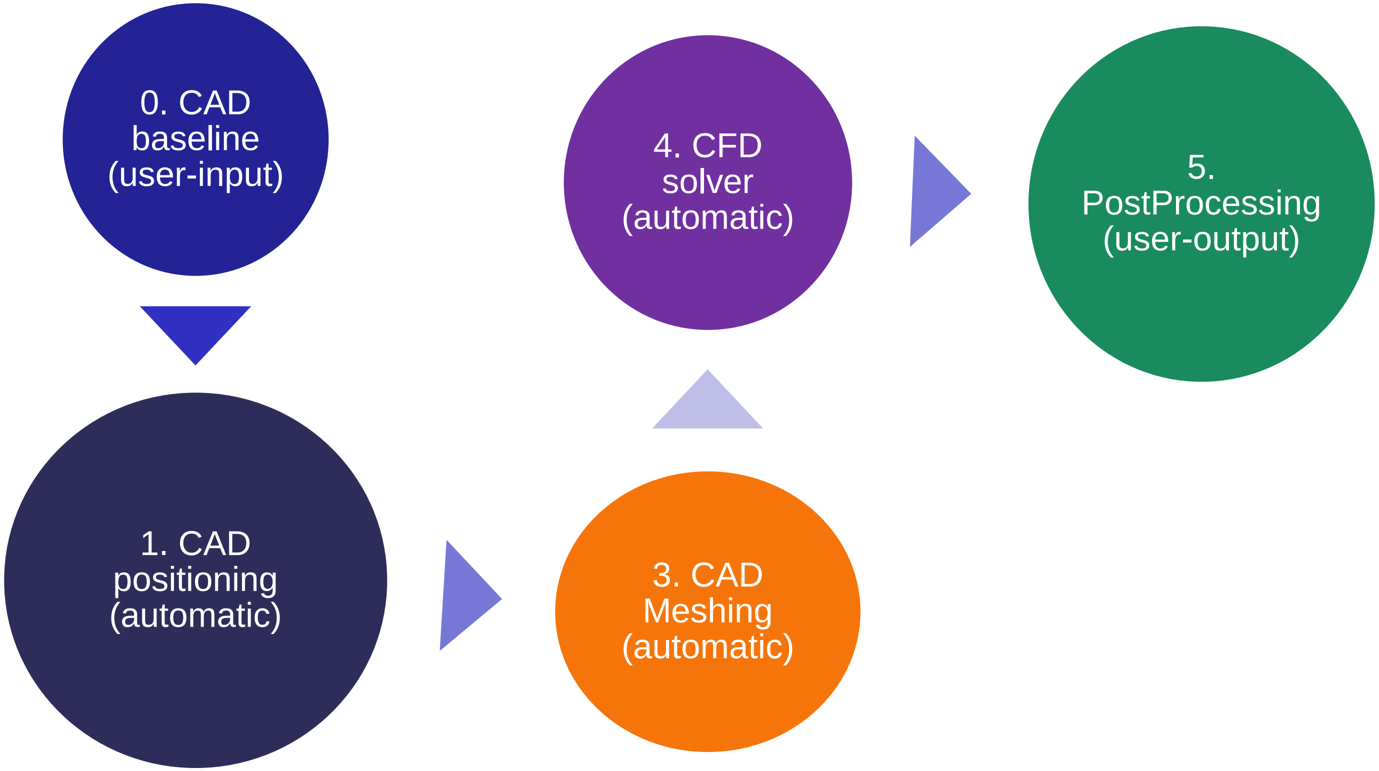
Pre-processing: openFoam (snappyHexMesh & cad positioning tools)

Computing: openFoam (simpleFoam)

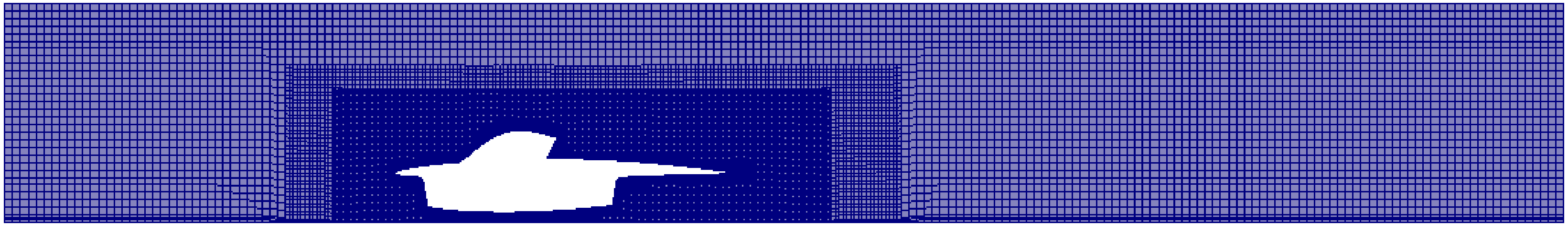
Post-processing: openFoam (VTK automatic data saving) and Python visualization modules

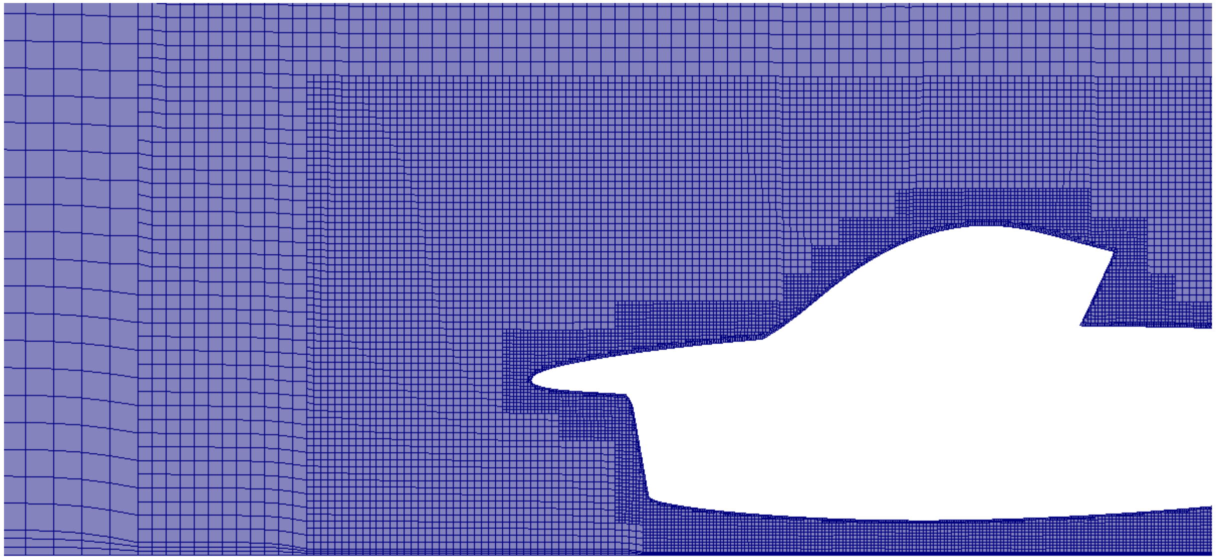
Automation and gluing: Python programming language

Implementation: the workflow

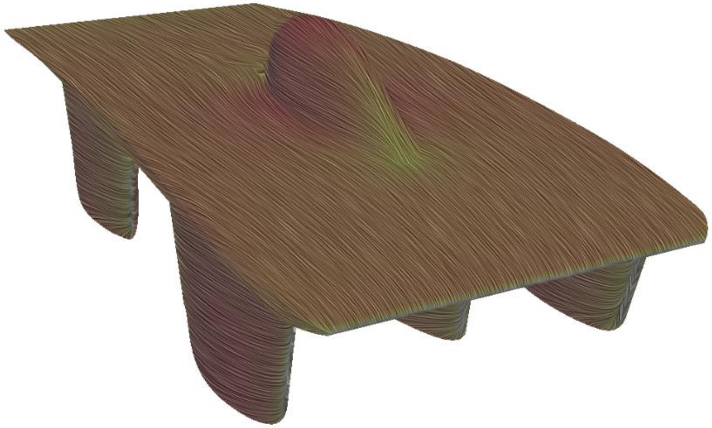


Implementation: the workflow





Implementation: the workflow



Expected benefits

- Severe cut off of human time required to perform a CFD computation

Activity	CAD Design	CAD Cleaning	Meshing	CFD modelling	Post Processing	Decision making
Human	100%	100%	**0%**	**0%**	**0%**	100%
Computing	0%	0%	**100%**	**100%**	**100%**	0%

- Dramatic reduction of time to result for the single CFD run thanks to parallel HPC systems performances

- Enlargement of the number of performable concurrent CFD runs thanks to the open-source software stack design

Conclusions

1. HPC platforms brings opportunity to become more productive adding more computational power to CAE workflows.
2. Nevertheless the way we decide to perform some basic activities (pre/post-processing) can impact the level of productivity since there are relevant bottlenecks related to these activities that can downscale the benefits of using HPC systems.

Conclusions

3. In the near future (I hope) we are going to move to web-based application that will speed-up the productivity and improve the ease of use:

- **CAD input files are designed remotely directly on a web server able to interact with the computational (HPC) infrastructure**
- **Pre-processing is performed on the HPC system automatically**
- **Calculations are performed on the HPC system automatically**
- **Post-processing is performed on the HPC system manually**
- **Synthetic results (figure, tables) are available remotely directly on the web server, conveniently placed in the user DB for visualization, comparisons and decision making**