

Motivation

The latest technological advances in computing have brought a significant change in the concept of new product design, production control, and autonomous systems. In the last few years, we have been witnessing a considerable transition to virtual prototyping and gradual pressure on integrating large parts of the industrial sector into the fourth industrial revolution, or Industry 4.0.

Starting using a supercomputer can be quite challenging task. Today's trend, i.e., HPC as a service, tries to provide a reasonable user experience for everyone who needs high performance computing (HPC).

The main objective of this thesis was to create graphical configuration tool for the ESPRESO solver's module for engineering simulations of heat transfer. The free licence for the developed package allows automatized simulation chains, based on HPC as a service, such as automatized systems for shape or topological optimization to be created on the top of the ESPRESO framework.

ESPRESO

- ExaScale PaRallel FETI Solver.
- Open-source package for engineering simulations.
- Developed at IT4Innovations National Supercomputing Center.
- Massively parallel approach for the best performance tested on 281,216 cores within the 17,576 nodes of ORNL Titan (5th in TOP500). See Figure 1.

Problem

- The ESPRESO configuration is performed via special text files called ECF.
- Inconvenient for new users due to hundreds of parameters, mandatory and compulsory parameters, and dependencies between parameters.

Solution

- Graphical user interface (GUI) powered by the Qt library (C++) serving as a "guide" through the configuration process.
- Graphical elements are assembled according to the ECF structure provided by ESPRESO. When the structure changes, the GUI reacts automatically.
- OpenGL 3D visualisation of a model that is the subject of a computation (e.g., a CPU cooler).
- Parallel execution (MPI, OpenMP) of GUI including parallel preprocessing of data for 3D visualisation.
- Possible connection with the ESPRESO solver – direct local execution, or remote execution.
- Figure 2 contains a simplified workflow of the configuration process.

Future work

- Extending features during PhD studies.
- Development of an online web-based GUI introducing the solver as a service model.
- The GUI will be presented at the ICNAAM 2018 conference.

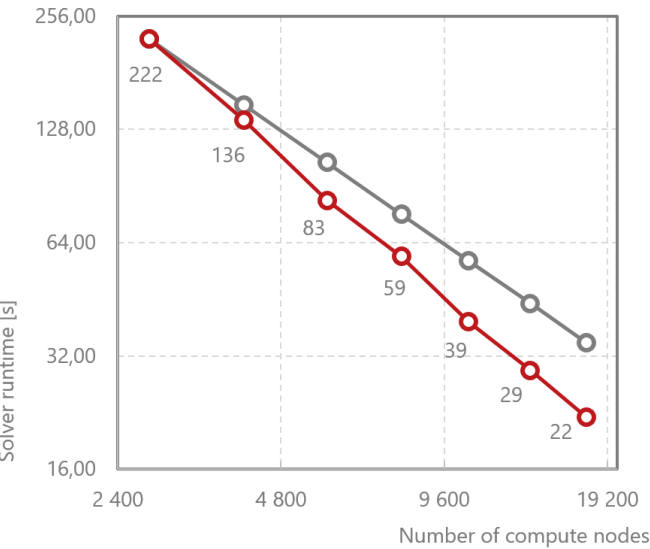


Figure 1: 3D heat transfer computation on ORNL Titan

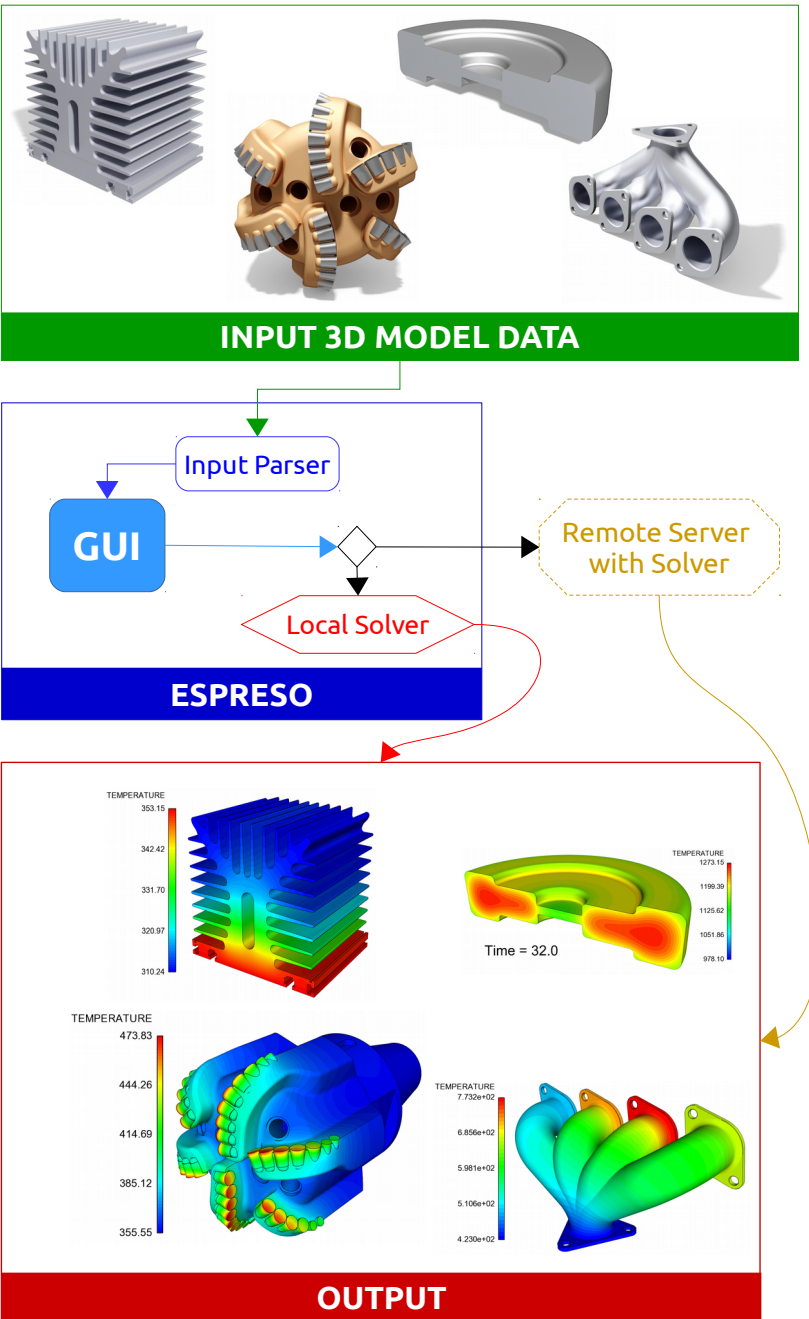


Figure 2: Graphical configuration tool workflow