

# **NEPTUNIUS: the ENEA HPC portal for multiphysics simulations**

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## **Abstract**

The goal of NEPTUNIUS [1], the ENEA CFD/Multiphysics virtual laboratory, is to bridge the gap between HPC-oriented CFD/multiphysics software implementations and field experts/researchers. NEPTUNIUS stands for **N**umerical **co**dEs for **co**m**Pu**Tational **flU**id **dy**Namics and **flU**id **strU**cture **int**eraction**S**; It's a web portal tailored around CFD/multiphysics simulations, acting as a gateway to the CRESCO [2] HPC infrastructure.

It provides access to HPC software packages, masking and simplifying the underlying job submission paradigm and user data input via a web based GUI, to less HPC-skilled users although experts in fluid dynamics and multiphysics interaction.

## **Introduction**

Multiphysics simulations are a well established modelling approach to complex phenomena. The ever growing computational capability available reflects on quality simulations and can increase simulation relevance in many fields like scientific prediction and engineering design.

The goal of NEPTUNIUS is to favour modelling experts, or in general the less HPC-skilled users, through an easy and unified access to:

- the available numerical codes related to multiphysics modelling;
- the HPC-related software components and their documentation (resource manager, web applications, distributed filesystems, etc.)
- the CRESCO main clusters, currently sections CRESCO3 [3] and CRESCO4 [4].

The multiphysics modelling environment requires a widespread user expertise: from Computational Fluid Dynamics (CFD) to Finite Element Methods (FEM) or Fluid-Structure Interactions (FSI); from Computer Aided Design (CAD) to programming and High Performance Computing (HPC).

These high profile and specific skills are generally distributed among different professional figures; a single individual unlikely has thorough knowledge of more than a few of the modelling disciplines mentioned. This is also true for other subjects, therefore ENEA provides the virtual laboratory approach: web portals tailored around several scientific or thematic fields aimed to exploit and streamline HPC usage.

NEPTUNIUS is the key for engineers and CFD/multiphysics modelling experts to an immediate and effective usage of HPC resources, automating key tasks such as running software in both interactive/developing mode and batch/production mode.

## **The NEPTUNIUS Portal**

In interactive mode users can launch the GUI of the codes running on dedicated CRESCO nodes and also prepare simulations and do pre/post-processing activities. In batch mode users can submit and keep track of their simulations running on CRESCO nodes.

<p><b>CFD</b></p> <ul style="list-style-type: none"> <li>• Ansys Fluent</li> <li>• Ansys CFX</li> <li>• OpenFOAM</li> <li>• STAR-CCM</li> </ul>	<p><b>FEM</b></p> <ul style="list-style-type: none"> <li>• Ansys</li> <li>• Nastran</li> <li>• Calculix</li> </ul>	<p><b>Multiphysics</b></p> <ul style="list-style-type: none"> <li>• Comsol</li> <li>• Ansys</li> <li>• STAR-CCM</li> </ul>	<p><b>FSI</b></p> <ul style="list-style-type: none"> <li>• MpCCI</li> </ul>
<p><b>Pre/Post-Processing</b></p> <ul style="list-style-type: none"> <li>• Paraview</li> <li>• Gambit</li> </ul>			

Table 1: NEPTUNIUS currently available codes roughly grouped by thematic fields

The listed codes are available, besides the standard ENEAGRID [5] access gateways and SSH clients, also through the NEPTUNIUS Java-based web portal. It can easily provide graphical interactive mode via NX technology [6]; NX software layer handles remote X Window System connections, it is developed by NoMachine and exploits data compression techniques to improve performance of the native X display protocol in order to provide a reliable and responsive graphical experience even on slow networks. SSL encryption is achieved encapsulating remote connections over SSH sessions. The NX main server is virtualized and a load balancing facility manages the CRESCO node pool involved, to improve availability.

Through NEPTUNIUS web portal it is possible to gain complete access to the main ENEAGRID capabilities and web applications such as FARO [7] to access directly CRESCO frontends, documentation archive, and other utilities (ticketing system, job monitoring, etc.).

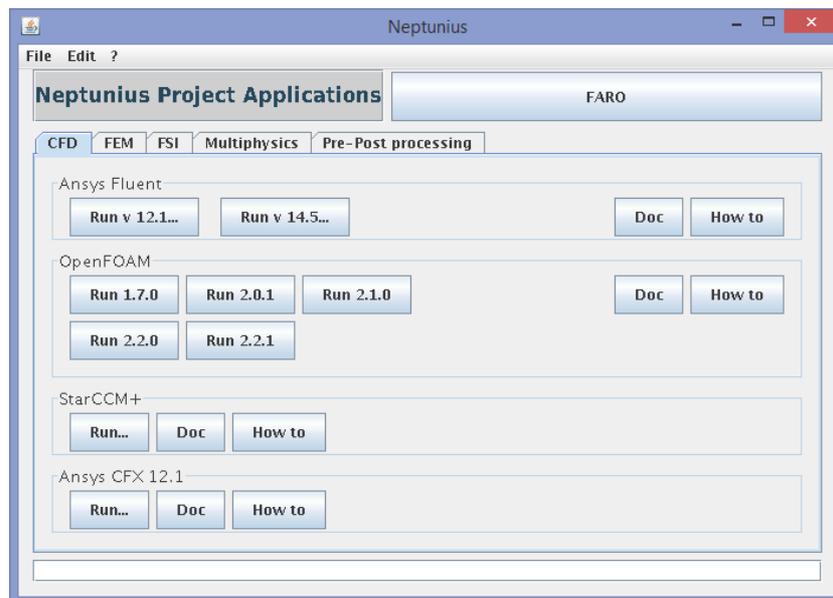


Figure 1: NEPTUNIUS Java gateway application

In figure 1 it is shown a snapshot of the Java GUI itself organized in subject tabs to provide easy access to CFD software in interactive mode. Note also the FARO launch button.

Figure 2 shows the Ansys Fluent simulation submission panel on CRESCO HPC system. It is possible to recognize some features aimed to simplify the tuning of various aspects related to HPC simulations that can be new for those used to work on their office workstation:

- ability to run batch simulations along interactive mode
- ENEAGRID middleware provides the Load Sharing Facility (LSF) resource manager [8] for batch scheduling, therefore users can choose submission queue, specify hardware resource

type, maximum job duration, output and error files and other things useful to monitor the submitted jobs.

- license management: CRESCO relies on ENEAGRID middleware also for licensing software runs via a virtualized central license server and LSF capability in license accounting and management. Users can also provide their own license and therefore ask for a dedicated queue.

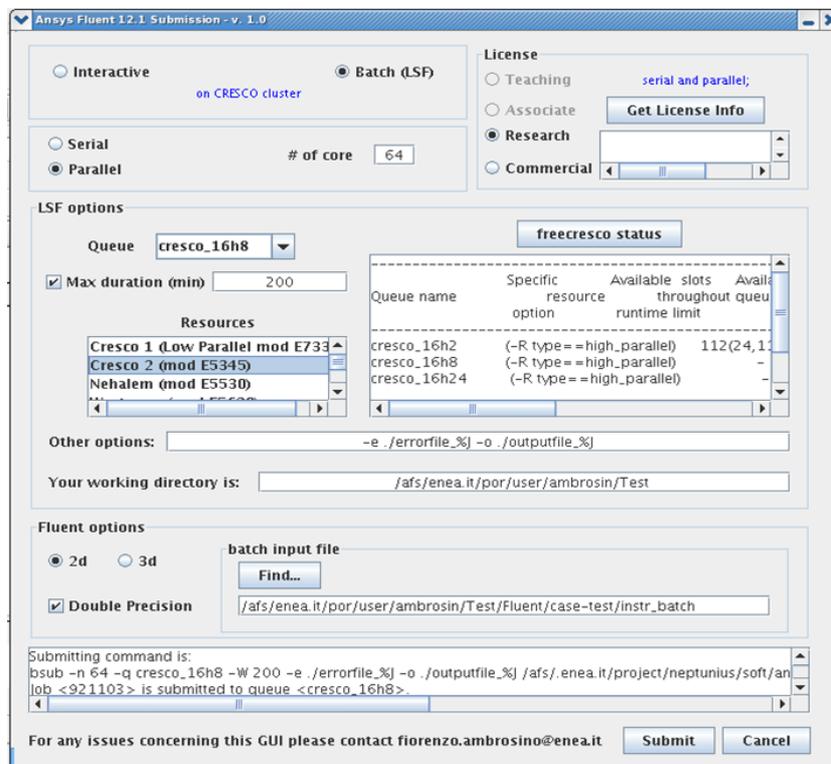


Figure 2: Ansys Fluent Java launcher

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## References

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