FUSION TECHNOLOGY
DESCRIPTION

EUROfusion
TECHNOLOGY TRANSFER PROGRAMME

e-Science MUSCLE3:
Enhancing multiscale computing with sensitivity and uncertainty quantification

In fusion technology MUSCLE3 helps coupling different codes, even if written in different languages, into a single workflow, while each code component maintains its internal state throughout. The aim of the technology is to develop generic methods and efficient algorithms for uncertainty quantification and sensitivity analysis for multiscale modelling and simulation. In addition, it implements these as high-quality modules of the publicly available Multiscale Modelling and Simulation Framework. This, in return, validates, verifies, and sensitively analyzes multiscale data. The applications of such a technology can tackle challenging multi data analysis in various sectors such as climate, energy, health, etc. This sensitivity analysis of multiscale workflows reduces the number of varied inputs and therefore cut down the sample size and cost.

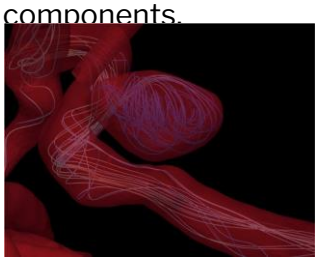
Description of the technology

In some systems, the interaction of multiple different processes at different scales, different times, and different spaces, is very challenging to monitor, analyze and control. Here arises the need for multiscale models of such physical systems that can simulate the workflow dynamics by connecting the transport, equilibrium and turbulence models together with a module that converts fluxes into transport coefficients. In other words, MUSCLE3 connects submodels together to simulate the whole multiscale process.

Although the submodels are connected to MUSCLE3 via an easy-to-use library (currently available in Python, C++, or Fortran), the submodels exchange information via peer-to-peer network connections. This makes the process possible even if different programming languages are used for different models. The library is then followed by a configuration file that describes how many instances of each model should be there and how models should connect together. As a result, single-scale models are coupled together into a multiscale workflow that is easier, cheaper, and more accurate to operate.

By using MUSCLE3, rewiring models becomes as easy as changing the configuration file and re-running. This allows for easy testing in different versions of a submodel, modifying or saving data being exchanged, or adding components for (semi-intrusive) UQ, which will also be included. Moreover, MUSCLE3 lets you configure the submodels' settings from the central configuration file, and allows adding components that modify settings on-the-fly, so that ensembles can be set up for UQ, or submodel parameters can be set based on output of another submodel.

Multi-physics simulations, like for ITER plasmas, need to couple together different physics codes, sometimes written in different languages. MUSCLE3 provides an elegant solution whereby the different codes are not tightly coupled together, but are run as independent components. MUSCLE3 coordinates the workflow and carries out the communication between components.



Muscle model, courtesy of the Netherlands' e-Science Center 2022©

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Innovation and advantages of the offer

Many of the quantitative research and engineering challenges in contemporary science, such as climate, energy, health and disease, are essentially multiscale system problems. Progress in most of these societal grand challenges is determined by our ability to design and implement multiscale models and simulations of the particular systems under study.

Historically, Uncertainty Quantification (UQ), used to measure level of certainty about a model's results, involve either intrusive UQ, which is time-consuming and not always possible, or non-intrusive UQ, which is computationally very expensive. However, MUSCLE3 uses novel semi-intrusive methods, which take advantage of the coupled-submodels nature of the multiscale model, and add some components to the model and rewire it without changing the individual submodels.

MUSCLE3 is publicly available on GitHub and comes with extensive documentation, a unit and integration test suite, and a well-defined process for community contributions.

Non-fusion Applications

MUSCLE3 is research-domain agnostic and can be used for multiscale models in any domain. Various multiscale system problems which usually contain complex data can have a direct gain from this technology. Sectors like climate, energy, health and disease, and many others are good candidates for non-fusion applications of MUSCLE3.

EUROfusion Heritage

MUSCLE 3 was used as the integrated modeling simulation framework for the fusion reactor ITER. The future simulation framework assists with predictions of plasma behavior in ITER's fusion reactor. These simulations are complicated due to multiple physics processes that all have to be modelled separately and tied together.

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