Scientific Workflows for the Linear MHD Stability Analysis Chain

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Introduction:

The European Task Force on Integrated Tokamak Modelling (ITM-TF) has the long term goal of providing the European fusion community with a validated suite of simulation tools for ITER exploitation. Starting from a set of previously largely unrelated numerical tools, which had been dedicated to specific physics problems and, for historial reasons, tightly connected to specific fusion laboratories, the ITM-TF has been striving for the integration of these numerical tools, sometimes major codes, into a unified workflow concept.

To this end, a standardized set of data structures has been defined which is sufficient to cover the wide range of physics topics of the European fusion community like equilibrium reconstruction, MHD stability, transport, turbulence, heating and current drive, and plasma waves [1]. The data structures are organized by physics problem into so called consistent physical objects (CPOs). The definition of these unique CPOs allows for the development of standardized code interfaces for data I/O and the definition of a Europe-wide data base for fusion simulations comprising all major fusion experiments within EFDA. It also allows for the implementation of a completely modular workflow concept by turning formerly autonomous physics codes and numerical tools into encapsulated modules which interact with each other via CPOs. Within a specific physics area, like for instance fixed boundary equilibrium reconstruction, these physics modules become interchangeable through polymorphism, i.e. standardized interface definitions. Communication with the ITM-TF data base is done via automatically generated access tools, referred to as the Universal Access Layer (UAL).

As one of its first sets of physics modules, the ITM-TF intends to release a set of codes for equilibrium reconstruction and linear MHD stability analysis. The codes to be released have been adapted to the ITM-TF interface standard using the equilibrium and MHD CPOs. A significant effort has lead to the integration of previously unrelated numerical tools into a general scientific workflow environment using the open source workflow system Kepler [2] as an orchestration

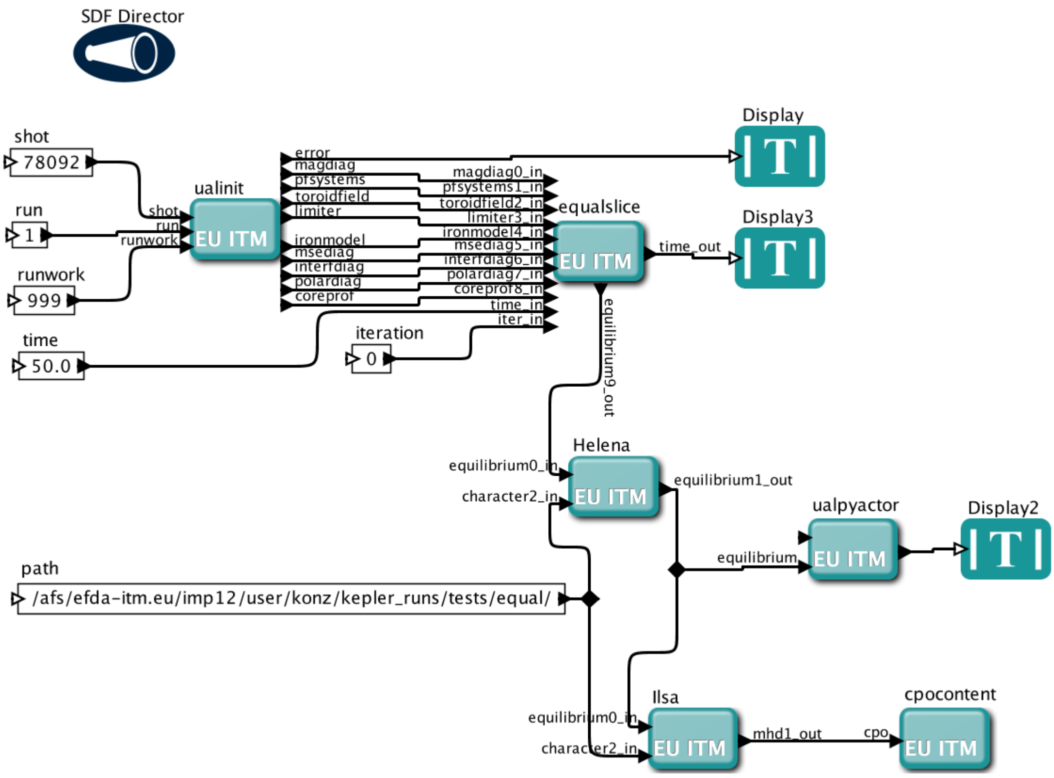

Figure 1: linear MHD stability chain

tool. We present two of the first scientific workflows resulting from this effort: the equilibrium reconstruction and linear MHD stability chain as well as a j-α stability workflow.

Linear MHD Stability Chain:

The workflow for the linear MHD stability chain consists of three physics modules: the free boundary equilibrium reconstruction code EQUAL [3], the high resolution fixed-boundary Grad-Shafranov solver HELENA [4], and the linear MHD stability module ILSA which is used here in MISHKA mode [5].

Fig. 1 shows the sequence of simulation modules as a Kepler workflow. Each of the boxes represents a so called actor, i.e. a module. Data flows along the arrows and is exchanged in memory between the actors. The modules developed by the ITM-TF are marked as 'EU ITM'.

The Kepler orchestration tool is a mixed language environment. While most physics modules in the ITM-TF have been written in Fortran, it also currently allows for C/C++, Java, Python, and Matlab code, thereby facilitating the coupling of physics codes which could not - or at least only with substantial difficulties - be coupled before. This approach allows for a vast number of workflow options including entire tokamak simulators and gains significantly over data transfer via files.

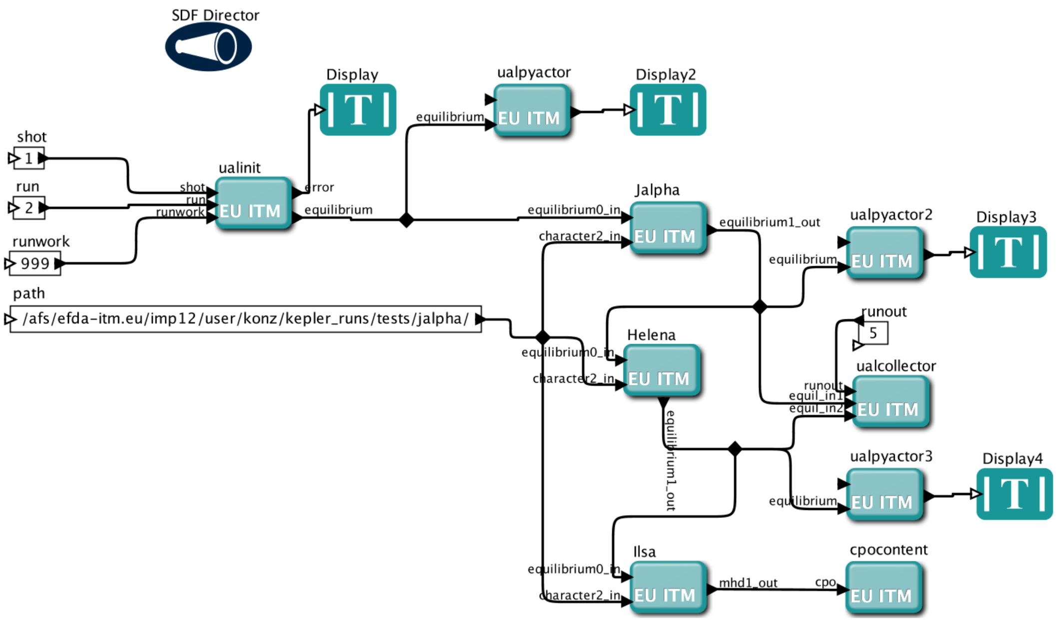

Figure 2: j-α stability workflow

The workflow presented here starts like any ITM-TF workflow with a `ualinit` actor which reads data from the data base and passes it on in form of CPOs to the following actor, in this case `equalslice` which calculates a free boundary equilibrium from the incoming signals (for more details see [6]). The resulting free boundary equilibrium is stored in an equilibrium CPO from which the HELENA actor extracts the plasma separatrix and the plasma profiles like pressure p and flux surface averaged current density $\langle j_{tor} \rangle$ for the calculation of a high resolution fixed boundary equilibrium within the separatrix. The resulting equilibrium together with the metric tensor for the straight field line coordinate system is passed on to the linear MHD stability module ILSA as well as to the visualization actor `ualpyactor`. The latter was created in collaboration with the EUFORIA project [7] and uses freely adaptable Python scripts to visualize the equilibrium. Finally, the ILSA actor computes the spectrum of growthrates for the given equilibrium within the framework of linear MHD.

j-α Stability:

The j-α stability workflow shown in Fig. 2 has a similar structure as the linear stability chain but differs by the fact that the `equalslice` module has been replaced by a module called `jalpha`. The `jalpha` module takes the pressure profile $p(\rho_{vol})$ and the flux surface averaged current density $\langle j_{tor} \rangle (\rho_{vol})$ from a previously calculated equilibrium (typically but not necessarily done with the HELENA module) and modifies them through multiplication by the factor

$$f = c_1 \left(\rho_{vol}^{\alpha_1} - \rho_{vol,ped}^{\alpha_1} \right)^{\alpha_2} H \left(\rho_{vol,ped} - \rho_{vol} \right) + c_2 \quad (1)$$

where $H\left(\rho_{\text{vol,ped}} - \rho_{\text{vol}}\right)$ denotes the Heaviside function and $\rho_{\text{vol}} = \sqrt{V/V_{\text{LCFS}}}$ with V_{LCFS} the volume within the last closed flux surface. The exponents α_1 and α_2 differ for the pressure and current density and may be chosen arbitrarily. The factors c_2 are direct scaling factors for the maximum edge pressure gradient and edge current density while c_1 is determined by maintaining the energy content W_{MHD} of the plasma and the total plasma current I_{p}.
The resulting profiles are then fed again into the HELENA module to calculate the new modified equilibrium which is passed on to the ILSA module for stability calculation. Thus, a standard j-α stability diagram may be calculated by repeatedly calling the above workflow with modified scaling parameters c_2.

Conclusions:

After significant integration efforts, the ITM-TF is about to release its first physics modules in form of the linear MHD stability chain. The data structures and physics modules have matured enough to allow for the versatile and fast creation and modification of physics workflows in the Kepler simulation environment. Strict encapsulation and polymorphism of the physics modules allows to exchange each module with another of the same kind, for instance fixed boundary equilibrium solvers. The usage of standardized interfaces facilitates the benchmarking and the validation of the employed modules. The ITM-TF ensures the completion of a series of verification and validation tests before a physics module is officially released. At the current pace, the ITM-TF will release its first modules in 2010 for equilibrium reconstruction and linear MHD stability analysis.

References

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