Development of the SOLPS-IO (5.3) code: Extended grids

Technical Specifications

	Version 1	*Date: 22/09/2013*
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Table of Contents

1 Purpose

ITER relies on computer simulation for the prediction of plasma behaviour. For the boundary region of the plasma, which interacts with the material surfaces of the containment vessel, the SOLPS code has been used to guide the design of the plasma facing components (PFCs), fuelling and pumping systems, and diagnostics. As construction begins and design work in these areas naturally concludes, SOLPS will increasingly be used to provide the data required for detailed operational planning.

For the past three years, ITER has run Task Agreements through F4E for the development of SOLPS5.3, which is a substantial upgrade of SOLPS4.3, the current ITER reference version. The primary objectives were to update the physical model used by the code and to align modeling tools at the IO with that of the wider fusion research community. For design continuity, an important and challenging constraint was that SOLPS5.3 be able to reproduce the simulation data generated by SOLPS4.3, which was successfully accomplished to a high order.

This contract focuses on the resolution of a notable limitation when applying SOLPS5.3 to ITER: extension of the computational domain so that it covers the entire volume inside the containment vessel, specifically the regions between the outermost grid boundaries and the main chamber surfaces.

The code currently only represents plasma contact with the divertor surfaces, and so the interaction of plasma with the material surfaces elsewhere in the vessel (the “main chamber”) are treated in an approximate way. This is an issue because main chamber plasma-wall interaction may be very important in ITER due to the close-fitting wall. Extending the code to include the entire volume is necessary for accurate estimation of wall armour lifetime, material migration around the machine (tritium retention and dust production), gas fuelling of the core plasma, and diagnostic performance (e.g. first mirror lifetime).

2 Scope

Given the maturity of the divertor and blanket (first wall panel) systems (TKM), the principle beneficiaries of SOLPS5.3 development will be operational planning (POP) and diagnostic design (CHD). No other activities at the IO are affected.

3 Definitions

For a complete list of ITER abbreviations see: [ITER Abbreviations (ITER_D_2MU6W5)](ITER_D_2MU6W5).

<u>Abbreviations</u>

B2	plasma fluid code included in SOLPS4.3
B2.5	more advanced plasma fluid code included in SOLPS5.3
CHD	CODAC, Heating & Diagnostics Directorate
EIRENE	kinetic neutral particle (gas and photons) transport computer code
EFDA	European Fusion Development Agency
FWP	first wall panel
FZJ	Forschungszentrum Jülich, Germany

IO	ITER Organization, France
IPP	Institut für Plasmaphysik, Germany
PFC	plasma facing component
POP	Plasma Operations Directorate
PWI	plasma-wall interaction
SOLPS	boundary plasma computer simulation code suite
TKM	Tokamak Directorate

Definitions

Standard grid – The reference computer code grid geometry used with the current generation of ITER simulations that does not have triangular cells at the grid boundary. This type of grid cannot be used to include plasma contract with the main wall of the containment vessel.

Extended grid – A more flexible grid system that can use trianglular cells at the grid boundary, which allows extension of the computational domain so that plasma contact with the main wall can be included. The modification of the boundary conditions in SOLPS5.3 to account for triangular cells is the main focus of this contract.

4 References

[1] M. Baelmans, P. Boerner, W. Dekeyser, and D. Reiter, "Tokamak plasma edge modelling including the main chamber", Nuclear Fusion 51 (2011) 083023.

5 Estimated Duration

18 months with a total effort of 0.7 ppy.

6 Work Description

As outlined in Section 1, this contract focuses on the extension of the computational domain in SOLPS5.3.

Extension of the Computational Domain

1) *Employ existing mesh generation tools to prepare an "extended grid" that covers the full volume of the ITER plasma chamber*. The computer codes use a mesh of connected polygons (a "grid") to represent the physical volume inside the containment vessel, but many standard grid generation tools can only produce the highly structured grids with are typically used by 2D plasma fluid codes. The extended grids required for representing plasma-wall contact in the main chamber can currently only be produced by software available from FZJ (GRIDADAP) and IPP (CARRE-2), and so the Contractor will need to arrange access to one of those codes.

2) *Global modifications to SOLPS5.3 (with the exception of the B2.5-EIRENE interface; see item 5 below) that allow the import and processing of the extended grid*. The code was originally written for a grids with a specific "rectangular" structure and "grid cuts" to connect different grid regions. This basic setup was used for modifying SOLPS4.3 for extended grids [1]. The same method could be used for SOLPS5.3. Alternatively, a generalisation of the code could be performed to allow fully unstructured grids. In the latter case, all of the routines that are affected by the unstructured geometry of the generalized

grids need to be modified. This would represent the largest modification to the code base associated with this contract.

3) *Modify the numerical boundary conditions for inclined surface elements, across which plasma fluxes parallel and perpendicular to the magnetic field are accommodated (rather than either purely parallel or purely perpendicular fluxes, as it is currently the case in SOLSP5.3).* This task is the most involved and difficult work element in the contract. Extended grids preserve orthogonality in the main chamber by allowing plasma transport to wall surfaces through the sides of grid polygons, which are orthogonal to the magnetic field (radial transport), rather than via the end surfaces (parallel transport), which is not currently supported by SOLPS5.3. The solution is to modify the boundary conditions when solving the plasma fluid equations in the near-wall grid cells, which is a challenging mathematical and numerical problem. Timely implementation will be greatly aided by prior knowledge of the solution methods employed in SOLPS5.3.

4) *Update the wall erosion (sputtering) model in SOLPS5.3*. The change in the near-target grid cell geometry will require that the ion velocity be modified, and so there will be some overlap with development activity outlined in the previous work item.

5) *Compare results from simulations with purely parallel and parallel/radial boundary conditions on the same computational volume*. As a test of the modified boundary conditions, a comparison shall be made with a standard SOLPS5.3 case for the same computational volume, that is, without extension of the grid to include plasma contact in the main chamber. This study also relates to the effect of non-orthogonality near vertical divertor target surfaces, which may (or may not) contribute to variations between the solutions for the different grid implementations. Test cases are to be run (Q=10, low density), selected from the ITER test simulations currently available for benchmarking:

   a. single-fluid (D)
   b. multi-fluid (D+He+Be+Ne)

   The IO will supply the input data for the standard grid runs.

   The required modifications to the SOLPS5.3 B2.5-EIRENE interface to support operation on extended grids have been conducted as part of a previous IO SOLPS5.3 development contract.

6) *ITER test cases with a generalized grid*. Representative cases (Q=10, medium density) shall be run on the generalized grids with extension of the computational domain so that main chamber plasma contact is explicitly included, with radial convection applied in the extended grid region. The following test simulations are required:

   a. single-fluid, $v_\perp = 10$ m s^{-1} in the far-SOL;
   b. single-fluid, $v_\perp = 100$ m s^{-1};
   c. multi-fluid, $v_\perp = 10$ m s^{-1} in the far-SOL, no wall sputtering;
   d. multi-fluid, $v_\perp = 10$ m s^{-1} in the far-SOL, wall sputtering included.

   The parameters for the reference test simulations (standard SOLPS5.3 setup) will be provided by the IO.

It is difficult to anticipate the time required to complete the above work programme, given the challenge of anticipating difficulties when specifying code development activity of this complexity. Regular IO monitoring is therefore required in order to ensure that the specified level of effort is being expended on this contract; see Section 11.

7 Responsibilities

The Contractor appoints a responsible person (C-RO) who shall represent the Contractor in all matters related to the implementation of this Contract.

The contractor will be responsible for the work described in Section 6, providing results according to the scope of the work outlined above and fulfilling the implementation plan and conditions of the present contract.

Details of the precise target design to be used in the experimental tests shall be decided in consultation between the IO-RO and the C-RO at contract kick-off.

8 List of deliverables and due dates

Month	Description
3	Report #1, illustrating the successful generation and importation of a generalized grid into SOLPS5.3 (work items 1 and 2).
9	Report #2, discussing the modification of the boundary conditions and sputtering model, i.e. results from test cases (non-ITER runs are acceptable) (work items 3 and 4).
12	Report #3, presenting a comparison between the standard SOLPS5.3 version and the modified code on a standard grid (plasma contact in the divertor only). (work item 5)
18	Final report summarizing the code development and verification activity, in particular the simulation results including plasma contact with the ITER wall in the main chamber. (all work items) Installation and successful compilation of the SOLPS5.3 source code on the IO computer cluster.

9 Acceptance Criteria

The Contractor should demonstrate that personnel assigned to the contract have the experience and technical capability to perform the work described in Section 6.

The Contractor should quote a fixed amount for the work package described in Section 6.

The contract will be considered complete once ITER has accepted the last deliverable.

10 Specific requirements and conditions

With its offer, the Bidder shall provide:

- Detailed CVs of key personnel proposed for execution of the work activities;

- Implementation Plan for execution of the contract to demonstrate how the work will comply with the requirements of this specification. The Implementation Plan shall include list of points which require ITER check and/or approval for continuation of the work.

It is noted that Contractor's personnel visiting the ITER project will be bound by the rules and regulations governing safety and security. The Contractor shall have and maintain the necessary equipment and licences to run the software tools required to produce the deliverables in accordance with the tools adopted by the IO.

The official language of the ITER project is English. Therefore all input and output documentation relevant to this Contract shall be in English. The Contractor shall ensure that all the professionals in charge of the Contract have an adequate knowledge of English, to allow easy communication and adequate drafting of technical documentation. This requirement also applies to the Contractor's staff working at the ITER site or participating in meetings with the IO.

Documentation developed shall be retained by the Contractor for a minimum of 5 years and then may be discarded at the direction of the IO. The use of computer software to perform a safety basis task activity such as analysis and/or modelling, etc. shall be reviewed and approved by the IO prior to its use, it should fulfil IO document on calculation code for safety analysis. The work may require the presence of the Contractor's personnel at the IO site, Route de Vinon sur Verdon, 13115 St Paul Lez Durance, France, for the purpose of meetings and data gathering.

11 Work Monitoring / Meeting Schedule

Monitoring should proceed through the following schedules meetings:

Scope of Meeting	Point of Check/Deliverable	Place of meeting
Kick-off of contract	Work programme	Videoconference or Contractor site
Meeting #1, month 3	Presentation of content related to Report #1	Videoconference or Contractor site
Meeting #1, month 9	Presentation of content related to Report #2	Videoconference or Contractor site
Meeting #1, month 12	Presentation of content related to Report #3	Videoconference or Contractor site
Closing contract meeting / contract completion	Presentation of content related to the Final Report	Videoconference or ITER site

To assure proper monitoring of activity, short progress meetings will be conducted every two weeks between the IO Responsible Officer and the Contractor, either by phone or video conference.

In addition, informal discussions which can be conducted at any time between the IO and the Contractor, as required.

12 Payment schedule / Cost and delivery time breakdown

Date	Fraction of Contract Value
Month 3	30%
Month 9	30%
Month 18	40%

13 Quality Assurance (QA) requirements

Prior to commencement of any work, a Quality Plan must be provided to IO for approval. This is a separate document which comprises:

1) a workplan with proposed time schedule and agreed preliminary dates for progress meetings,

2) a statement of those involved in the activity and their approximate role and contribution in time,

3) a statement of what work (if any) will be subcontracted and who will responsible for checking this.