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Technical Specifications (In-Cash Procurement)

Technical Specifications for SOLPS-ITER matrix solver numerical improvement contract

This document contains the technical specifications for a contract aimed at improving the numerical robustness of the matrix solver used to compute plasma fluid transport inside the B2.5 component of the SOLPS-ITER code suite.

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1 Preamble

This Technical Specification is to be read in combination with the General Management Specification for Service and Supply (GM3S) – [Ref 1] that constitutes a full part of the technical requirements.

In case of conflict, the content of the Technical Specification supersedes the content of Ref [1].

2 Purpose

The design of the ITER divertor and estimates of the required fuelling throughput for safe operation have relied for many years on simulations performed by use of the SOLPS plasma edge modeling tool. In 2014, a new version of this code package was adopted, named SOLPS-ITER [2]. The SOLPS-ITER suite contains the B2.5 code as its main solver for the plasma transport, and uses the EIRENE code as its main workhorse for solving the transport equations related to neutral atomic and molecular species, as well as for radicals and molecular ions. In 2022, the code was significantly expanded with a Wide Grids capability, moving to an unstructured (though still field-aligned) geometry description [3]. More recently, the code was migrated to a GitHub distribution and made available as open-source software for the fusion community at large.

The scope of the present contract is to improve the robustness of the matrix solver methods used in the B2.5 fluid plasma transport component of the SOLPS-ITER code to handle non-orthogonal grids, particularly those found in converted cases from older SOLPS versions that used structured grids. These structured grids often needed to be strongly distorted near the target plates, to try and simultaneously satisfy the requirements of field alignment, target shape matching, and a rectangular computational domain. Running the Wide Grids SOLPS-ITER version on a case with such a (narrow) grid, including those from the ITER divertor design database, quickly leads to crashes. These crashes are often triggered by densities dropping to zero in very elongated grid cells and make the older cases unusable with the Wide Grids code version. The inability to run such legacy cases is an obstacle in the IO's long-term goal to make the Wide Grids SOLPS-ITER code version the reference code version and to no longer need to maintain both structured and unstructured code versions.

Several schemes exist in the literature of numerical algorithms designed to avoid such issues, for example slope limiters [4]. The aim of the contract is thus to evaluate such schemes in the B2.5 Wide Grids context and implement the most promising solution. The measure of success in any new scheme implementation will be the ability to re-converge representative cases from the ITER divertor design database and demonstrate accuracy of the numerical results by benchmarking them against reference structured SOLPS-ITER run output.

3 Acronyms & Definitions

3.1 Acronyms

The following acronyms are the main ones relevant to this document.

Abbreviation	Description
AD	Algorithmic Differentiation
CI	Continuous Integration
CRO	Contract Responsible Officer
GM3S	General Management Specification for Service and Supply
IO	ITER Organization
KOM	Kick-Off Meeting
PRO	Procurement Responsible Officer
SDCC	Scientific Data and Computing Cluster
SOLPS	Scrape-Off Layer Plasma Simulator
TRO	Technical Responsible Officer

3.2 Definitions

Contractor: shall mean an economic operator who have signed the Contract in which this document is referenced.

Kick-Off Meeting: initial meeting between Contractor and TRO that will mark the beginning of the Contract timeline.

Technical Responsible Officer: shall mean the IO staff member(s) in charge of monitoring the Contract progress and the point of contact for the Contractor regarding all technical matters

4 Applicable Documents & Codes and standards

4.1 Applicable Documents

It is the responsibility of the Contractor to identify and request any documents that would not have been transmitted by IO, including the below list of reference documents.

This Technical Specification takes precedence over the referenced documents. In case of conflicting information, it is the responsibility of the contractor to seek clarification from IO.

Upon notification of any revision of the applicable documents transmitted officially to the Contractor, the Contractor shall advise within 4 weeks of any impact on the execution of the contract. Without any response after this period, no impact will be considered.

Ref	Title	IDM Doc ID	Version
1	General Management Specification for Service and Supply (GM3S)	82MXQK	1.4

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2	X. Bonnin *et al.*, Plasma Fus. Res. **11** (2016) 1403102		
3	W. Dekeyser *et al.*, NME **27** (2021) 100999		
4	P. Sharma *et al.*, J. Comp. Phys. **227** (2007) 123		

4.2 Applicable Codes and Standards

It is the responsibility of the contractor to procure the relevant Codes and Standards applicable to that scope of work.

Ref	Title	Doc Ref.	Version
CS1	SOLPS-ITER CONTRIBUTING rules		3.2.1

5 Scope of Work

This section defines the specific scope of work for the service, in addition to the contract execution requirements as defined in Ref [1].

5.1 Scope of work

The work envisioned in this Contract aims at providing a more robust solution method for the fluid plasma transport equations used in the B2.5 Wide Grids unstructured 3.2.1 code version, in the context of the SOLPS-ITER code suite with the same version number. As such it will need to demonstrate the ability to provide accurate and well-converged solutions, in a reasonable amount of CPU time (roughly the same as current B2.5 execution), for cases currently known to crash with the current solver implementation.

The demonstration of the new capability will be performed upon the set of cases from the stored examples that are part of the structured SOLPS-ITER code distribution, and available as Zenodo records at https://zenodo.org/communities/solps/. From these demonstrations cases, a new set of example cases for the unstructured code version will be built, along with a relevant set of CI test scripts making use of them, at least covering the same ground as the existing structured code CI tests, and, in addition, some tests aimed at ensuring that the new scheme remains accurate, by means of comparisons against known analytic solutions or using the MMS method. The material for these new CI tests will be stored as a new SOLPS-ITER Zenodo record alongside the existing ones.

In order to minimize the impact of the Contractor's work on other B2.5 or SOLPS-ITER developments, the work should be performed within dedicated branches on the *iterorganization* GitHub repositories (https://github.com/iterorganization), which will have to be kept current with any code updates arising from other SOLPS-ITER project contributors. Backward-compatibility shall be maintained, i.e. existing Wide Grids cases must be able to be continued without change if the old solver numerics are being used. To this end, any new numerical treatment options should have some switch governing their usage, although it may be decided by the TRO after sufficient testing to make the new treatment the default one used in future code runs.

The set of examples on which the new numerical method must be demonstrated is the one found in the *master* branch of the SOLPS-ITER repository, in the *$SOLPSTOP/runs/examples* directory, namely:

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- *test_slab_ortho_standalone*: An orthogonal slab test case for **B2.5** standalone;
- *AUG_16151_D*: ASDEX-Upgrade D-only benchmark cases, including **B2.5** standalone, coupled and single **Eirene** call run directories;
- *AUG_16151_D+C+He*: ASDEX-Upgrade multi-fluid benchmark cases, including **B2.5** standalone, coupled and single **Eirene** call run directories;
- *AUG_28903_D+N_drifts*: ASDEX-Upgrade D+N case including drifts;
- *AUG_28903_D+Ne_drifts*: ASDEX-Upgrade D+Ne case including drifts;
- *DIIID_3106_DN_D+C*: DIII-D disconnected double-null case including Carbon chemical sputtering;
- *ITER_2171_D+He+Be+Ne*: ITER full performance case with Ne injection and Be sputtering;
- *ITER_2264_0.6Ne_100MW*: Another ITER full performance case with Ne injection;
- *ITER_2275_Donly_20MW*: ITER low power case at low density (D-fuelled);
- *ITER_2292_Honly_20MW*: ITER low power case at low density (H-fuelled);
- *ITER_2294_Honly_20MW*: Same as above, but increasing density;
- *ITER_2296_Honly_20MW*: Same as above, but continuing density scan;
- *ITER_2297_Honly_20MW*: Same as above, continuing scan;
- *ITER_2298_Honly_20MW*: Same as above, continuing scan;
- *ITER_2299_Honly_20MW*: Same as above, continuing scan, reaching detachment;
- *ITER_2308_Honly_20MW*: Same as above, continuing scan, detached conditions;
- *ITER_2360_0.95He+0.05H_40MW*: ITER Helium plasma case at mid-power (also contains an example with metastable-resolved Helium neutrals);
- *ITER_2588_drifts*: ITER **B2.5** standalone D-only demonstration case with and without drifts;
- *ITER_535_D+He+Ar*: ITER full power case with Ar injection;
- *ITER_Be-W_D+T+He+Ne*: ITER full power case with 98 species;
- *JTEXT_Limiter_H*: J-TEXT limiter case (H-only, full drifts);
- *MAST_U_SFminus_Donly*: Lower snowflake-minus case at low power with D-only.

5.2 Description

The sequence of tasks envisioned for this contract is as follows:

1. As a first deliverable, the Contractor will perform a literature search about solution methods for finite-volume fluid solvers such as the one used by B2.5, with an emphasis on numerical robustness and stability, and propose implementation of one of more of these methods in the existing code base. A report about this activity is to be provided to the IO six (6) weeks after the start of the Contract work.
2. Choice of the numerical method(s) to implement, to be made at a dedicated meeting between the Contractor and the TRO within 2 weeks after receipt of the first deliverable report. The selection will be based on the following criteria (in no particular order):
    a. Public availability of the needed software
    b. Portability of the software across compilers and platforms
    c. Compatibility with OpenMP and MPI parallelization schemes
    d. Adherence to Fortran 2003 standards
    e. Ease of implementation and integration into the existing B2.5 data structures
    f. Existing numerical accuracy and robustness literature

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3. Implementation of the new numerics methods, in a backward-compatible fashion, with demonstration of accuracy and convergence properties against known analytical solutions and/or using MMS tools.
4. Modify the conversion workflow taking legacy results obtained with the structured code to new starting points using the unstructured code, but still able to use the original grids.
5. Demonstrate convergence of the ITER legacy examples with the new numerical method and rebuild the full library of them.
6. Demonstrate convergence of the examples for slab, limiter, DN, and snowflake topologies and rebuild them.
7. Publish a new Zenodo record with all the updated examples.
8. Modify the CI test scripts to use the updated Zenodo record and include an analytic or MMS test of the solution method.

5.3 Service Duration

The maximum expected duration for this activity is 6 months. See Section 8 for the Deliverables schedule.

6 Location for Scope of Work Execution

The work envisioned in this contract is expected to be done on the Contractor's premises.

Code development is to be performed on a fork from the SOLPS-ITER and B2.5 GitHub repositories (https://github.com/iterorganization/SOLPS-ITER and https://github.com/iterorganization/B2.5, respectively). These forks should be based at the tip of the respective *feature/wg-release* branches, and must be kept current throughout the contract period, in order to catch any potential conflicts as soon as they arise.

B2.5 and SOLPS-ITER runs may be performed either on the Contractor's own computer infrastructure or on the SDCC cluster at ITER.

7 IO Documents

Under this scope of work, IO will deliver the following documents by the stated date:

Ref	Title	Doc ID	Expected date
1	Provide access to *iterorganization* GitHub domain with "Write" permissions on SOLPS-ITER and B2.5 repositories		T0 + 2 weeks
2	Provide Contractor with an SDCC cluster account to run B2.5 and SOLPS-ITER cases at ITER		T0 + 2 weeks

8 List of deliverables and due dates

The Supplier shall provide IO with the documents and data required in the application of this technical specification, the GM3S Ref [1] and any other requirement derived from the application of the contract.

A minimum, but not limited to, list of documents is available hereafter with associated due dates:

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Technical Design Family (TDF)	Generic Document Title (GTD)	Further Description	Expected date (T0 + x) *
Review or Decision or Recommendations Report	Progress Report	Literature search and applicability analysis of available numerical methods	T0 + 6 weeks
Commissioning Record or Report	Software Test Report	Final report showing implementation results	T0 + 6 months

(*) T0 = Commencement Date of the contract (KOM); X in months.

The T0 start of the Contract will coincide with the date of the Kick-Off Meeting. The KOM may be held remotely via videoconference.

The software prepared by the Contractor is to be delivered in the form of Pull Requests on the relevant GitHub repositories and the delivery will only be considered complete once these Pull Requests pass all required CI tests and are merged by the TRO. The Contractor is urged to make these Pull Requests as atomic and focussed as possible to simplify and speed up the code review by the TRO. The TRO may invite external reviewers to examine the Pull Requests if it is felt that they would have relevant expertise or tests cases with which to challenge the proposed code.

The Pull Requests will be done within the *iterorganization* GitHub domain, so that the IO CI server can immediately take notice of them and run the standard set of CI test cases which are already in use for the SOLPS-ITER Wide Grids code version. These CI tests must be passed before a Pull Request will be considered for merging into the main development branches.

Since an expansion of the list of CI test cases is an integral part of this Contract, the Contractor must also deliver updates to the CI test scripts that add the new CI test cases to be considered, which must, as a minimum, contain several of the cases from the structured SOLPS-ITER code CI test case database. These new cases should be delivered as a Zenodo record, in a manner compatible with the current CI workflow, at https://zenodo.org/communities/solps/ . The final version of the Wide Grids code version CI test scripts, provided by the Contractor by the end of the Contract, should cover at least the same ground as already done for the structured code version, namely **B2.5** standalone and coupled **B2.5-Eirene** code operation; check for restart effects; serial, debug, MPI-, and OpenMP-parallelized operation; single- and multi-fluid runs; and single- and double-null topologies, in addition to the AD code tests already performed for the Wide Grids code version. The current CI scripts can be found in the *$SOLPSTOP/scripts* directory. An AD version of the code delivered by the Contractor is not required, unless the Contractor has access to a Tapenade® licence (not provided by the IO) and can build the differentiated code (tangent, adjoint, and Hessian variants) using their own infrastructure.

The Supplier is requested to prepare their document schedule based on the above and using the template available in the GM3S Ref [1] appendix II (click here to download).

9 Quality Assurance requirements

The Quality class under this contract is QC4, [Ref 1] GM3S section 8 applies in line with the defined Quality Class.

10 Safety requirements

No specific safety requirement related to PIC and/or PIA and/or PE/NPE components apply.

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11 Special Management requirements

Requirement for [Ref 1] GM3S section 6 applies in full.

12 Appendices

None