EFDA EUROPEAN FUSION DEVELOPMENT AGREEMENT
Integrated Tokamak Modelling

Preliminary draft

Guidelines for the Validation & Verification procedures

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Introduction

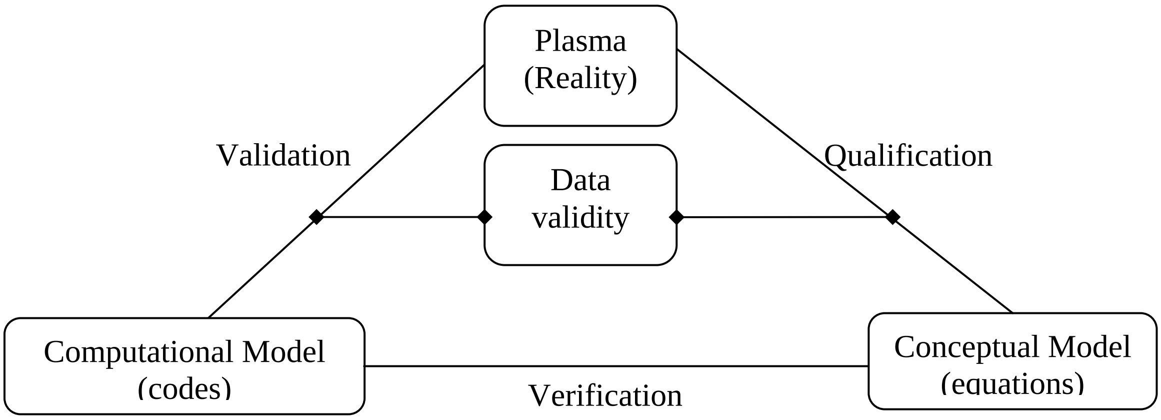
The European Task Force on Integrated Tokamak Modelling has been set up to provide modelling tools for future ITER exploitation. The STAC steering document puts strong emphasis on the quality and reliability of the simulation tools to be provided:

The aim of the task force is to co-ordinate the development of a coherent set of validated simulation tools for the purpose of benchmarking on existing tokamak experiments, with the ultimate aim of providing a comprehensive simulation package for ITER plasmas.
The remit of the Task Force would extend to the development of the necessary standardized software tools for interfacing code modules and for accessing experimental data.
In the medium term, this task force's work would support the development of ITER-relevant scenarios in current experiments, while in the long term it would aim to provide a validated set of European modelling tools for ITER exploitation **(EFDA(03)-21/4.9.2)**

To meet this goal a validation and verification process has been developed with the aim to quantify the impact that limitations and uncertainties in theory and modelling as well as error bars in experimental data have on our ability to model the plasma conditions achieved in current day experiments. Ultimately this characterization of uncertainty should provide quantification of the predictive capability in predicting plasma behaviour outside the validation domain. For most predictive tools involving multiple physics components this will be a complicated task where several steps in the process of formulating, writing and exercising the code need to be assessed, tested and documented. Generally this will be an iterative process involving a range of tests and comparisons at different levels of interaction between theory, modelling and experimental communities. At the core of the experimental validation is the integrity and quality of the experimental data used to benchmark the predictions. Available experimental data need to be assessed not only with respect to diagnostic uncertainties but also for how appropriate it is for the particular validation effort at hand. In addition, the level of confidence in the predictive performance of a code or model is closely related to how much of an extrapolation from the validation domain the prediction is.

The basis of the validation procedure

The validation procedure has been designed to be used in a broad range of integrated modelling projects. For this reason the procedure document has the character of general guidelines where detailed descriptions and requirements have been left out and will have to be formulated within each of the separate validation projects it is being used. The structure of the procedure is largely based on the identification of a few key components believed to be fundamental in building confidence in the predictive capability of any code or module. The components are: Qualification, verification and experimental validation together with an assessment of data validity appropriateness.



Qualification (assessing the validity of the conceptual model): Are the equations we are solving providing a sufficiently detailed description of the underlying phenomena and are they valid within the intended context of the model? Frequently the assumptions made in deriving a set of governing equations for a system will limit the domain of validity of the model. Knowing the range of validity and the specific assumptions made in the derivation may help understand the outcome of a validation exercise as well as help evaluate the predictive performance of the model. For cases where different model are being assessed knowledge of the differences in physics basis between the modules may help discriminate between the models and help construct dedicated experimental validation test. Different models purported to describe the same physics may have different detailed physical contents and assumptions built into them. Care need to be taken as to highlight these differences within the validation and benchmarking process to help provide a deeper understanding of the physics basis and to ensure that we achieve a proper understanding of the predictive capability when going beyond the validation domain.

Verification (assessing the validity of the computational model): Is the implementation correct and free from coding errors? To what accuracy are we obtaining correct solutions? Finding coding errors in complex codes is a necessary, non-trivial and often time consuming task of any project. Static debuggers and enforcing strict standard conformance during code compilation may help. Special care needs to be exercised in mixed-language settings where interface issues may cause portability problems and may yield hard to diagnose system dependent errors.
The process of estimating the accuracy and reliability of a code is a purely numerical exercise: Grid convergence tests, conserved quantities, analytical test cases as well as code-to-code benchmarking is but a few possible means. For cases when part of the validation exercise is to benchmark different models the numerical testing should also be expanded to include physics based tests and comparisons where the objective is to highlight model differences and find quantities with systematic deviations that can be tested experimentally.

The qualification and verification steps provide a convenient mechanism for reviewing the code documentation and implementation but the main importance from a code validation point of view is to ensure the applicability of the code for the current validation task at hand and to provide the domain of validity of the theory and the accuracy of the numerical implementation.

Validation (assessing the ability of the code to accurately model experiments): For codes or models that come reasonably close to describing measured quantities to merit a direct comparison with experiments, the validation step should provide a detailed comparison of the code calculations against validated experimental data. The range of plasma parameters scanned should be as broad as possible (within the validity of the model) and also take into account the uncertainties and physics bias uncovered through the qualification and verification steps. Known experimental errors should be assessed. The validation metrics should be carefully chosen and employed to provide quantitative measures of code performance and help provide detailed information on the sensitivity of simulation results to variations in model inputs and parameters.

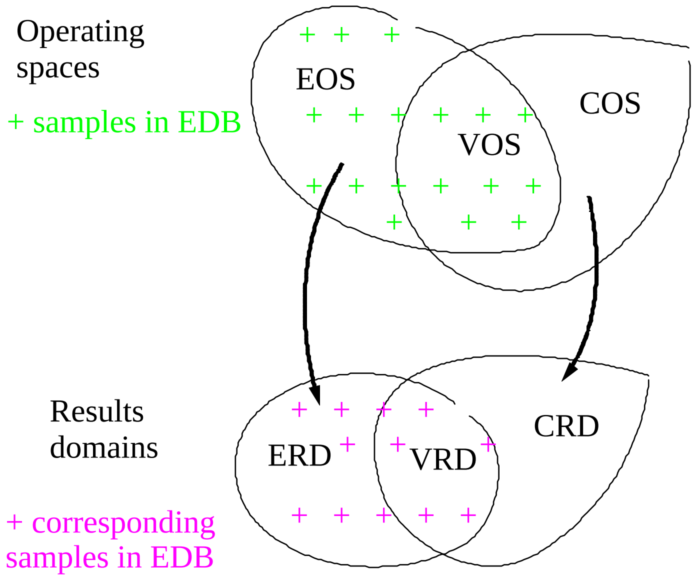
In particular, the validation metrics need to be chosen with care when different modules describing the same or similar physics are being benchmarked. In these cases validation tests should be complemented with experimental comparisons targeted to discriminate between the different models. In these physics validation tests, the aim is to see if experimental trends of a measurable quantity with respect to some dimensionless parameters for instance are recovered using any the models.

Not all codes and modules will be possible to completely validate against experimental data; no measurable quantity may be obtainable to compare simulations with or only secondary effects are calculated that fall into the validation domain. For these qualification and verification may be as far as the validation can go without new diagnostics being available.

Not all codes can be exercised to span equal amounts of the database. For large time-consuming codes only a smaller number of runs may be possible whereas for faster codes the whole database can be covered including a detailed assessment of variations in free modelling parameters and experimental error bars.

Experiments, codes and free modelling parameters.

The quality and integrity of the available data is a very important aspect for the quality and outcome of the validation effort as a whole. In particular, the range of the experimental data used has direct impact on the confidence in the predictive performance. An integral part of the validation work as a whole is the creation of experimental multi-device databases. These will store discharges defining the general validation domain, as well as profiles from dedicated experiments for benchmarking modules and physics models. Understanding device to device differences and diagnostics as well as providing high quality consistent data will require a high degree of coordination and interaction between the modellers and experimentalists. To maximize the efficiently of the validation effort a deep understanding of the different operating spaces of the both the codes (COS) to be validated and the experiments (EOS) are needed. The EOS is characterised by the experimental input parameters and the corresponding experimental results, deemed to be reproducible. Both codes and experiments produce results that are mapped into corresponding results domains. The ERD is defined by the set of all the measurements that are produced. For the code definitions are analogous, except that the input of the code is not restricted to the EOS parameters and will in general contain some measured parameters, as well as some assumed parameters. The overlap between the experimental and code domains constitutes the validation operating space and validation results domain.



In addition to understanding the operating spaces it is equally important to understand and assess the impact on free modelling parameters have on the predictive capability of the code.

Outcome of the validation exercise.

What should the outcome of a validation exercise be? First of all the systematic analysis of the physics basis, numerical implementation and validity of the experimental data performed throughout the process should provide deeper insights in all three of those areas. Limitations and problems in derivations and implementations uncovered should provide a basis for further exploration and research to increase the fidelity of the physics basis of the models and improve the numerical methods and algorithms we are using. Further experimentation may be needed to help discriminate between models and model predictions. The call for quantitative estimates throughout the process will lead to quantitative estimates on how well the simulations can represent current day experiments and may at the same time by systematic exploration of the validation domain provide means for steering future model developments.

The validation procedure - a schematic outline

Scope and aim of validation exercise

Provide: A brief description of the scope, aim and requirements of the model/code to be validated

Qualification — Interface/communicate: Theory/modelling

Provide: Documentation of the physics model or code (References and pointers to relevant material)
Define: Domain of validity (derived from model limitations)

Assess: Suitability of code/module to describe required physics

Conformance — Interface/communicate: Code developer(s)/ modellers

Assess: Adherence to Taskforce software and coding standards.

Verification

Provide: Documentation on existing code verification work

Assess: Accuracy of calculated solutions
Impact of "free" parameters in the model

Define: plan for extended verification testing if needed

Validation and benchmarking — Interface/communicate: Experimentalists and modellers

Define: Quantitative validation/benchmarking metrics
(sensitivity to variations in input and model parameters)
Standard protocol for code operation
Need for experimental data (input and diagnostics).

Provide: List of discharges suitable for this validation effort

Assess: Quality and accessibility of experimental data
Uncertainties in the data inputs. (i.e., error bars)

Provide: Detailed description of the code performance in terms of validation metrics(taking uncertainties in data, modelling etc into account).

Define: Plan for extended validation testing if needed.
new experiments in support of the validation effort

Provide: Files, run scripts, data and code to assure reproducibility and provide a basis for impact and regression testing of new code and physics model updates.

Summary and recommendations:

Provide: A summary of the findings and recommendation for use of the model together with further validation and benchmarking work to be performed.

Qualification – Validity of the conceptual model

The purpose of the qualification assessment is to assess and describe the physics basis of the code(s) or module(s) in order to:

- Ensure that the physics description is appropriate for the codes intended use.
- Highlight any intrinsic limitations of the model in view of its intended use.
- Provide an explicit statement of the domain of validity of the model as a basis for the experimental validation process.

Process and procedure

The qualification step requires code documentation to be assembled (depending on what documents are already available within the project). An assessment and/or review of the physics model(s) should be performed and documented.

Review: The following should be provided for the codes and modules being used.

Physics Basis: A description (with references) of the physics basis of the code or module.
Limitations: A discussion of the limitations in derivations, underlying assumptions and methodologies employed in the code with emphasis on specific features particular to the code compared to other models.
Modelling assumptions: Any intrinsic free parameters and other model dependent parameters should be discussed.

The basic purpose of the qualification step is to define the conditions under which the model should provide a sufficiently detailed description of the phenomena to be studied. The following criteria's should then be assessed:

Evaluation: Based on the model review, define or assess

- The domain of validity for the model.
- The free parameters or model specific assumptions in the formulation of the model.
- The general applicability of the model for its intended use.
- Highlight theoretical differences between models to be benchmarked.

Possible actions:

If the physics basis of the code for any reason is found to be insufficient a discussion should be initiated with theory/developers to help improve the situation. This discussion should also be initiated if possibilities for improvements become evident during the review process.

Verification – validity of the computational model

The purpose of the verification procedure is to establish the accuracy and correctness of the computer code implementation of the physics model.

Process and procedure

The verification step requires a description of the numerical implementation to be given and analysed. Both static (code review) and dynamic (convergence tests etc) analysis should be performed and the results documented in detail. Conformance to the Task Force interface standards and published language standards should be reviewed.

Review: The following should be provided for the codes and modules being used.

> **Numerical Implementation:** Provide a description (with references) of the numerical methods and algorithms used in the computational model.
> **Limitations:** A discussion of the limitations and performance of the methods and algorithms used in the model should be given with emphasis on specific features particular to the code compared to other models.
> **Conformance:** Does the code or module adhere to the interface standards defined by the task force? Formal language definitions and accepted coding conventions?

There are a number of steps and tests that can be performed in order to verify the correct implementation of the model and to evaluate the accuracy of a code implementation:

Static analysis: Analysing code to minimize the chance for formal coding errors:

- Review of code listings.
- Exercising static debuggers whenever available.
- Compile code on different systems/compiler combinations as possible using strict syntax checking.

Dynamic analysis: Test code performance with respect to:

- Analytical test cases.
- Convergence tests as appropriate for the application.
- Conserved properties
- Other codes providing the same capabilities (benchmarking)
- Application of other formal test protocols (e.g., Method of Manufactured Solutions)

The results of any code verification should be documented and run scripts, test drivers, data and other related results should be stored electronically and made publicly available.

Evaluation: Based on the code review and testing the following should be provided:

- A detailed list of code input/output quantities for the model
- An evaluation of the impact of any free parameters used in the model.
- An estimate of the accuracy of calculated output quantities.
- Provide a systematic analysis of the differences between models being benchmarked if applicable.

Possible actions: A plan for further verification tests should be defined as needed.

Validation

The purpose of the validation procedure is to establish confidence in the predictive performance of the code through extensive comparisons of simulations with experimental data.

Process and procedure

The validation step requires the validation metrics and other figure of merits to be used in the comparisons with experimental data to be defined. A plan for the validation effort should be formulated based on the information collected in the qualification and verification. Special care need to be taken that the full range of uncertainties to be characterized and propagated through the code(s). The validation plan should be revisited and updated as work progresses through code calibration, physics development and new experimental data becomes available.

Review: An analysis of the validation database with respect to the intended use of the mode or model should be performed

- Review and make a selection of the data to be used in the validation benchmarking
- Identify specific subsets of the experimental data that can be used for detailed physics comparisons in support of the physics benchmarking of the code
- Identify possible gaps in the validation database. Initiate work to expand the database (in collaboration with the data coordinating group) and possibly suggest new experiments to be performed.

The review and analysis of the data should be done with the intended use of the code or model to be validated in mind.

Define: The following items need to be provided.

- Detailed quantitative validation metrics.
- How to incorporate the uncertainties in input quantities and modelling parameters in sensitivity studies with respect to code simulation results as a supplement to the validation metrics.
- A plan for the simulation /benchmarking work to be performed. Making sure that an appropriate subset of the parameter space is explored.

Ideally the simulation results should be stored in an standardized database complimentary to the experimental databases. This has several benefits:

- New validation metrics can be introduced at any pointing the validation process and data simply reprocessed
- New or updated versions or parts of a code can be evaluated in detail against previous versions (code-to-code benchmarking) as well as the full experimental database.

Glossary of terms

Adapted mainly from American Institute of Aeronautics and Astronautics (AIAA), *"Guide for the Verification and Validation of Computational Fluid Dynamics Simulations"*, AIAA G-077-1998.

Validation: *The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.*

Verification: *The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model.*

Prediction: *Use of a model to foretell the state of a physical system under conditions for which the model has not been validated.*

Calibration: *The process of adjusting numerical or physical modelling parameters in the computational model for the purpose of improving agreement with experimental data.*

Modelling: *The process of construction or modification of a model*

Simulation: *The exercise or use of a model.*

Model: *A representation of a physical system or process intended to enhance our ability to understand, predict, or control its behaviour.*

> *A* **conceptual model** *consists of the observations, mathematical modelling data, and mathematical (e.g., partial differential) equations that describe the physical system. It will also include initial and boundary conditions.*
>
> *The* **computational model** *is the computer program or code that implements the conceptual model. It includes the algorithms and iterative strategies. Parameters for the computational model include the number of grid points, algorithm inputs, and similar parameters, etc.*

Error: *A recognisable deficiency in any phase or activity of modelling and simulation that is not due to lack of knowledge.*

Uncertainty: *A potential deficiency in any phase or activity of the modelling process that is due to the lack of knowledge.*