UK Atomic Energy Authority

ExCALIBUR

D3.1 Software Requirements Specification

RB/1 Tokamak Science Requirements Specification

Abstract
This document provides a description of tokamak science physicists' requirements for NEPTUNE. It forms part of the requirements baseline (RB).

UKAEA REFERENCE AND APPROVAL SHEET

	Client Reference:	
	UKAEA Reference:	CD/EXCALIBUR-FMS/0054/RB/1
	Issue:	1.00
	Date:	26 October 2021

Project Name: ExCALIBUR Fusion Modelling System

	Name and Department	Signature	Date
Prepared By:	Fulvio Militello James Harrison Tok Sci	N/A N/A	5 November 2020 5 November 2020
Reviewed By:	Wayne Arter BD		26 October 2021
Approved By:	Rob Akers Advanced Computing Dept. Manager		26 October 2021

Requirement specification for new UKAEA exhaust code (Tokamak Science Perspective):

The new UKAEA Exhaust code needs to be able to capture parallel and perpendicular transport of charged and neutral particles in 3D, full geometry and in a time dependent way. Turbulence should be self-consistently modelled, as well as energy transfer physics between charged particles, neutrals and photons (radiation). While perturbations need to be 3D, a minimal requirement for the code is that it can simulate realistic axisymmetric equilibrium configurations with complex topologies and wall designs. The aim of the code should be to:

1. Efficiently and reliably model exhaust in next generation experiments, like e.g. MAST-U, JT60-SA, and especially ITER (the latter is a stringent requirement for the code).
2. Allow predictive exhaust capability for future reactor relevant machines like STEP or DEMO.

Overall capabilities

- Hierarchical approach with multiple models, going from low fidelity (e.g. laminar fluid and fluid-kinetic runs in 2D) to medium fidelity (e.g. fluid runs with neutrals and turbulence – multispecies, but with reduced number of species) and high fidelity (e.g. full kinetic or hybrid kinetic/fluid runs with turbulence and multispecies approach).
- Numerically efficiency, obtained for example through scalability to large number of cores (given the expected computational resources, the code should be designed to take: $\sim$1 week for low fidelity parametric scans; $\lesssim$1 month for medium-high fidelity runs for advanced design; $\lesssim$3 months for high fidelity physics studies).
- Focus on stability of the code, using (preferably) unconditionally stable numerical schemes and capability to diagnose and re-start failed runs. Ensure a small failed simulation rate for common configurations. Provide ccapability to model exhaust physics all the way from sheath limited to strongly detached regimes;
- Modern software design with modular approach (independent and efficient libraries);
- Ability to integrate with other codes (for example with IMAS);
- Modern visualization tools;
- Accessibility (output easily catalogued and interrogated – big data);
- Version control and user support.

Physics model

- General requirements for the plasma model(s):
  - Equations need to be applicable to arbitrary aspect ratio devices;

- The collision operators between plasma components, plasma and impurities and plasma and neutrals have to be sufficiently accurate to properly describe the radiation generated and the energy transfer between species;
  - Photon opacity effects need to be included in the model;
  - The equations need to be capable of dealing with multiple species in non-trace amounts (at least D, T, He and seeding impurities);
  - The equations should not rely on the Boussinesq approximation;
  - The code should evolve both the electron and ion energy (temperature)
  - It would be acceptable to have only axisymmetric equilibria, potentially corrected through small perturbations.

- For high fidelity simulations:
  - In high fidelity simulations, kinetic/fluid transition for both plasma and neutrals has to be properly captured, potentially using a multi-region approach exploiting different models in different parts of the machine could be considered (for both neutrals and plasma);
  - Boundary conditions need to consider improved sheath physics (collisional & shallow angles);
  - Ideally, the model should be able to treat de-magnetized ions in the divertor region;
  - Electromagnetic effects should be included, but a perturbation approach would be acceptable;

- Neutrals and impurities:
  - Different levels of multispecies capabilities should be considered;
  - In medium to high fidelity models, neutrals and heavy species should be treated fully kinetically (the latter have a large Larmor radius, the former potentially low collisionality and they are not bound by the magnetic field).
  - In high fidelity models, dynamical neutral evolution on the turbulence time scale would be preferable, if possible;
  - Ability to model pumps (either directly or via pumping surfaces) should be included;
  - Pellets the code should enable simulation of, or coupling to models that can model, pellet fuelling.

Physics capabilities:

The code needs to be able to give reliable predictions of:

- Divertor loads:
  - Reliable calculation of upstream particle and heat flux profiles: proper drift physics and upstream turbulence;

  - Divertor turbulence: turbulence spreading in the divertor region, effect of magnetic shear next to the X-point(s) to understand upstream/downstream connection;
  - Multifluid capacity to model radiation and detachment physics;
  - Reliable calculation of the electric field (collisionless physics near the separatrix, proper reflection of neutrals at the target);
  - Able to capture in/out and top/down asymmetries (geometry, drifts, radiation and detachment)

- Wall loads:
  - Should be able to predict filamentary transport and role of hot ion confinement (wall erosion)
  - Should calculate radiation and neutral loads (may require dedicated modules, same for divertor loads);

- Impurity transport, pumping and fueling:
  - Ability to track low (He Be), medium (C, N, Ne) and high Z impurities (W, Ar, Xe) with multiple charge states;
  - Reliable kinetic modelling of neutrals to assess fueling and pumping capacity;
  - Ability to handle non-trace species (D, T, He, seeded species), which requires new closures for the equations (if fluid, beyond Braginskii $\Longrightarrow$ Zhdanov or better);
  - Accurate model of friction forces (turbulence + neoclassical on open field lines);
  - In high fidelity models, the code should be able to simulate localized gas puffs, via injection of neutral particles.
  - Dust the code should enable coupling to codes to simulate dust generation, transport and ablation, via exchange of fluxes and sources.

Geometry

- Ability to handle complex topologies and novel geometries:
  - Capacity to treat different topologies with multiple X-points ($>$2), possibly in a dynamic way, or at least implemented in a way that does not preclude time-varying equilibria being modelled in future;
  - Ability to handle singularities in the grid (null points) or to develop accurate scheme(s) that do not have singularities;
  - Ability to interface with 3D CAD designs of the machine;
  - Capability to handle conformal grids that go all the way to the wall for both neutrals and plasma;
  - Capability to treat subdivertor structures (only neutrals).

References