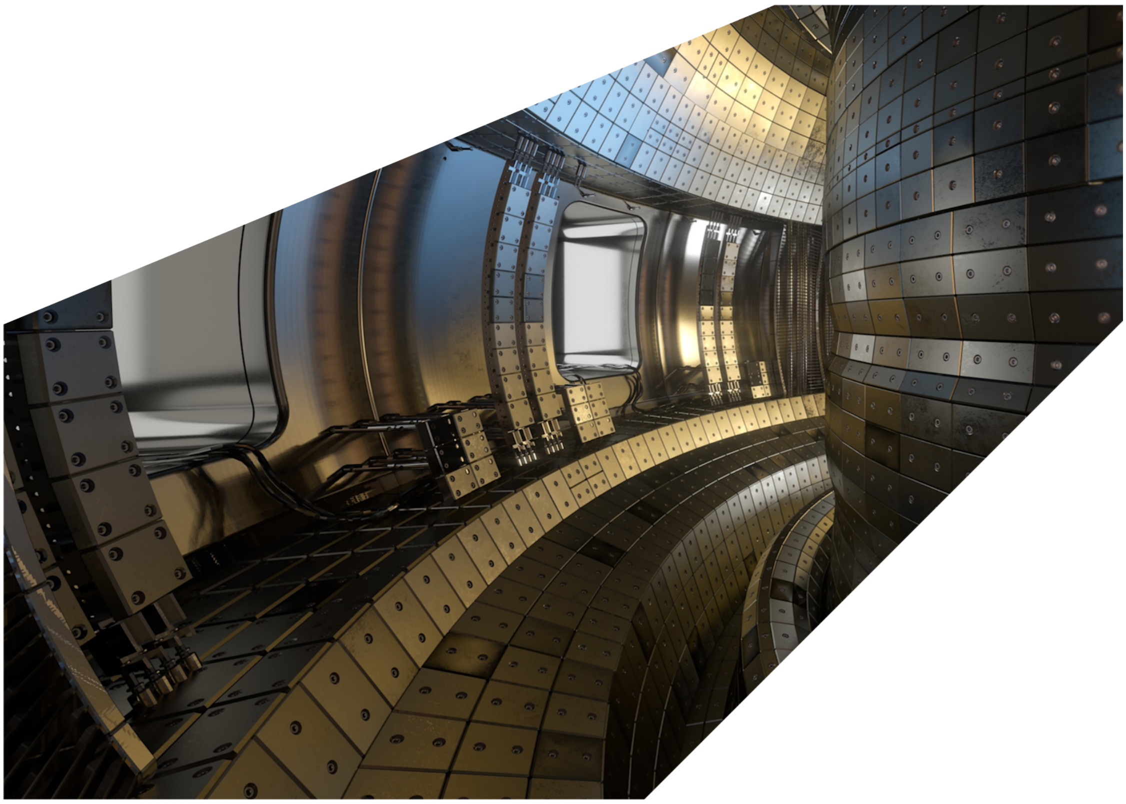
ExCALIBUR

Selection of the physics models

M2.8.1

Abstract
The report describes work for ExCALIBUR project NEPTUNE at Milestone 2.8.1. Minutes of meeting to form report on technical progress.



UKAEA REFERENCE AND APPROVAL SHEET

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1 NEPTUNE Meeting: 20 April 2021 2-3pm BST

Present

- Chair: Wayne Arter, UKAEA
- Felix Parra, Oxford
- Michael Barnes, Oxford
- Sarah Newton, UKAEA
- John Omotani, UKAEA
- Joseph Parker, UKAEA
- Ed Threlfall, UKAEA

2 Minutes

WA started by discussing the recent report '03' by Oxford, *Physics in the edge of fusion devices* [1]. (Two other reports [2, 3] have already been produced.) He commended the very good report, praising an accessible (ie. to other NEPTUNE grant holders) introduction, followed by an authoritative literature survey (4 pages of references). The reviewer had passed the report subject to only minor details. WA thought the focus on drift-ordered fluid models interesting and FP confirmed that this was the approach taken in most of the current state-of-the-art models. WA said the fundamental dimension is the size of the flow ie. the size of the boundary sheath, but mentioned there could be an alternative expansion for higher flows - FP agreed and cited the case where there is a potential difference across the wall (some machines do this eg. rotating mirrors, but not tokamaks; he also mentioned biasing the divertor though this idea seems to have been abandoned years ago for reasons that were unclear). WA said potential differences made performance worse and that the pedestal does not 'like' having flow.

WA moved on to discuss the novel research content of the report; it was not clear what model would be best ie. full gyrokinetics, or drift kinetics with small corrections (easier). FP added that drift-plus-corrections might be acceptable; WA stated that the main worry with this approach is a proper energy conservation relation; however, a cheap model is certainly needed, in order to perform many runs with the aim of assessing the effect of damping terms. WA mentioned that lots of diverging types of calculations were performed in the 1990s. WA suggested formulating the new physics in the form of a variational principle, compatible with new work involving adding a variational-based DSL to NEKTAR++ as part of ExCALIBUR cross-cutting theme work (this could allow the easy passage of the new physics into an exascale-enabled code in the next three years). FP mentioned that there are many variational approaches, automatic differentiation etc. so many possible ways of formulating physics models.

WA returned to his own questions regarding the report and asked FP how he planned to proceed next. FP responded that he proposes to explore three areas where existing work is lacking:

1. Address neutrals, with a charge-exchange operator;
2. Wall boundary conditions;
3. Calculation of the electric field (difficult).

The electric field is obtained from a pressure balance equation and there is a trick in gyrokinetics for calculating it from a small polarization density term. Material on the pressure balance approach is included in FP's first report (the new thing is to try this in the higher-moment approach, meaning the electric field can be derived from the parallel momentum equation). FP is not sure it will work as it involves a rather artificial 'split' of an equation. WA then asked about similarities to the asymptotic-preserving schemes as used by Patrick Farrell; FP said this problem is similar - it involves the asymptotic behaviour of a small parameter (here, the gyroradius) though it does not clearly fall into the strict ambit of asymptotic-preserving problems. WA mentioned that even if implemented using asymptotic-preserving methods, PF's work shows that a degree of numerical ingenuity is still required. It seemed that FP had talked with PF after the last progress meeting to revisit a problem FP had worked on (without success) in the past - it seems they are working on this but there were no details.

WA steered the discussion back to the report; he was a little confused by the discussion of particle methods (a kinetic model may be attacked as a 5-D fluid system or as a particle system). FP stated that the continuum equations are integrable using particles; WA said the the physics suggests this is so but that electromagnetism is then a challenge. FP said his method is not exclusive to fluid or particle approaches; fluid methods are attractive as it is clear how to do a spectral implementation, as in MB's work (there was some confusion about whether a spectral particle code is even possible). The *HAGIS* code [4] (particles coupled to spectral force fields) was cited - Fourier spectral field representation provides a nice cut-off here. WA said he had brought up particles because of sheath effects meaning it is not clear what boundary conditions to use for fluids near the wall. In this context, FP has extended work by Geraldini et al [5] to derive the distribution of ions at a domain end (extension involves replacing adiabatic electrons with kinetic ones); this distribution is input into a (complicated) code by Geraldini that calculates the potential at the wall, and which electrons come back, given the ion distribution at the presheath. WA wanted to understand how this all fitted together. FP said for ExCALIBUR , the full sheath code would be replaced by something simpler eg. assuming ions always leave and that this assumption determines the potential drop, hence a simplified boundary condition. The motivation here was not to start simulations with a full-blown code whose true results are unknown. WA mentioned that PIC modelling could be used to check the outputs of this boundary code. FP agreed and also said the Geraldini boundary code might prove unstable. Regarding PIC coupling, WA asked about how to couple the different representations used in different domains, having talked previously to a worker on the *XGC* boundary code who had admitted that the determination of the sizes of overlap regions was done largely by trial and error. WA had previously mentioned methodological concerns about instabilities in the US *GENE* simulation code. FP expressed his own confusion why there is currently work to couple *XGC* and *GENE*, given that these are both kinetic codes (*XGC* is gyrokinetic PIC and *GENE* treats a 5-D continuum model. WA mentioned that NASA need to solve the particles / fluids dichotomy; he thought *XGC* was best for boundaries and *GENE* for bulk. WA agrees that one can use a continuum representation but worries that collision operators are problematic; further to this, FP asked whether particle methods were better for collisions. WA said that collisions have been done for many years and the trade-off is accurate microphysics but much noise / sampling error; he mentioned it might not be necessary for us to get the momentum balance strictly correct. FP thinks collisions are a problem in PIC too; he sees why the neutronics field uses particle codes but thinks either particle or continuum appropriate for plasmas. WA mentions collisions in fluids are harder because both particles are moving and generally a hard problem to identify a particle 'collision' without using a mesh. FP said particle vs. continuum is not considered in his report. WA said he has never looked into rigorous maths behind this in detail and opined that a definitive theory is needed here. WA then mentioned that in classical fluids, the mean free path is used to determine what overlap is needed (ie. between regions simulated using continuum and particle descriptions) - can this be applied in plasmas? FP opined that he favours fluid / drift models for two reasons: 1) the 11-moment equation can be used to compute the electric field and 2) one has better control over the energy; in different regions of different temperatures, their grids can rescale 'automatically'. There is scope for a diagnostic in this code that detects that the distribution is Maxwellian and triggers use of Braginskii theory. WA mentioned that in space applications, he thought he recollected that the mean free path is used to determine whether a particle description is needed (it is clearly more attractive to simulate a fluid by default and switch unresolved regions to use a more expensive particle description as required, rather than defaulting to particles); NASA applications involve compression and heating near a nose cone giving a hot, collisionless gas (and indeed a plasma). WA asked whether there exists a simple problem using FP's formalism in which the need for a particle description can be detected. FP answered that, in his experience, the need for kinetics is determined heuristically (he used the phrase 'fudge factor'); he noted that even if the mean free path is relatively small, collisionless processes involve high energy particles which can nevertheless contribute significantly to transport eg. heat fluxes.

WA invited FP to talk about his plans for future work and FP handed over to MB, who has implemented a 1+1-D drift kinetic solver which evolves the distribution function, see the '02' report [3]. The results from this agree with kinetic solvers (once they apply 'corrections'). Technical details: implemented in Julia using the FFTW3 library; Chebyshev pseudospectral elements; no explicit artificial viscosity but uses an upwind flux at element boundaries so it has slight numerical dissipation: apparently they deal with this by 're-normalizing' the integral over velocity space so it remains constant. They still want to test solving for the electromagnetic field in this code (this would conclude their work with periodic boundaries). WA mentioned that a similar code could be implemented in MATLAB but that this would run slowly; MB added that JO had tested the Julia code vs. C++ and found little difference in speed.

There followed a brief discussion on DSLs (unfortunately FP and MB missed the recent DSL meeting due to other commitments). WA mentioned that FIREDRAKE is build around Python and it calls C code, giving a possible challenge for integrating NEKTAR++ into the DSL of FIREDRAKE as part of a forthcoming cross-cutting ExCALIBUR bid. MB added that Julia can call C++ or Fortran code.

WA closed the meeting. FP checked it was OK for JO to be a co-author on their publication; WA said there was no issue here so long as the bidding process is seen to be transparent and fair. He reiterated that the aim of UKAEA is to make codes that come out of NEPTUNE as widely-available as possible.

Acknowledgement

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References

[1] F.I Parra, M. Barnes, and M.R. Hardman. Physics in the edge of fusion devices. Technical Report 2047357-TN-03-01, UKAEA Project Neptune, 2021.

[2] F.I Parra, M. Barnes, and M.R. Hardman. 1D drift kinetic models with periodic boundary conditions. Technical Report 2047357-TN-01-02, UKAEA Project Neptune, 2021.

[3] M. Barnes, F.I. Parra, and M.R. Hardman. Numerical study of 1D drift kinetic models with periodic boundary conditions. Technical Report 2047357-TN-02-01, UKAEA Project Neptune, 2021.

[4] S.D. Pinches, L.C. Appel, J. Candy, S.E. Sharapov, H.L. Berk, D. Borba, B.N. Breizman, T.C. Hender, K.I. Hopcraft, G.T.A. Huysmans, and W. Kerner. The HAGIS self-consistent nonlinear wave-particle interaction model. *Computer Physics Communications*, 111(1):133–149, 1998.

[5] A. Geraldini, F.I. Parra, and F. Militello. Dependence on ion temperature of shallow-angle magnetic presheaths with adiabatic electrons. *Journal of Plasma Physics*, 85(6), 2019.