NEPTUNE Workshop 6 September 2022

1 Topic, Location

Topic Physics equations

Moderator, Assistant Sarah Newton, Wayne Arter

Time 11:30am-1pm

Location Abbey Rm, Guildhall

2 Notes

The discussion started with the equations governing atomic processes, when Matthew Barton described the model of radiation he had implemented in the SMARDDA modules as SMARDDA-PFCR, using ADAS data. WA pointed out that it would be more appropriate to take this further in the dedicated afternoon session, and explore other edge-relevant equations in the present session.

Discussion then focussed on the sheath, and in particular how sheath models might be coupled to fluid models of the SOL. There was general agreement that the work of Geraldini et al [1] was state-of-the-art for analytic theory of the magnetised sheath, whereas the work of David Tskhakaya using BIT1 was state-of-the-art for sheath modelling. BIT1 is a 1D3V Particle-in-Cell (PIC) code, although variants that model 2-D and 3-D space exist. There was some discussion of PIC in general, although again it was pointed out that there was a more appropriate breakout session for this. It was not known whether BIT1 was current or charge conserving (WA note: Tskhakaya et al [2], 2010, shows that it likely uses the standard 'charge conserving' formalism because BIT1 is a development of the Berkeley PIC codes which employ a Poisson-solve, and incidentally allow for collisions via Monte-Carlo algorithms. Vasileska et al 2021 [3] have recently 'loosely' coupled BIT1 to SOLPS-ITER.)

Since BIT1 was only 1-D in space, there was speculation as to why calculations using BIT1 could become extremely costly (sometimes days of cpu), was it due to poor coding and implementation, or inherent in physical attributes such as a large number of species, the cost of collision modelling or stiffness due to disparate atomic masses? This lead to a general discussion as to how to treat physical processes that involved very disparate time scales. WA felt that there were stiff ODE solution techniques that were demonstrably adequate (eg. LSODES package as used in UKAEA's FISPACT-II neutronics software https://fispact.ukaea.uk/) for calculating steady states given an almost unlimited range of timescales, provided that all oscillations were well damped over the time of the calculation. Problems remain when oscillations persist over long times, or when accurate transient calculation is needed. WA had seen work by numerical analysts at the SIAM NA20 online conference that addressed this issue, notably Variable Stepsize, Variable Order (VSVO) schemes by Victor DeCaria, and Multirate schemes as reviewed by David Reynolds - this to be investigated further by STFC.

In the context of continuum, particularly fluid equations, the question of collision operators was raised. Simple damping 'Krook' like operators were often used with little discussion as to the implications for accuracy and physical realism (ie. UQ). This led to general discussion about the lack of a consistent derivation of the SOLPS-fluid equations accounting for kinetic effects. The view seemed to be that there were relatively few instances when kinetic effects could be definitely be shown to be untreatable as corrections to fluid models, although this was expected to change with improved models and diagnostics of the plasma edge, when the NEPTUNE-funded work of Parra et al, eg. ref [4] might be expected to bear fruit.

References

[1] 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.

[2] D. Tskhakaya, A. Soba, R. Schneider, M. Borchardt, E. Yurtesen, and J. Westerholm. PIC/MC code BIT1 for plasma simulations on HPC. In *Proceedings of 18-th Euromicro Conference on Parallel, Distributed and Network-based Processing*, pages 476–481. IEEE Computer Society, 2010.

[3] I. Vasileska, X. Bonnin, and L. Kos. Kinetic-fluid coupling simulations of ITER Type I ELM. *Fusion Engineering and Design*, 168:112407, 2021.

[4] F. I. Parra, M. Barnes, and M. Hardman. 1D drift kinetic models with wall boundary conditions. Technical Report 2047357-TN-05-01, UKAEA Project Neptune, 2021. `https://github.com/ExCALIBUR-NEPTUNE/Documents/blob/main/reports/2047357/TN-05.pdf`.