Warwick University: PIC methods.

Note that this is a modified summary of the bid document accounting for modifications that occurred after initial submission, so is intended to present information about Warwick's bid in an easy-to-follow way. That is, this is not a redacted version of the agreed contract document.

1 Purpose of Document

This document provides a statement of how and when the Research Plan's objectives would be achieved, by showing the major products, activities and resources required of the Research Plan.

There are two major products:

1) An exploratory proxy-app, in which disruptive PIC numerical methods will be implemented, and which will also enable UQ exploration.
2) Reports on the feasibility and limitations of the disruptive methodologies employed, and on UQ aspects in PIC.

The single activity, which involves carrying out the research plan, comprises several parts, which may temporally overlap:

1) Literature survey, consultation with relevant experts (e.g. at the Met Office and UKAEA), and draft specification of additional features for the proxy-app.
2) Development of the proxy-app features by the project team.
3) Exploitation of the proxy-app, to determine the practicality and limitations of the potentially disruptive features, and UQ studies.
4) Reporting on these aspects, to enable this work to be integrated within the ongoing NEPTUNE project.

Timing of individual work elements is described in detail in the list of milestones, the overall project leads will be responsible for ensuring on-time delivery of milestones, and redeploying effort as required to ensure full delivery before the end of the 9 month project period.

Resources required are the following

1) A proportion of the time of each of the project participants.
2) Access to journals, which will be provided by the University of Warwick
3) Access to desktop PCs and workspaces, which would normally be provided by the University.
4) Access to workstation-level HPC, which is provided by the university.

There are two major objectives, which we will now provide contextual information on, including some relevant literature, and describe in detail.

Objective 1: Co-design.

We will work together, early-on in the project, with other successful co-bidders to determine whether the proposed particle methods will be compatible with the proposed fluid methods and adapt them as needed. Due to the very short timeline of the project, it is however necessary to work in parallel on other aspects of the project on the assumption that such adaptions will be possible and relatively minor. We will also need to, as part of the work towards this milestone, develop familiarity with the spectral-hp method and the chosen software infrastructure in which it is embedded (e.g. Nektar++). This milestone will assume the availability and willingness of the lead organisation and other relevant successful bidders to commit time and resources early-on in the project. We note that coupling between PIC methods and fluid methods has previously been achieved, and we think that the advanced-PIC aspects and advanced-fluid aspects of the project should in-principle be compatible. The basic PIC algorithm itself is quite flexible in terms of grid and field representation (e.g. high order finite element methods are common e.g. ORB5), and the proposed PIC extensions are not highly sensitive to the choice of field discretisation.

We will also work with the other successful bidders to examine how the gyrokinetic theory of interest may be implemented in a kinetic scheme, and which features of PIC algorithms need to feed in to the design of the uncertainty quantification.

This work will initially be expected to involve literature search, discussions with other partners, and training of staff, for example on PIC and Spectral-HP methods. This will allow the best approaches to the couplings between these NEPTUNE subprojects be identified, which will be described in the milestone report.

Objective 2: Implicit timestepping and transformative PIC algorithms

The finite-difference time-domain (FDTD) method is the de facto industry standard time-integration algorithm for particle in cell (PIC) codes. However, its temporal stability constraints render it inefficient for modelling systems with a large disparity in timescales, where implicit [e.g. 1, 2] or semi-implicit [3] methods are preferable. Additionally (semi-)implicit methods can provide physically desirable behaviour, such as energy conservation, which explicit time-integration methods cannot.

Leveraging implicit PIC methods on Exascale systems is unlikely to be straightforward. In addition to the algorithmic considerations relevant to explicit PIC, implicit PIC requires the efficient inversion of a non-linear system. Interestingly, both Chen et al. [1] and Markidis and Lapenta [2] utilise the Jacobian-free Newton-Krylov (JFNK) method. JFNK methods do not explicitly form the Jacobian matrix, thus avoiding the high-memory requirements of conventional implicit methods. A third possible time-integration method is the semi-implicit method of Lapenta [3], which offers the advantages of implicit methods (no temporal stability constraints, exact energy conservation) whilst maintaining the lower algorithmic complexity of explicit methods.

Unfortunately decoupling the performance benefits of existing methods from the differences arising from data-structures, linear-solvers, and numerous other implementation details is at best difficult, and at worst impossible. In order to disentangle these issues, we are proposing to produce a prototype mini-app to assess the relative merits of different algorithms, whilst using the same underlying computational framework. The choice of time-integration algorithm is complex. Even restricting the discussion to JFNK based time-implicit methods using particle enslavement, one must decide on a method to solve for the enslaved motion, for example the Picard method [1] and the Newton-Raphson method [2] have both been used. Furthermore design decisions regarding spatial filtering, particle substepping, and even the possibility of preconditioning the JFNK system must be made. As JFNK methods don’t explicitly form the matrix, these methods typically require bespoke physics-based preconditioners (e.g. [4-5]).

The questions raised in the preceding paragraph are far beyond the scope of this initial nine month study. Instead this work package will deliver a key first step for further work, an extendable, easily deployed, time-implicit mini-app, upon which future investigations and comparisons can be built.

Especially in a tokamak context, the rapid gyration time can be an equally or more severe limit on the particle timestep as an explicit field solve. To overcome this limitation, several methodologies have been developed, including substepping and gyrokinetic techniques. Particle substepping is known to be compatible with implicit methods in general, and, although it increases in computational complexity per particle per timestep, does not require significant additional memory bandwidth so is appealing on the pathway to exascale. Both a reduced (simplified, long-wavelength) gyrokinetic particle tracking method and direct substepping will be implemented in the PIC mini-app and compared, as a full-scale integrated edge code will likely have particles of such widely varying gyrofrequency/gyroradius that both types of methods will be required.

Low-noise particle methods generally depend on improved sampling of the particle velocity space and on knowledge of an appropriate underlying smooth distribution function. One way to do this is via fluid-entrainment techniques. A control-variates method has been implemented in EPOCH, and this will be ported to the EPOCH-miniapp; an extension to allow background evolution consistent with the fluid equations (closed with PIC moments) will be implemented and investigated.

[1] Chen, Guangye, Luis Chacón, and Daniel C. Barnes. "An energy-and charge-conserving, implicit, electrostatic particle-in-cell algorithm." *Journal of Computational Physics* 230.18 (2011): 7018-7036.

[2] Markidis, Stefano, and Giovanni Lapenta. "The energy conserving particle-in-cell method." *Journal of Computational Physics* 230.18 (2011): 7037-7052.

[3] Lapenta, Giovanni. "Exactly energy conserving semi-implicit particle in cell formulation." *Journal of Computational Physics*334 (2017): 349-366.

[4] Knoll, Dana A., and David E. Keyes. "Jacobian-free Newton–Krylov methods: a survey of approaches and applications." *Journal of Computational Physics* 193.2 (2004): 357-397.

[5] Chen, Guangye, et al. "Fluid preconditioning for Newton–Krylov-based, fully implicit, electrostatic particle-in-cell simulations." *Journal of computational physics* 258 (2014): 555-567.

2 Benefits and alignment to Work Package objectives

Please evidence below how the submission aligns to the Work Package objectives outlined in Part 1 Section 2.3.

This submission directly works towards several of the objectives in Part 1 Section 2.1.

Firstly, the issue of timestep limitations in particle tracing will be tackled by both advanced particle update schemes and an implicit time-solver for the coupled field-plasma problem that is, it addresses the ‘task work’ described in section 2.3 and 2.4. In addition, low noise techniques, including low-dispersion sampling, and control variates will be explored, probing the questions in section 2.2 of the task work.

As required by the call, each disruptive approach tested will be examined by performing appropriate literature surveys, and by implementing proof-of-principle code in the PIC proxy-app. The overall findings will be documented to determine their applicability in NEPTUNE.

We will provide the (existing) PIC proxy-app to the broader community and support its application and use by NEPTUNE participants to deliver the broader project aims; in particular, this will allow HPC experts to explore the HPC and scaling aspects of PIC algorithms.

3 Scope

3.1 Key Deliverables and/or Desired Outcomes

1) Write a report addressing co-design aspects related to PIC, particularly with respect to spectral-HP.

2) Implement an implicit electromagnetic solver, advanced low-noise methods, and advanced particle tracing (to mitigate restrictions due to the gyro-time) within a PIC mini-app, report on issues, and identify potential solutions.

3.2 Exclusions

Activities/topic areas that are out of scope of the Bid and which will not be undertaken (may also include things that Bidder would like to do but are not currently in scope)

1) Examine coupling of fluid methods to PIC.

2) Examine interface of PIC with spectral-HP elements scheme. This may be performed outside the bid framework as a PhD student is currently investigating advanced Galerkin-type representations for the purpose of representing anisotropic variations.

3) Some aspects of PIC data storage and sub-MPI task tiling to mitigate memory-throughput related performance limitations were investigated on historical HPC using the EPOCH mini-app [1] [2]. Reviewing and extending work on data layout and locality with reference to advanced HPC would thus be a natural extension of the proposed work but we don’t have experience staff available to perform this at the moment.

[1] Bird, Robert F., et al. "Mini-app driven optimisation of inertial confinement fusion codes." *2015 IEEE International Conference on Cluster Computing*. IEEE, 2015.

[2] Bird, Robert F., et al. "Performance Optimisation of Inertial Confinement Fusion Codes using Mini-applications." *The International Journal of High Performance Computing Applications* 32.4 (2018): 570-581.

3.3 Constraints

Restrictions that affect proposals of the project by imposing limitations such costs, resources or project schedule, which may affect the execution of the Bid.

- This project is designed to feed in to a collaborative activity and potential fusion of the PIC method explored here with a range of other approaches for specification of a complete edge model. This bid was prepared without a clear picture of these elements, and in the absence of a clear strategy for this process to occur.
- The tight project schedule, with certain milestones due within the first three months, probably precludes any significant modification to the project plan, or significant renegotiation of milestones etc., after the start date, without substantially impacting on the scope of the work.

4 Approach

Describe how will the work be undertaken, including a definition of methodology that will be used in the project to deliver the work package and call objectives.

Numerical science will commence with a review of the relevant literature, for work-packages where there is not an existing identified numerics strategy. This will be a collaborative process chaired by Ben McMillan and Tony Arber. To give an example where value for money can be provided by short-circuiting this process, the implicit field solver ties in with an existing project of a project member (Tom Goffrey) and this literature review and identification of the numerical methods is already complete; the implementation in the PIC proxy-app thus can begin immediately.

We note that there is an existing proxy-app based on a heavily simplified version of the EPOCH PIC code, developed by several of the team members: this combination of experience and existing code-base allows rapid pursuit of the advanced numerics targets. Indeed, this code has previously been used to examine scaling and data-arrangement issues on earlier-generation architecture.

The numerical algorithms chosen to meet the milestones will be fed into a streamlined software engineering process to allow agile development of proxy-app extensions. A lightweight code specification will be developed by the lead on each milestone, and approved by the lead scientists.

5 Activity Plan

Identify activities plans for the Research Plan (please add and use as many activity templates as required into the document and complete Annex B with schedule). Please include any relevant planning assumptions.

We note that Annex B was not included as part of the bid documents: the work schedule may be inferred from the below.

Duplicate this table for each Activity	**Activity No**	**1**
Activity:		

Exascale PIC **Assignee:** Ben McMillan		
Objective 1: UQ for PIC methodology. **Objective 2:** Implicit timestepping.		
Key Deliverables: **1) Report on findings of codesign process and implications for further algorithm development.** **2) Implement advanced methods (low-noise methods, implicit field solver, advance particle tracing) within a PIC mini-app.**	**Start and Completion date:** **1) 01/01/2021 – 20/03/2021** **2) 01/01/2021 - 01/09/2021**	**Assignee:** **1) Ben McMillan** **2) Tom Goffrey**
Milestones towards deliverables: **1) Report on co-design.** **2) Implicit field solver baseline implementation in mini-app.** **3) Advanced particle orbit solver implementation in mini-app.** **4) Low noise techniques implementation in proxy-app.**	**Completion date:** **1) 20/03/2021** **2) 01/09/2021** **3) 20/03/2021** **4) 01/09/2021**	**Assignee:** **1) Ben McMillan** **2) Tom Goffrey** **3) Ben McMillan** **4) Ben McMillan**

10 Financial Schedule

10.1 Payment schedule

Activity number	Milestone number	Payment Value	On completion of associated activities (please provide relevant activity number) *	Start Date	End Date
2	3			04/01/2021	01/09/2021
			Associated Output of Milestone: Mini-app with implicit field solver baseline implemented. Dependencies: none		
	4			04/01/2021	20/03/2021
			Associated Output of Milestone: Mini-app with advanced particle orbit solver implemented. Dependencies: None		
	5			04/01/2021	20/03/2021

			Associated Output of Milestone: Low-noise control variates implementation in proxy-app. Dependencies: None		
1	6			04/01/2021	20/03/2021
			Associated Output of milestone: Report on findings of co-design process, assessing the impact of spectral-hp fluid and gyrokinetic/drift-kinetic model on design of advanced PIC methods. Dependencies: none		
	Total Value:				