Agenda, 14 January 2021

- Wayne Arter, UKAEA 9.05-9.20 Introduction
- Ben Dudson, York 9.20-9.45 Plasma fluid referent model via exploratory proxyapps
- Steven Wright, York 9.45-10.00 Investigate DSL and code generation techniques
- —Break—
- Dave Moxey, Exeter 10.20-10.50 Performance of Spectral Elements
- Felix Parra, Oxford 10.50-11.10 Referent model for plasma edge region
- —Break—
- Peter Challenor, Exeter 11.20-11.35 UQ (UKAEA funding outside ExCALIBUR)
- Sue Thorne, STFC 11.35-11.50 Investigate matrix-preconditioning techniques
- Peter Coveney, UCL 11.50-12.05 Study of Uncertainty Quantification (UQ) techniques
- Serge Guillas, UCL 12.05-12.20 Study of Model Order Reduction (MOR) Techniques
- Ben McMillan, Warwick 12.20-12.35 Optimal Use of Particles
- —Short break—
- Discussion 12.40-end

*Slides of the talks, where subsequently submitted, appear as files listed by first speaker's surname.

Rob Akers PI Neptune in chair

indicated that the importance of this meeting to the project as two-thirds of Neptune was to be sourced outside UKAEA. In particular, the presenters should explain their proposed contributions to Neptune, concentrating particularly on first 6-9 months.

Wayne Arter

was introduced as technical lead for Neptune. [The script for Wayne Arter's introductory talk appears in this (KOM) directory as intro_wa.md (Markdown format).] He thanked the attendees for their bid work and remarked upon its high quality despite the circumstances. He emphasised that the attendees should take the opportunity in the next few months to examine options for the software, as by late summer 2021, Neptune needed to be transitioning to a full-on software development phase.

Ben Dudson

focussed on the most complicated model in his portfolio, which includes nonlinear, time dependent, highly anisotropic tensor coefficients, and the challenges presented to finite elements, notably SHP (spectral/hp element). He particularly indicated the relationship with the work packages of other presenters, nicely summarised on one slide:

- Conventional neglect of the (speed of) light-timescale leads to an elliptic problem for the electric potential which may be a major bottleneck, hence good preconditioning important.
- Sources from the particle model involve reaction rates with uncertainties.
- The multispecies aspect leads to additional complexity where DSL could be helpful.
- The kinetic proxyapp would benefit from development of a gyro-averaged model.

Peter Hill (dudson.pdf)

explained the Excalibur-Neptune github 'organisation' which he was setting up, as an "umbrella" for entire project, so that the downloader of Excalibur-Neptune/Neptune gets all the software used by the project. Individual repositories (repos) become submodules of the github organisation, e.g. Documentation, with Nektar++ expected. The project encourages use of a common open-source licence BSD 3 - "do what you like, but must acknowledge, and not use name if change source" All issues should be raised in Excalibur-Neptune/Neptune, and classified as "being done", "done" etc. The standard github development workflow was explained, with a recommendation for test-driven development, with automated testing by github actions. A common code style will be enforced using clang-format or black, and the recommendation is to use latest language standards such as C++20 and Fortran 2018 as far as Exascale machines permit.

Discussion

Slack was mentioned for user feedback. Peter Coveney provoked a discussion on accessible HPC hardware. Rob Akers explained that all bid respondents offered to use their own machines, and noted that UKAEA was contributing £1M per year to CSD3 (Cambridge Service for Data-Driven Discovery) for use under DiRAC so that 6000 cores of Cascade Lake were available and 2 racks of the latest 60Gbtye Nvidia Ampere cards were to arrive in Spring. Neptune may however also have to use ARCHER2 because of "turbulence" in EPSRC budget. Peter Coveney stated that Europe will have 3 machines comparable to US Summit this year, but UK use of these machines is subject to negotiation.

Steven Wright

introduced himself as from York Computer Science dept. His task was to coordinate code development and set standards, beginning with a survey of available hardware and software, including DSLs and proxyapps particularly ones directed towards software with characteristics of BOUT++ and Nektar++. The metric to be used was due to Pennycook, Sewall & Lee et al Future Gen Computer Systems 2019 https://doi.org/10.1016/j.future.2017.08.007 He expected coordination, especially when related to providing a programming model, to involve extensive user feedback, to be provided via Slack.

Introductions at Break

- Chris Cantwell introduced himself as having 10 years' experience of spectral elements, intending to be working on proxyapps for Neptune.
- Gihan Mudalige introduced himself as working on several Excalibur projects, for Neptune specifically DSLs.
- Nigel Woods introduced himself as looking after the science side of the Met Office's weather and climate Excalibur use case, and publicised recent appearence of the Excalibur cross-cut call.
- Louise Kimpton introduced herself as a recent Peter Challenor PhD, who had just become a postdoc working with Tim Dodwell.

David Moxey

with Chris Cantwell and Spencer Sherwin, will focus on a prototypical 2-D anisotropic heat transport problem. He gave a brief introduction to spectral/hp element methods (SHP) with reference to techniques for generating meshes with curved edges and surfaces, notably by variational weighted optimisation within Nekmesh (weight corresponding to linear- or hyper-elasticity or Winslow or Laplacian smoothing). He illustrated mesh r-adaptation including nodes that slid along a surface, with particular reference to treating the vicinity of the X-point for Neptune. Concerning the spectral element calculation, he planned to extend efficient matrix-free implementation from x86 to GPU and other architectures. Regarding engagement with other partners, he mentioned use of CWIPI for code coupling. He also introduced Nektar++ as a open-source framework for high-order finite element methods for wide application, and mentioned recent developments facilitating use by docker, and Jupyter (nearly complete, but remaining a work in progress) with continuous delivery as well-advanced, for automating the entire software release process. He advertised a vacancy for a post-doc to work with him on Neptune.

In response to Rob Akers' question regarding adaptive meshing, David Moxey indicated that he was developing adaptive r-refinement, but that he currently mainly used p-adaptation, with a longer term plan for coupled h-adaptation driven by errors detected in the numerical solution. Replying to Wayne Arter, he agreed that training needs should be expressed via Slack channels, and although difficult for Dave Moxey to address in short terms beyond say a two-hour seminar, things should ease after say Easter, when other Nektar++ project members should be able to help. In response to Rob Akers' question regarding separation of concerns, Dave Moxey stated that combining e.g. Kokkos with pre-existing code such as Nektar++ could be difficult. Two possibilities to be investigated were the identification of kernels that could be optimised for GPU, and better memory management based on discussions planned with Nvidia. Rob Akers encouraged discussion of separation of concerns.

Felix Parra

apologised for absence of Michael Barnes and postdoc Michael Hardman due to teaching commitments, and introduced himself as a physicist principally concerned with analytic calculation. He explained that kinetic effects matter when lack of collisions means that contributions from particles distant from a point are important at the point, and plasma has additional complication of electromagnetic (EM) effects. Collisionality is low in the core plasma, and the fluid approximation may also break down in the divertor where electrons (and ions) are energetic and so collide less. He does not think a simple fluid model with corrections will be adequate. Plasma presents the problem of quasi-neutrality when the light timescale is neglected, which implies that there must be a very accurate balance between positive and negative charge in the plasma. Plasma confinement by large magnetic field B implies a short lengthscale of gyro-radius of ion motion which can be avoided by gyro-averaging, likely best done analytically. He presented a schematic form of kinetic equations noting the appearance of the perpendicular drift velocity resulting from gyro-averaging. The tininess of any net charge implies not only a near-solenoidal electric field E, but also a near divergence-free current, and there results a very stiff equation for the time evolution of the electric potential. The aim of his analytic approach is try to avoid this stiffness by splitting particle distribution function into kinetic and fluid parts in a special way indicated.

Wayne Arter's question revealed that Felix Parra's fluid is not necessarily Maxwellian. The deviation of the particle distribution function from Maxwellian is very involved in the core but probably more simply skewed in the edge region. Though the electric field may be large in the edge, it is believed that quasi-neutrality fails only on short electron timescales. As a result of question by Rob Akers, Ben Dudson mentioned the existence of Swiss work on gyro-averaged models for the plasma edge.

Rob Akers emphasised importance of UQ to UKAEA programme going forwards, consequently that Peter Challenor was present as a result of funding directly from UKAEA budget.

Peter Challenor

defined the direct problem y=f(x), and the inverse problem as, given measurements of y to find corresponding x. Uncertainty Quantification (UQ) was defined as the subject of treating prediction with uncertainty, sensitivity analysis, uncertainty analysis, and inverse modelling with uncertainty. Fast models use Monte-Carlo (MC), Markov Chain MC (MCMC), and Quasi-MC (QMC). To proceed with slow problems need to produce fast surrogates that include a measure of uncertainty, referred to as 'emulators'. Neural networks (NNs) tend not to include uncertainty measures, hence Gaussian Process Emulation (GPE) preferred.

- f(.) as a sum of a mean function + zero mean Gaussian Process (GP) with covariance function C(.,.) + 'nugget' is white noise term.

C(.,.) may be Gaussian in cases of smooth f. For more irregular f behaviour, the square in the Gaussian should not simply be replaced by modulus but rather the Gaussian replaced by a special function after Matern. Priors for GPE are form of mean function (which could be a Fourier series or polynomial), C(.,.), and the nugget amplitude. Analysis typically proceeds by designing a training set, building the emulator, and validating use LOO = "leave one out" or by conducting other experiments. Designs use Latin hypercube sampling, Sobol, sequential sampling. Emulation may not work because of model discrepancy. The widely used approach of Kennedy and O'Hagan has problems that means Peter Challenor prefers to use "History Matching", also this has problems of statistical interpretation and also caused by empty sets of NROY= "not ruled out yet". History matching can cope with hierarchical models and with a mix of fidelities. Rob Akers indicated work could be useful to STEP, was reassured that the use of Gaussians ensured extrapolation beyond boundaries of the data prevented dramatically divergent behaviour, however it did pose difficulties for imposing positivity constraints.

Sue Thorne

gave apologies for Anton Lebedev and Emre Sahin. Preconditioning speeds iterative solution of Ax=b for x, find B= inv(P) A so By=c goes faster for y= inv(Q) x. Coupling is an important issue, gives rise to a block structure in A to try to exploit. Preconditioning within a block may use knowledge of physics of system (elliptic/hyperbolic, elliptic particularly allows use of multigrid) or involve SPAI (sparse approximate inverse) or use MCMCMI (MCMC for approximate matrix inversion) to approximate inv(A). Neumann series for diagonally dominant matrices, implemented using MPI, OpenMP and range of GPUs, see Vassil and Vassil https://ieeexplore.ieee.org/document/8638012, outperforms MSPAI (Monte-Carlo SPAI). Implicit-factorisation to treat both loosely and strongly coupled, also hope to examine novel reduced subspace iteration. Example of a 3x3 block system where 3rd row and column specially constrained. Rob Akers' question revealed MCMCMI as a new (2018) and exciting approach. Patrick Farrell asked how MCMCMI worked matrix-free, but the STFC team were momentarily unable to provide a detailed answer, and it was suggested by Rob Akers that the question be pursued via Slack.

Peter Coveney

introduced Maxime Vassaux, who revealed he had MD experience coupling particle and continuum models for materials. Objective to recommend UQ techniques for Neptune longer-term, and for workflows, not only EasyVVUQ which is being developed under Framework programme project VECMA but also Multi-output GP (MOGP) from ATI. V & V as verification (that equations are correctly solved) and validation (by comparison with experiment). [Barry Boehm defines validation as answering the question "Are we building the right product?", and verification as "Are we building the product right?"]

Two classes of uncertainty recognised, namely

- Systemic - uncertainty in parameters
- Aleatoric - random, stochastic contribution

He publicised UQ Neptune workshop on 18/1/21 and VECMA Hackathon 19/1/21 where attendees should find EasyVVUQ to be "easy" to use. VECMA is an open development (notably involving Coster and Lakhlili from the German fusion lab IPP), producing a modular toolkit called VECMAtk which allows complex workflows and includes "Pilot job" for managing a campaign, typically an ensemble of UQ calculations. He described two pieces of work applying VECMA to (1) high systemic uncertainty - Neill Ferguson's Covid-Sim about 15 minutes on single node, noting the importance of parameter identification, finding 940 which were reduced down to 20 significant ones by expert discussion and a dimension adaptive methodology, see Edeling et al https://www.researchsquare.com/article/rs-82122/latest.pdf and (2) high aleatoric uncertainty - MD simulation using 2 million core-hours, identifying most important parameters.

Serge Guillas

Introduced Deyu Ming, joining the project on 1st February, who revealed he has been working on statistics of coupling tsunami to earthquake. Serge Guillas noted Deyu's linkage via earthquake modelling work with Eric Daub, and his own Met Office link. He emphasised the n-cubed scaling of GP fitting if f n-dimensional, and two publications related to MOR, for

- Dimension reduction, see Liu & Guillas - http://www.siam.org/journals/juq/5/M109064.html, and
- Sequential design, see Beck & Guillas http://www.siam.org/journals/juq/4/98961.html, where parameters are chosen on the basis of previous simulations.

1. Dimension reduction of outputs (wave heights) in Cascadia tsunami temporal problem, using Outer product emulator (OPE) f = Sum (alpha g) + e , alpha=Sum (beta g) where choice of basis g may be splines, polynomials etc depending on problem. Use of functional principal components beats Fourier, as validated by LOO. OPE also successfully applied to a spatial problem, namely parameterised gravity waves from NCAR climate model CSM which is 1.2M lines of code, calibrating using spherical harmonics.
2. Dimension reduction of inputs (sample sea depths) in tsunami prediction using synthetic bathymetry, where 150 training runs reduced 3200 inputs to 5, then emulator was built using gKDR (gradient-based kernel dimension reduction). This approach was compared with others on a range of test problems and generally found to be superior.
3. In MOR for multi-physics or even multi-disciplinary applications, it was found to be very powerful to use knowledge of components of system to construct a "linked emulator" (term now preferred to "integrated emulator" as used in the slides), see Ming & Guillas https://arxiv.org/pdf/1912.09468

Ben McMillan

with Tom Goffrey, advised by Tony Arber with computational expert Keith Bennett. Ben McMillan described use of particles to deal with kinetic effects, noting the usefulness of reducing 6-D phase-space to 5-D by gyro-averaging, here solving the resulting problems by a Lagrangian (particle) method, cf. Felix Parra is using Eulerian approach. Ben McMillan described a PIC (Particle-in-Cell) code, where (macro-)particles are driven by an electromagnetic (EM) force, using an EM field calculated typically on a finite difference grid. He referred to Arber's 2015 review article https://iopscience.iop.org/article/10.1088/0741-3335/57/11/113001 which acts as a reference for Warwick's EPOCH (6-D) PIC code, important as Neptune work will employ an EPOCH proxyapp. [The review by Wayne Arter http://dx.doi.org/10.1088/0034-4885/58/1/001 although older covers particle modelling for fusion in Sec.3.] Ben McMillan explained how gyro-averaged (5-D) PIC moves "rings of charge", and how he has extensive experience of the implementation in ORB5 software, which will be transferred to EPOCH proxyapp. Ben saw his project work as intended to demonstrate proof-of-principle for algorithmic features of particle substepping, Jacobian-free Newton-Krylov (JFNK) for implict PIC solution, gyro-averaging, delta-f (control variates as perturbations to fluid model), and ultimately to help design coupling to SHP.

Concluding Remarks

[The slide Wayne Arter presented at this point is joined to the end of his introductory talk slides.] Wayne Arter in points arising, noted that presenters were allowed to edit slides before they became part of the Neptune "archive" however ultimately defined. He recommended training in git for all but the most experienced users. He drew attention to the "sub module" repo Excalibur-NEPTUNE/Documents, particularly a collection of acronyms and symbols in subdirectory tex He emphasised that at least for the current FY, project reporting would be lightened as far as possible, to help with consequences of lockdown.

Rob Akers thanked presenters and encouraged submission of slides within the week, reminded attendees that Neptune was a £5M project continuing until at least 2024. Invoices should be in by 19th March, slides presented at the March workshop acceptable as deliverables provisionally. Peter Hill mentioned that readthedocs will have to be public, so in Neptune subdirectory of Excalibur-Neptune, suggested acronyms and symbols moved to readthedocs.