Monday 20 November

Session 1 - Introduction Lectures I

1.1 - (Invited) Introduction to computational plasma physics
T Arber
University of Warwick, UK

1.2 - (Invited) Software practices in computational science
R Guichard
University College London, UK

Research Software Development group, Research IT Services, London WC1E 6BT, United Kingdom In this talk, I will overview current software practices and actions that are now in place in the development of scientific codes for research. Through the emergence of the UK Research Software Engineer (RSE) community, to concrete examples and teaching events, the academic sector now acknowledges the value in quality, reusable and sustainable software. These software practices have now become inseparable from the expected reliability and reproducibility requirements for high-standard research outputs.

1.3 - (Invited) Trends in computer science for scientific high performance computing (HPC)
P Gillies
ECMWF, UK

It has now been more than 10 years since the end of ever increasing processor clock frequencies. Up to that point improved performance was almost guaranteed since any new processor would have a higher clock frequency than the previous generation. Those days are now long gone. Since then processor manufacturers have continued to deliver increased performance instead providing multiple cores on a single processor die. Now we are routinely seeing more than 20 cores on a standard processor for HPC. This has meant that scientific programmers wishing to make use of the increase in performance on a processor must ensure that their applications expose sufficient parallelism to be able to scale to higher numbers of cores. To further increase the performance of processors, wider vector units are being added to increase the number of floating-point operations that can be carried out at each clock cycle. To achieve the peak performance of a processor, programs must be able to vectorise so that they can use these vector units.

There are a number of ways to use the multi-core capability of modern processors. The first assumes that an application is already able to run in parallel, perhaps using the Message Passing Interface (MPI). With multi-core processors the program can just treat each core as a separate processing element. Requiring little additional effort it is clearly an attractive option, however it relies on the program being able to scale to much higher numbers of MPI ranks for a given problem size. For some applications that can scale to very
large numbers of MPI ranks this may be sufficient, however others may not be able to scale so well. An
alternative approach is to explicitly program for multi-core processors. The dominant programming model for
on-node parallelism is OpenMP. OpenMP is a shared memory parallel programming model. Since all the
cores in a multi-core processor share the same memory an OpenMP thread can run on each core, with all
threads working on the same memory space. It is possible to use both MPI and OpenMP together in a hybrid
fashion to control parallelism both within the node and between nodes.

Vectorisation allows the same operation to be carried out on multiple data elements in a single instruction.
Generation of the vector instructions is done automatically by the compiler, but only if the program is written
in such a way that operations can be done in parallel. For example, a loop can be vectorised if it is valid for
multiple iterations to be performed simultaneously. This can’t be done when an iteration depends on the
result from an earlier iteration, in this case the loop would have to be executed in serial.

In addition to the trends in processor technology it is important to take note of the trends in memory
technology as these too have a significant impact on the performance of HPC applications. Before a
processor is able to perform any floating-point operations it must load that data in from memory. The DDR
memory in current HPC platforms takes tens of processor clock cycles to get data from memory, whereas
processors can perform up to 32 floating point operations per cycle. This could lead to programs not
achieving the full performance of the processor. There are high bandwidth caches on the processor to help
mitigate this latency, but without efficient memory access patterns in the application performance will be
limited by the memory bandwidth of the system. This is the scenario faced by many scientific codes whose
performance is limited by the memory bandwidth of the system rather than the floating-point capability of
the processor. It is therefore important for developers to understand and optimise for efficient memory
access, maximising the use of data while it is in cache.

With every generation of processor it is becoming ever more challenging to achieve high performance.
Scientific code developers must have an understanding of how these processors operate if they are to
develop efficient code.

Session 2 – Introduction Lectures II

2.1 - (Invited) Introduction to PIC methods
H Ratcliffe
University of Warwick, UK

Particle-in-cell codes aim to simulate the full behaviour of a plasma and its interactions with EM fields. They
do this by approximating plasma particles as small “clouds” with single centre-of-mass velocity, moving
through a grid on which fields are defined. This talk aims to introduce the basics of PIC methods; introduce
some of the more advanced concepts essential to an efficient, correct code; and give a brief overview of
some of the limitations and things to beware of when using these codes, along with the practical
considerations for using a PIC code in your research.
2.2 - (Invited) Advanced techniques for accuracy and speed of novel particle accelerator concepts

J Smith
Tech-X, UK

The standard Yee-Cell PIC as applied in 3D to full scale laser plasma interaction and particle acceleration problems is too computationally expensive for many problems, even when using leadership class facilities. This presentation will outline extensions to the FDTD PIC method to allow it to compute faster, or with more accuracy for extreme cases, such as the beam frame poisson solve. Lorentz boosting, and the envelope approximation are discussed in the context of field advancement, and next generation particle pushers are discussed.

2.3 - (Invited) Gyrokinetics, and the control variates (delta-f) method for general plasma physics problems with small fluctuations.

B McMillan
University of Warwick, UK

We first introduce the gyrokinetic formalism for describing low-frequency dynamics in magnetised plasmas, most typically MCF devices (e.g. tokamaks and stellarators). Gyrokinetics allows much faster simulations of behaviour below the cyclotron frequency as they solving for the drift motion of rings of charge, so that gyration does not need to be explicitly modelled. This formalism may be implemented numerically via Lagrangian (i.e. Particle-In-Cell) or Eulerian methods. We will explain how to implement gyrokinetics in a PIC code: the main barrier is the relatively large amount of numerical noise in a naive implementation, when compared with the small fluctuations typically present in MCF plasmas. This brings us to the second part of the talk, which is a means for reducing noise levels in PIC codes, the control variates method, also known as delta-f. The idea in control variates is to exploit the knowledge that the perturbed distribution function, f, is close to some known analytic distribution function, f₀, and to use the markers (computational particles) to evaluate the moments (currents and charges) of δf = f - f₀. The overall currents/charges in the system can then be found by adding the analytically known currents/charges due to f₀. This leads to much lower overall numerical noise, with RMS levels reduced by a factor of (δf/f). We illustrate the use of the control variates method with some results from the gyrokinetic PIC code ORB5 and the general plasma PIC code EPOCH.
3.1 - (Invited) Continuum vlasov solvers

A P L Robinson
Central Laser Facility, STFC-Rutherford-Appleton Laboratory, UK

Although Particle-in-Cells codes are probably the dominant computational model used for kinetic problems across plasma physics, there are a number of alternatives. One of these is the continuum Vlasov solver. Here the distribution function is represented directly on a n-dimensional grid, and evolved in time using a finite-difference approximation to Vlasov’s equation.

In this lecture we will examine the pros and cons of this model, the algorithms used to implement the model, problems it has been applied to, and extensions of the model.

3.2 - (Invited) Introduction to Vlasov-Fokker-Planck numerical methods

R Kingham
Imperial College London, UK

Vlasov-Fokker-Planck codes are continuum, kinetic codes that evolve the particle distribution function, including the effect of Coulomb collisions. They usually solve Maxwell’s equations self-consistently too. They are most widely used in ICF, HEDP and MCF (for parallel transport in the later case) to describe particle and energy transport under extreme conditions which are semi-collisional. This lecture aims to; (1) describe where VFP codes fit in the zoo of plasma physics codes, (2) provide an overview of the model & numerical method and (3) give some key examples of their use. The emphasis will be on solving for the electron distribution and the use of angular-expansion methods in velocity space.
4.1 - (Invited) Introduction to Eulerian hydrodynamics and Adaptive Mesh Refinement (AMR)

J Macey
AWE, UK

This training talk will discuss some aspects of massively parallel hydrocodes and then focus on Adaptive Mesh Refinement.

After a quick look at Lagrangian, Eulerian and Arbitrary Lagrange Eulerian hydrocode techniques, we will consider some of the practical requirements of these codes (which are often the most time consuming aspects but are frequently glossed over).

We will then look in detail at Adaptive Mesh Refinement (AMR). The real world frequently has widely disparate length scales; AMR techniques allow us to place spatial resolution where the numerical accuracy and physical length scales require. AMR codes are being used within the worldwide astrophysics and laser communities to look at phenomena such as MHD field lines around the sun, stellar equations of state, accretion disks, star bursts, collapse of supernovae, ICF and laser target debris. In this talk we will focus on building AMR methods in to a hydrodynamics solver.

4.2 - (Invited) Lagrangian and Arbitrary Lagrangian-Eulerian (ALE) hydrodynamics

T Arber
University of Warwick, UK

Most laser-driven fusion facilities have a computational problem which involves an imploding pellet of DT fuel surrounded by a plastic ablation layer. This ablation is often doped with a high Z material to prevent hard X-ray fuel preheat. The implosion is a radius reduction by a factor of 20-30. During this implosion it is important to prevent numerical diffusion of materials as this would lead to an incorrect modelling of the field mix. The most common solution to this is to have a grid which moves with the fluid (Lagrangian) as this naturally tracks the implosion and maintains resolution. It also allows different materials to be separated into cells which due to the Lagrangian model cannot mix. This is all fine unless the grid becomes too distorted. At this point the kid needs to relax to a less distorted grid, possibly even locking the grid (Eulerian) to allow fluid motion through the grid. The ideal mix is an Arbitrary-Eulerian-Lagrangian (ALE) code and this talk will introduce the basic principles of this approach.
Session 5 - Numerical Approaches

5.1 - (Invited) Adaptive mesh methods for systems of hyperbolic conservation laws in plasma physics

S V Loo
University of Leeds, UK

The equations of ideal Magnetohydrodynamics (MHD) are a set of hyperbolic conservation laws, which means that one can use standard conservative, upwind, shock capturing schemes. However, MHD presents some unique difficulties: the Riemann problem is far too complicated for an exact solver to be viable and one has to deal with the constraint that the divergence of the magnetic field should vanish. The complexity of the Riemann problem presents no great difficulty since one can use approximate Riemann solvers that give excellent results. The divergence constraint is more problematic, but there are various ways of dealing with it. Some of these methods are easier to combine with Adaptive Mesh Refinement (AMR) than others. It is also possible to add non-ideal effects to such codes, such as ambipolar diffusion and Hall resistivity. In this talk I will discuss these issues and illustrate them with simulations of astrophysical shocks and will also briefly touch upon the possibility of using AMR in Vlasov codes.

5.2 - The Current Status of the Arbitrary Lagrangian Eulerian Radiation-Hydrodynamics Code, Odin

T Goffrey¹, M Read², K Bennett¹, T D Arber¹, R H H Scott³, C S Brady¹, C P Ridgers², K McGlinchey⁴, J P Chittenden⁴, R Kingham⁴, and S Rose⁴

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The UK is home to world-leading groups in theoretical and experimental plasma physics. The continued success of these groups is reliant on access to an adequate suite of suitable codes. While the UK is well resourced in terms of kinetic, Vlasov-Fokker-Planck and atomic physics codes, no suitable radiation-hydrodynamics code is available to the UK community. In order to redress this, we have developed the Arbitrary Lagrangian Eulerian, radiation-hydrodynamics code, Odin. Odin is a multimaterial, Arbitrary Lagrangian Eulerian (ALE) radiation- hydrodynamics code. ALE codes seek to exploit the strengths of Lagrangian codes, whilst having an optional remap phase to avoid their key weakness, robustness. I will discuss the development and benchmarking of the core Lagrangian multimaterial phase and the remap. Additionally I will review the ideal-magnetohydrodynamic algorithm, as well as non-ideal effects, such as the Biermann-battery mechanism. The thermal conduction, currently modelled using a super-stepping time-integration[1] method will be examined. Finally I will comment on future development.

Magnetic confinement fusion offers the prospect of abundant clean energy, but the practical challenges remain very great. One key difficulty is plasma turbulence: at the extremely high temperatures required for nuclear fusion, instabilities in the plasma drive turbulence which transports particles and heat out the machine, preventing sustained fusion. Considerable progress has been made towards understanding and minimizing turbulence, with valuable insights increasingly being made through numerical simulation.

Turbulence in the core of fusion devices is described by the gyrokinetic equations, a nonlinear partial differential equation system for the distribution function – the number density of particles with a given position and velocity – and consistent electromagnetic fields. Since both position and velocity are coordinates, the system is high-dimensional. Moreover, the system incorporates disparate length and time scales, from the fast, small-scale electron Larmor motion (with typical period $\sim 10^{-11}$ s and radius $\sim 10^{-4}$ m), to the slow, large-scale transport of the equilibrium profiles (which typically evolve over the energy confinement time $\sim 1$ s and length scale $\sim 1$ m). Consequently, problem sizes are very large, and simulations push the limit of what is feasible on High Performance Computing platforms. Gyrokinetic computations involve the evolution of huge distribution functions, which must be distributed across many processors so that work can be done in parallel. To make optimal use of resources, it is imperative that we write parallel code that scales – that is, if we double the number of CPUs, the code should run twice as fast. The extent to which parallel scaling can be achieved is somewhat limited by the nature of the gyrokinetic equations, because common operations (like integrations, Fourier transforms and collisions) require data from different parts of the distribution function, which might be held on different CPUs. Communicating data between CPUs can take a significant part of run time and prevents the code from scaling, a problem exacerbated (at fixed problem size) as we use larger machines with more CPUs. To scale to higher CPU counts, we must carefully design algorithms and data layouts to minimize communication.

In this presentation, we introduce the gyrokinetic equations and the features which make their solution computationally challenging. We also introduce some fundamental principles of code optimization, and discuss how these guide numerical implementations of the gyrokinetic equations in various different codes. Finally, we present some recent examples of code development from the gyrokinetics code GS2, where changing the order of operations, introducing load imbalances, and using Shared Memory have each improved code scalability, allowing GS2 to better exploit High Performance Computing platforms.
5.4 - Incorporating kinetic effects on magnetized transport in inertial fusion simulations


1University of York, UK, 2Livermore, USA, 3University of California, USA, 4University of Technology, The Netherlands, 5University of Manchester, UK, 6University of Bath, UK, 7Imperial College London, London, UK

Inhibition of heat transport by magnetic fields can allow for hotter hohlraum fill in inertial fusion experiments. This advantage is somewhat diminished by the Nernst effect, which advects magnetic fields down temperature gradients. Direct-drive simulations require flux-limiters on the Nernst term to match experimental measurements; the same is likely to be true with indirect-drive. However, introducing another free parameter into design codes is undesirable; we therefore suggest three possible methods for incorporating corrections to the Nernst term motivated by comparisons with Vlasov-Fokker-Planck simulations: (a) obtaining independent fits for the Nernst and thermal flux-limiters as a function of magnetization (b) tying the Nernst flux-limiter to the thermal flux-limiter, and (c) tying the Nernst velocity directly to the heat flow, which could instead be obtained by an existing nonlocal model.

Magnetic field profiles after 50 ps relaxation of a 1 keV to 150 eV thermal ramp for a $5 \times 10^{20} \text{ cm}^{-3}$ helium plasma with an initial uniform magnetic field of 1.5 T. It is observed that using only a flux-limiter on the heat flow $f_Q$ leads to over-amplification of the magnetic field compared to a fully kinetic Vlasov-Fokker-Planck simulation (VFP). Introducing a finite flux-limiter on the Nernst velocity $f_N = f_Q$ reduces the discrepancy but still underestimates the degree of advection beyond ~150 µm. Additionally, it is seen that using no flux-limiters at all (both set to infinity) agrees better with VFP than just using a thermal flux-limiter.

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Tuesday 21 November

Session 6 – Applications I

6.1 - Higher order Kerr terms vs. plasma: Saturation of the nonlinear refractive index

R Guichard¹, C Köhler and L Berg², E Lorin³, S Chelkowski and A D Bandrauk⁴, S Skupin⁵

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In this talk, I will present a study on atomic nonlinear polarization induced by high-intensity ultrashort laser pulses in hydrogen by numerically solving the time-dependent Schrödinger equation. The aim is to reveal the origin of the nonlinear index saturation and subsequent intensity clamping in femtosecond _laments. This allows for the comparison between the proposed model of the higher-order Kerr effect (HOKE) and two versions of the standard model for femtosecond _lamentation, including either a multiphoton or tunnel ionization rate. We find that around the clamping intensity the instantaneous HOKE model does not reproduce the temporal structure of the nonlinear response obtained from the quantum-mechanical results. In contrast, the noninstantaneous charge contributions included in the standard models ensure a reasonable quantitative agreement. Therefore, the physical origin for the observed saturation of the overall electron response is confirmed to mainly result from contributions of free or nearly-free electrons.

6.2 - Preparatory simulation studies for the laboratory experiment of cosmic-ray driven magnetic field fluctuations

C-S Jao¹, Y Chen¹, M Gross¹, M Krasilnikov¹, G Loisch¹, T Mehrling², J Niemiec³, A Oppelt¹, A M la Ossa⁴, J Osterhoff², M Pohl¹,⁵, F Stephan¹ and S Vafin¹,⁵

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For the source of PeV-scale high energy cosmic ray particles, the diffusive shock acceleration process at the forward shocks of supernova remnants is considered as the principal mechanism. For efficient acceleration, a nonresonant instability driven by cosmic ray current is suggested as a candidate for providing the required magnetic turbulence in the upstream region of the shock [1]. Previous magnetohydrodynamic and kinetic numerical studies had shown this nonresonant instability could generate the magnetic field fluctuations stronger than the background interstellar field as theoretical prediction [1,2]. In order to examine the saturation level and mechanism of this cosmic-ray driven instability in the laboratory, we attempt to develop an experiment by using the plasma cell and electron source of the PITZ group of DESY. We here present the pre-experiment numerical investigations[3] that study physical conditions for the beam-driven nonresonant instability to occur in the laboratory experiment and its expected properties.

6.3 - Finite banana width effect on NTM Threshold Physics

K Imada¹, J W Connor, A Dudkovskaia¹, P Hill¹ and H R Wilson¹²

¹University of York, UK, ²Culham Centre for Fusion Energy, UK

The successful operation of future tokamaks, such as ITER, depends on the control of MHD instabilities, including neoclassical tearing modes (NTMs). Characterised by the formation and evolution of magnetic islands, NTMs can degrade the plasma confinement due to enhanced radial transport across the island, which reduces the core pressure. If left uncontrolled, NTMs can trigger a disruption, which must be avoided in future larger devices. NTM control systems rely on the understanding of the island threshold physics, whereby a sufficiently small seed island tends to heal itself. Theory and experiments suggest that the threshold island width, \( w_c \), below which the island heals, is comparable to the banana orbit width of trapped ions, \( \rho_b \) (typically \( O(1\text{cm}) \)). In toroidal geometry, the finite banana width effect gives rise to the neoclassical polarisation current, which is induced when the magnetic island chain is in relative motion with respect to the plasma. This in turn generates a parallel return current, which contributes to the magnetic island evolution via the modified Rutherford equation. Whether stabilising or destabilising, it will influence the threshold island width, when \( w_c \sim \rho_b \).

By expanding in the small ratio of \( w/r \), where \( r \) is the minor radius at the island location, but retaining the ordering \( w \sim \rho_b \) we have developed a new drift kinetic theory for the ion response to the magnetic island. This results in a 4D particle orbit-averaged kinetic equation in toroidal geometry, where the solution depends on the toroidal canonical momentum \( p_p \), (representing poloidal flux, \( \psi \)), the helical angle \( \xi \) (labelling the field lines at the rational surface), pitch angle \( \lambda \) and kinetic energy \( v^2 \). Our new code solves the above equation for the perturbed ion distribution function, taking into account momentum conservation and quasineutrality, both of which are crucial for determining bootstrap and neoclassical polarisation current perturbations. We have developed a novel iteration scheme to calculate the momentum conservation term and electrostatic potential, both of which require the velocity space integral (parallel flow and density moments, respectively). This allows us to decouple the explicit dependence on \( v \), leaving a 3D kinetic equation. This is solved using the “shooting method” in the pitch angle (\( \lambda \)) direction, with the resulting 2D equation solved at each of the \( \lambda \) grid points. This enables us to solve what is initially a computationally demanding 4D problem at sufficiently high resolution, without the need for excessive computational resources.

In this paper, we present our new results on the ion response to the magnetic island perturbation. When collisions are neglected, the ion distribution function is flattened across the drift-island structure, which is similar to the island geometry, but shifted radially by an amount proportional to \( \rho_\Omega \) (\( \rho_\Omega \) is the poloidal Larmor radius; \( \rho_\Omega = \varepsilon^{1/2} \rho_b \Omega \) and \( \varepsilon \) is the inverse aspect ratio). Our numerical calculations show that, even for a moderately small ratio of \( \rho_\Omega / w \), the finite orbit width effects are significant, particularly around the island separatrix layer. Not only is the density flattening across the island incomplete (with consequences for the bootstrap current perturbation), but there exists a substantially wider ion parallel flow layer than predicted by the analytic theory. There is also a substantial flow within the island, which had not been considered in earlier works. This is likely to have a significant contribution to the modified Rutherford equation, and hence to the island threshold physics.
This talk will describe the hierarchy of models of increasing sophistication that are required to capture the phenomena observed in plasma physics experiments and the challenges associated with adapting these models to advanced computer architectures based on accelerator technologies. The talk focuses on the author personal experiences and contributions [1-3] to developing computational approaches for modelling the X-ray propagation.

The focus of the talk will be on hohlraum driven targets, which convert the laser energy into an incident X-ray drive. This intense source of thermal X-rays interacts with the laser target, enabling complex processes which occur under extreme conditions to be examined in the laboratory. We discuss the synergies between the equations being simulated to model the X-ray transport and those relevant to the plasma evolution and the associated computational techniques used to model the plasma dynamics.

X-ray transport models must be able to simultaneously capture the details of the asymmetries in the radiation drive on the laser target, whilst also accurately capturing the diffusive energy losses into the hohlraum wall. The need to model these different phenomena means that the transport models must be simultaneously capable of representing long range propagation through semi-transparent media (a hyperbolic system of equations), while transitioning to a locally coupled diffusive transport process both within the hohlraum walls and in the interior of the target (a scalar elliptic equation).

The associated algorithms have inherently different characteristics in terms of their ability to map to future HPC platforms, with the requirements for exposing greater concurrency at both coarse and fine granularity in order to efficiently exploit many-core architectures. AWE and its collaborators are proactively investing these challenges and this talk will present highlights of recent progress.

The current computational models are able to accurately reproduce certain phenomena observed in the laboratory based on two-dimensional (2D) approximations of the geometry. However, there is still a long way to go before the codes are able to accurately predict a wide range of target designs with high confidence. Particular challenges include the need to capture the three-dimensional (3D) features which arise due to the experimental geometry and the need to accurately model turbulent instability growth, which is an inherently 3D process. The current algorithms need to be adapted to take advantage of innovations in HPC architectures in order to meet the 3D modelling challenges ahead.

7.2 - Diagnosing the Effect of Radiation Asymmetries and Isolated Defects on an ICF HotSpot

K McGlinchey, J P Chittenden and B Appelbe
Imperial College London, UK

Radiation asymmetries and hydrodynamic instabilities lead to strong variations in the areal density of an imploding ICF capsule [1], inducing residual flow and driving the stagnation conditions away from spherical compression. We report on simulations of ICF experiments using the 3D radiation-hydrodynamic code Chimera to investigate the influence of these mechanisms.

Large scale multi-dimensional simulations with radiation asymmetries, tent scars and the fill tube are presented, looking at the each individual perturbation and their combined role in either enhancing or diminishing each other. The role of each perturbation is quantified in both its early time and late time behaviour.

Each perturbation is evaluated in terms of its effect on hot spot conditions, and their viability to be diagnosed through x-ray backlighting and neutron detectors. Any unique signature left by the perturbation allows a catalogue of signatures to be developed that can be applied to the output of future experiments to diagnose failure modes.

[1] D. Clark et al., Three-dimensional simulations of low foot and high foot implosion experiments on the National Ignition Facility, PoP, 2016

Session 8 - Scientific Software Development I

8.1 - (Invited) HPC with Fortran 2008 and 2015 Coarrays

A Shterenlikht
University of Bristol, UK

Fortran 2008 standard includes coarrays - a native Fortran means for SPMD programming. The next standard, about to be published soon, Fortran 2015 substantially expanded the set of coarray features, including teams, collectives, events and facilities for dealing with hardware or software failures.

After a brief introduction to coarray design, we look at an example of coarray use in cellular automata simulations, a structured grid problem, with scaling data on Tier-1 (UK) and Tier-0 (EU) systems. Coarrays should be very appealing to existing Fortran programmers because they offer a lot of parallel flexibility with very little new syntax. We conclude with a brief discussion of the activities of the Fortran specialist group of BCS and of the IoP computational physics group and how these intersect with the interests of CPPC audience.
8.2 - Exploring Arm Architecture, Porting and Optimization

N J Sircombe

Arm, UK

Arm is the world’s leading architecture, used in everything from the vast majority of mobile phones, to the tiny processors embedded in the rapidly growing world of IoT devices. We work with over 1,200 partners to deliver an entire hardware and software ecosystem to help seamlessly deploy our technology wherever computing happens. In 2012 Arm launched its 64-bit instruction set opening up the worlds of enterprise servers, data centres and High Performance Computing (HPC).

We will explore the growing Arm HPC ecosystem, including the Arm Compiler for HPC, Arm Performance Libraries, Allinea Forge and the open source OpenHPC stack. We will detail the porting and initial profiling of plasma physics’ most ubiquitous numerical model, the Particle In Cell, or PIC, code - taking the EPOCH code[1], which has become part of the fabric of plasma physics modelling in the UK, and the highly vectorised VPIC code[2], which has frequently been demonstrated on leadership-class platforms in the US, as examples.

We will touch on the exciting future in Arm-based HPC, including the planned exascale Post-K system in Japan and the potential of Arm’s new Scalable Vector Extension (SVE)[3], which allows chip designers to build systems with vector lengths of up to 2048 bits.


9.1 - Performance of Second Order Particle-in-Cell Methods on Modern Many-Core Architectures

D A S Brown¹, M T Bettencourt², S A Wright¹, J P Jones³ and S A Jarvis¹

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The emergence of modern many-core architectures that offer an extreme level of parallelism makes methods that were previously infeasible due to computational expense now achievable. Particle-in-Cell (PIC) codes often fail to fully leverage this increased performance potential due to their high use of memory bandwidth. The use of higher order PIC methods may offer a solution to this by improving simulation accuracy significantly for an increase in computational intensity when compared to their first order counterparts. This greater expense is accompanied with only a minor increase in the amount of memory throughput required during the simulation.

In this presentation we will show the performance of a second order PIC algorithm. Our implementation uses second order finite elements and particles that are represented with a collection of surrounding ghost particles. These ghost particles each have associated weights and offsets around the true particle position and therefore represent a charge distribution.

We test our PIC implementation against a first order algorithm on various modern compute architectures including Intel’s Knights Landing (KNL) and NVIDIA’s Tesla P100.

Our preliminary results show the viability of second order methods for PIC applications on these architectures when compared to previous generations of many-core hardware. Specifically, we see an order of magnitude improvement in performance for second order methods between the Pascal and Kepler GPU architectures, despite only a 4_ improvement in theoretical peak performance between the architectures. Although these initial results show a large increase in runtime over first order methods, we hope to be able to show improved scaling behaviour and increased simulation accuracy in the future.

Figure 1: Execution time of a two stream problem using 1 million particles, 500 steps
9.2 - Case studies in Successful Scientific Simulation Software

C Brady and H Ratcliffe
University of Warwick, UK

Scientific software is, at core, about getting the correct (enough!) answer to the scientific problem that it is used to solve. But correctness on its own is a necessary but not sufficient condition to make software valuable to its community. As the use of simulations expands further and further beyond the traditional “computational physicist”, and the size of development teams for scientific software continues to grow, the value of “non–scientific” elements of scientific software development, such as version control and testing, will only grow. In this presentation, I will consider case studies of scientific software and demonstrate that other qualities such as ease of use, continuing and reliable support, the ability to guarantee replicatable results and the ability to not only give correct results, but demonstrate the correctness of the results given add significant and essential value beyond that of simple technical correctness.

9.3 - Improving the sustainability of BOUT++

P Hill and The BOUT++ Team
University of York, UK

BOUT++ is an internationally used framework for solving fluid equations, originally developed at York, with an emphasis on plasma modelling. It has been successfully used for a wide variety of physics models, in numerous fusion, space, and industry relevant plasma devices. Some particularly successful physics models include those of edge localised modes (ELMs) and plasma filaments in the scrape-off-layer of tokamaks.

Outside of plasma physics, applications to fluid flow are also being explored.

Recent efforts have been taken to improve the sustainability of BOUT++. In the context of software, sustainability is about increasing the lifetime of the software, ensuring that it continues to be available and supported in the future. This is naturally linked to the idea of reproducible research, that is, making available all the tools and data necessary to reproducing a piece of research: not just the physical parameters used, but also the software itself, input files and data, as well as the analysis chain used to produce the end figures and tables. Software sustainability therefore underpins reproducible research, allowing future researchers to revisit earlier work.

Here we present improvements to the sustainability of BOUT++ since 2014, when Research Software Engineer (RSE) Peter Hill joined the project. We will look at four specific sustainability features: the merging/development process, testing, documentation and visibility. Improvements to these features cover both technical solutions, such as automatically running tests on commits to the public code repository, and procedural solutions, such as mandatory code reviews on pull requests, and have led to a measurable increase in code quality.
10.1 - (Invited) Integrated Modelling Frameworks in Magnetic Confinement Fusion

M Romanelli
Culham Science Centre, UK

Design and operation of present and future Tokamak reactors require extensive integrated modelling enabling to optimize engineering parameters as well as maximising physics performance. In order to simultaneously predict quantities such as: particle and energy confinement time, fusion yield, power deposited to the wall and wall load from fast particles, modellers need computational frameworks allowing for the integrated simulation of different regions of the reactor, characterized by very different space / time scales and symmetries. Complex simulations of turbulent structures based on gyrokinetic equations help exploring ion-electron drift scales while transport codes based on fluid equations and reduced transport models allow simulating entire plasma discharges during different operational phases. These simulations make use of different integration frameworks offering different level of flexibility. As an example, the XGC1 edge/SOL/divertor gyrokinetic code [1] makes use of the ADIOS framework [2] to couple neoclassical transport, wall physics and turbulence. XGC1 is run on exascale super-computers to study e.g. the width of the heat-flux to divertor plates in attached plasma conditions. The BOUT++ framework [3] couples gyrofluid codes, such as CENTORI [4], along with neutral Montecarlo codes and is optimised on HPC infrastructures to allow extending global transport studies to confinement time scales. A new modular European Transport Simulator (ETS) [5], has been developed within the EU-Integrated Modelling framework building on a data and communication ontology, incorporating both simulated and experimental data. A similar approach has been adopted by ITER in IMAS [6]. The ETS has now reached a capability equivalent to the state-of-the-art integrated modelling transport codes, including a number of interchangeable physics modules for the Tokamak equilibrium, transport, impurities (all ionization states), heating and current drive sources including all the heating schemes and fuelling. Another framework for integrated Tokamak modelling is JINTRAC [7], a system of 25 interfaced Tokamak-physics codes used at JET for the integrated simulation of all phases of a Tokamak scenario. Integrated modelling codes predictions reflect the physics and assumptions implemented in each module and extensive comparison with experimental data is ongoing to allow validation of the models and improvement of Tokamak-physics understanding. The choice of the appropriate integrated modelling framework can be crucial to facilitate the above validation.

10.2 - Enhanced control of the ionization rate in radio-frequency plasmas with structured electrodes via tailored voltage waveforms

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Radio-frequency (rf) capacitively coupled plasmas that incorporate structured electrodes enable increases in the electron density within spatially localised regions through the hollow cathode effect¹. This enables enhanced control over the spatial profile of the plasma density, which is useful for several applications including materials processing, lighting and spacecraft propulsion. However, asymmetries in the powered and grounded electrode areas inherent to the hollow cathode geometry lead to the formation of a time averaged dc self-bias voltage at the powered electrode. This bias alters the energy and flux of secondary electrons leaving the surface of the cathode and consequentially can moderate the increased localized ionization afforded by the hollow cathode discharge. In this work, two-dimensional fluid-kinetic simulations are used to demonstrate control of the dc self-bias voltage in a dual-frequency driven (13.56 MHz, 27.12 MHz), hollow cathode enhanced, capacitively coupled argon plasma over the 0.5-1.5 Torr pressure range. By varying the phase offset of the 27.12 MHz voltage waveform, the dc self-bias voltage varies by 10-15 % over an applied peak-to-peak voltage range of 600-1000 V, with lower voltages showing higher modulation. Resulting ionization rates due to secondary electrons within the hollow cathode cavity vary by a factor of 3 at constant voltage amplitude, demonstrating the ability to control plasma properties relevant for maintaining and enhancing the hollow cathode effect.


10.3 - Linear Gyrokinetic Study of Kinetic Ballooning Mode (KBM) Width and Stability in Tokamaks

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Achievement of economical fusion energy using tokamaks faces many challenges, including the problems of: turbulence; lossy and damaging edge localised modes (ELMs); and understanding the H-mode pedestal. Gyrokinetics is the leading simulation tool for studying the microinstabilities involved in these processes. One particular microinstability, the kinetic ballooning mode (KBM), has been implicated in pedestal growth and the ELM cycle, and the control of ELMs via resonant magnetic perturbations. This talk reports a linear gyrokinetic study of KBMs in tokamaks. First, the global mode is reconstructed from an array of local simulations. This offers significant computational cost savings compared with using a global simulation directly. The work includes newly developed techniques to correctly track the mode of interest (in this case, KBMs) across parameter space while maintaining high performance in the simulations. The results are compared to the well studied ion temperature gradient driven mode. Next, the problem of very narrow KBMs in experimentally relevant equilibria is introduced. Following this, an investigation is presented looking into the effect of plasma shaping, geometry and other equilibrium modifying parameters on KBM stability and width. This uses analytical approximations to the experimental equilibrium, rather than numerical equilibria, as this enables easier modification of parameters.
Session 11 – Scientific Software Development and Applications II

11.1 - (Invited) Parallel in time integration – a step towards exascale computing in Plasma Physics

D Samaddar¹, D P Coster², X Bonnin³, W R Elwasif⁴, D B Batchelor⁴, L A Berry⁴, E Havlickova¹, T Casper³, S H Kim³, D E Newman⁵ and R Sanchez⁶

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Arguably, one of the 21st century’s greatest HPC Grand Challenges is ‘long time scale simulations of magnetically confined fusion plasma’. While parallel computing plays an important role in achieving these computations, a saturation in terms of improving computational gain with respect to increasing computing cores is encountered on existing Petascale supercomputers. With the inexorable march towards the ExaScale (10¹⁸ floating point calculations per second), Plasma Physicists will likely have access to such hardware by ~2023. Without significant investment in new algorithms that can exploit the emerging Exascale architectures however, it is unlikely that the ultimate goal of solving the plasma turbulence Grand Challenge will be realized. Temporal parallelization provides a crucial step in exploiting the computing power of modern supercomputers. Since time is intrinsically a sequential domain, parallelizing it might seem counter-intuitive. However, there are a variety of mathematical algorithms, such as Parareal and PFASST, that achieve this aim. Of these, the Parareal algorithm has so far been the most widely studied method in fusion plasma, reducing wall clock times by factors of 10 and 20 in complex non-linear problems. This talk will give an introduction to time parallelization and an overview of the various algorithms. It will then discuss a series of applications in fusion plasma, ranging from core turbulence and tokamak scenario modelling to multi-fluid scrape off layer simulations. Since the Parareal algorithm relies on a predictor-corrector approach, choosing a suitable coarse predictor often becomes the focal point of research and this will be illustrated. For the various applications, the talk will highlight the success stories as well as the difficulties encountered along this journey.

The views and opinions expressed herein do not necessarily reflect those of the European Commission or the ITER Organization.

Self-generated magnetic fields by the Biermann Battery mechanism are present in both astrophysical [1] and laboratory plasmas [2]. However, the accurate computation of the growth of these fields is mired with numerical difficulties [3]. Numerical tests of the Biermann Battery term will be presented, along with estimates of the impact of self-generated magnetic fields on the performance of capsule implosions on the National Ignition Facility [4].

The so-called ‘Biermann Catastrophe’ [3] can occur numerically due to discontinuities in plasma properties at shock fronts, resulting in unphysical magnetic field generation rates. Graziani’s algorithmic implementation can help to mitigate these problems [3], but has limitations, which will be discussed. Tests of magnetic field generation both in smooth and discontinuous regions will be shown.

Magnetic fields are self-generated in the hot fuel of asymmetric ICF implosions. These fields are estimated to be above 10,000T in strength, magnetising the thermal conduction out of the hot-spot. High-mode perturbations are found to generate the largest magnetic fields, but are confined to the cold and dense hot-spot surface, which is hard to magnetise. When both low and high-mode perturbations are present, the magnetic fields are injected into the core of the hot-spot, resulting in large magnetisations ($w_e T_e > 1$). In this magnetisation regime both the Nernst and Righi-Leduc effects are significant, and their impact on the energy containment of the hot-spot will be discussed.

Session 12 – Beyond the Laboratory

12.1 - (Invited) Astrophysical Collisional-Radiative Modelling

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AWE, UK

Spectroscopy has proved an invaluable tool to understand the properties of astrophysical plasmas. The light which is received encodes information about the density, temperature, elemental abundances and kinematics of the material which is observed, and even the magnetic field which passes through it. However, to fully exploit this information usually requires a detailed microphysical model of the source. I will describe the scope of astrophysical collisional-radiative modelling, with particular reference to the open-source code Cloudy (most recently described in [1]). While most astrophysical plasmas are of very low density compared to those typically found in laboratory experiments, they can contain a multiplicity of species: atoms, ions, molecules, solid grains and ices. Modelling the state of these species and all their interactions provides many challenges, for example in the acquisition and management of fundamental data, and the development of efficient and accurate algorithms. Processes, such as charge transfer, which introduce strong inter-couplings can undermine simple partitioning schemes. I will discuss recent progress on some of these issues.


12.2 - Hybrid simulations of pickup ion instabilities in space plasmas

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The ionisation of neutral material in space plasmas can give rise to a rich variety of electromagnetic plasma wave phenomena. The resultant instabilities and wave-particle interactions can be observed by in-situ spacecraft to infer the ion species present, their spatial and temporal distributions, and the distribution of free-energy throughout the medium. In this study we present self-consistent hybrid (kinetic ion, massless fluid electron) simulations of ion pickup and Alfvén-Cyclotron waves observed in the Jovian and Saturnian magnetospheres and draw comparisons to supra-Alfvénic pickup at planetary bodies immersed directly in the solar wind. In particular, we show how the hybrid simulation technique is able to self-consistently reproduce the growth of positively and negative ion instabilities in the Europan plasma environment and reveal how the left-hand and right-hand instabilities result in a non-linear coupling and wave amplitudes twice as high as expected [1]. We also show how hybrid simulation of non-gyrotropic ion distributions, as observed at the Saturnian moons Rhea and Titan, result in significantly enhanced instability growth rates and saturation amplitudes. This rapid release of energy is suggested as a possible mechanism to explain the lack of pickup ion-generated waves at these moons.

P:01 Particle-in-cell Simulations of Laser-Plasma Instabilities in Shock Ignition

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In recent years the shock ignition (SI) approach to Inertial Confinement Fusion (ICF) has been the subject of considerable interest due to its potential to drastically reduce the energy required of the laser driver[1]. A crucial issue for this scheme is understanding how laser-plasma instabilities (LPIs) driven by the high laser-intensity spike will affect its performance. Depending on their energy, hot electrons from LPIs may either enhance the ignitor shock or preheat fuel[2], while scattering of the laser reduces drive efficiency. Initial simulation work has been done in this regime[3][4][5], however these studies either investigated relatively small-scale plasmas, lacked realistic speckle profiles or had low numbers of particles per cell. Further, only a couple of different sets of simulation parameters were typically attempted. Here we describe initial progress on a campaign of PIC simulations in which we attempt to address these issues. We investigate conditions representative of experiments to be performed at the OMEGA laser[6] which will attempt to investigate ignition-scale SI.


P:02 Electron laser wakefield acceleration for production of nuclear isomers

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The ELI-NP facility [1] presents a unique opportunity for exploring problems in fundamental physics, combining a 2x10 PW high-power laser system (HPLS) and a high-brilliance gamma-beam system (GBS) with energies of up to 19.5 MeV. The laser system consists of two synchronized arms, each with three optical compressors that allow pulse extraction at different powers, ie. 100 TW at 10 Hz, 1 PW at 1 Hz, and 10 PW at 0.016 Hz, with a pulse duration around 20 fs. The GBS photons are produced by inverse Compton backscattering of laser pulses off electron bunches accelerated by a LINAC up to 720 MeV.

One of the proposed first-phase experiments [2] aims at studying in the laboratory the conditions normally encountered in nuclear astrophysics, namely inducing photoexcitation on a nuclear isomeric state. In a nutshell, electrons are accelerated by the 100 TW laser pulse to MeV energies, and they hit a tungsten target, producing Bremsstrahlung gamma radiation that impacts a secondary target with the nucleus of interest, producing isomers. These isomers are photo-excited just above the neutron threshold by the GBS.
We performed 3D PIC simulations using the EPOCH code [3] in order to study the electron beam generated by laser wakefield acceleration (LWFA), as follows. An electron beam with a total charge of 3.3 nC is produced from a LWFA consisting of a 1-mm-long gas cell filled with pure nitrogen. The relevant parameters of the LWFA can be determined by using the scaling law of nonlinear plasma wakefields in the bubble regime [4-6]. A laser pulse with 121 TW peak power and 20 fs duration is focused on a spot with a 20 µm radius at the entrance of the gas cell, operated at a plasma density of \( \sim 10^{19} \) cm\(^{-3}\). As a result, strong nonlinear wakefields can be generated so that the electron bunch could be trapped due to ionization-induced injection [7, 8] and accelerated up to \( \sim 250 \) MeV [9]. Figure 1 shows preliminary results of the PIC simulations, where we fixed the width of the gas-filled region from the nozzle jet to 1 mm and obtained an accelerated electron beam with an angular divergence of 6.6°.

![Figure 1: Momentum (left) and energy (right) distribution for LWFA electrons from PIC simulations. The driving laser has a Gaussian profile, with a wavelength of 800 nm. Parameters: focal waist 20 µm, peak power 121 TW and plasma density 2.83*10^{19} \) cm\(^{-3}\).](image)

P:03 Modelling Gamma-Ray Emission and Pair Production in High-Intensity Laser-Plasma Interactions

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In high-intensity (> $10^{21}$W/cm$^2$) laser-matter interactions gamma-ray photon emission by the electrons can strongly affect the electron's dynamics and copious numbers of electron-positron pairs can be produced by the emitted photons. We show how these processes can be included in simulations by coupling a Monte-Carlo algorithm describing the emission to a particle-in-cell code. The Monte-Carlo algorithm includes quantum corrections to the photon emission, which we show must be included if the pair production rate is to be correctly determined. The accuracy, convergence and energy conservation properties of the Monte-Carlo algorithm are analysed in simple test problems.

P:04 2D Vlasov-Fokker-Planck simulations of laser-ablated plasmas under ICF-relevant conditions

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Irradiation non-uniformity can be a major source of degrading target performance in direct-drive ICF implosions$^1$. Perturbations to electron temperature at the critical surface (location of laser absorption) feed through to the ablation surface whereupon they seed the Rayleigh Taylor instability. To some extent, lateral thermal transport in this ‘conduction zone’ attenuates the perturbations before they can imprint themselves on the ablation surface. The conduction region has density and temperature scale lengths comparable to the electron mean free path, therefore, a kinetic model must be used to model the thermal transport.

We will present 2D kinetic simulations of a planar ablating target irradiated by a perturbed laser using the fully-implicit, parallel, VFP code, IMPACT2. This improves upon previous 2D calculations$^3$, by including plasma flow (rather than assuming static density ramps) and magnetic field. The simulations focus on the conduction zone; in order to incorporate the plasma flow, novel inflow and outflow boundary conditions were required. Implementation proved to be quite challenging, and will be discussed. We also present improvements to the hydrodynamic ion model and laser package. Key findings from these simulations will be presented. Self-generated magnetic fields are found to have a significant effect on heat flow dynamics within the conduction zone, causing an inversion and enhancement of perturbation amplitudes; a result that contrasts with previous hydrodynamic studies$^4$. The role of kinetic effects and modifications from classical (Braginskii) transport will be discussed.

P:05 Modelling Laser Propagation with Magnetised Transport in Plasmas

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Inertial fusion schemes and high-energy density experiments use high-power lasers to produce very high temperature plasmas. Magnetic fields further increase the complexity of the physics by the introduction of new terms and magnetised transport. In a magnetised plasma, the transport of heat across magnetic field lines can be restricted by collisional effects [1] and this mechanism has been suggested as a means to ensure greater deposition of laser energy into the hohlraum [2] or to aid the confinement of energy in magnetised linear fusion experiments [3]. Building on previous 2D laser propagation work [4], a new full Braginskii [1] magnetised transport plasma physics code PARAMAGNET has been written with paraxial model laser solver to investigate the effects of the magnetic field on the laser-plasma physics. The plasma model is fully implicit and solved using a matrix free Newton method via the PETSc library. We will present progress on the development of the numerical methods used in the code as well as investigations on the effect of magnetic fields and magnetised transport on the filamentation and propagation of laser light in plasmas.


P:06 Charged particle transport for alpha-heating in the radiation hydrodynamics code Chimera

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We present a new 3D charged particle transport package for the radiation hydrodynamics code Chimera, developed at Imperial College London. The burn package consists of Monte-Carlo transport using a Particle-In-Cell framework, and is based on Sherlock’s framework for implementing Coulomb collisions in a hybrid particle-fluid model [1]. We compare the charged particle slowing in our model to results from established models, in addition to recent work undergone to magnetise the particle transport. We present results using the model for the transport of fast alpha-particles in inertial confinement fusion (ICF) capsules in 1D and 3D. We illustrate the influence of burn physics on the energetics of a homogeneous, unperturbed ICF hotspot in 1D based on the high-foot radiation drive shot N130927, breaking down the heat flow out of the hotspot via processes of alpha-transport, radiation transport and thermal conduction. We then consider the impact of a single Rayleigh-Taylor spike of cold fuel on this heat flow in 3...
P:07 Charged Particle Stopping Power Experiments on Orion


AWE plc, UK

The Orion laser facility provides a platform for performing direct drive capsule implosions using a thin shell 'exploding pusher' design, which is desirable both for robustness and for future charged particle stopping power experiments to validate current stopping power theories; important in high energy density physics. Stopping power experiments require a well-known source of particles (a proton source - the exploding pusher target), a well-characterized plasma (secondary target), and an accurate measurement of the energy loss (downshift in energy of the particle traversing the plasma). DD implosions generate 3MeV protons, which will then interact with the secondary target heated isochorically by a short pulse laser to ~200-300 eV at solid density (n_e ~ 2 x 10^{23} g/cc). The optimum exploding pusher capsule, selected from a 1D design study, taking into account facility and target fabrication constraints, satisfied design criteria on the 1D clean fusion yield, capsule dynamics and implosion time. The nominal target was a silica glass shell of radius 250±10µm and thickness 2.3±0.5µm, filled with 10atm. of DD gas. The preliminary secondary target was a plastic cuboid (PyN) of ~ 70x70x50µm dimensions. In order to accurately measure the downshift in energy of the protons from the exploding pusher target, the secondary target needs to be uniformly heated to approximately 200eV throughout the plasma. Therefore, 2D/3D simulations of the short pulse laser interactions with the
secondary target were conducted to look at the uniformity of the heating and the electron temperatures
produced for the above cuboid dimensions and for slightly different dimensions and laser energies/spot
sizes to see how this impacts the heating of the target.

The work presented here will briefly discuss the 1D design study for the exploding pusher target before
focussing on optimising the secondary target using EPOCH (a Particle in Cell code) and THOR (an electron
transport code), as well as using fully integrated modelling with EPOCH, THOR and CORVUS (a radiation-
hydrodynamics code).

P:08 Studying nano-thin graphene film for laser-driven ion acceleration

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Developing methods for generating high-energy ion bunches are important for applications relevant to ICF
and medicine. One approach focuses on inducing a highly intense highcontrast laser pulse on ultra-thin solid
targets. To achieve this and advance on current studies [1, 2] greater understanding of the acceleration
mechanisms and emerging instabilities are required. We work on studies coupling reproducible high-
contrast, ultraintense laser experiments with computational modeling on nano-thin graphene films. Here we
discuss studying the laser contrast and intensity with target thickness using hydrodynamic and particle-in-
cell simulations in order to understand the acceleration mechanisms and interaction physics.


P:09 A Code Comparison Project on Short Pulse Laser Heating of Solid Density Plasma

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High intensity, short pulse lasers are an effective means of generating the conditions necessary for high
energy density physics studies. However, there are many questions regarding the dynamics of the laser-
target interaction, such as the distribution of energetic electrons generated by the laser interaction, the
coupling of the electron energy to the background plasma, and the spatial and temporal dependence of the
heating. Computational methods can be used to attempt to answer these questions. However, these
methods require validation and verification. To aid in this, a code comparison project was initiated in early
2016. We present the results of the test problems to date.
This work aims at the analyzing the temporal evolution of species, heating and other physical quantities in a gaseous mixture subjected to electric discharges, similarly than a commercial spark plug. An electric field is produced in the gaseous mixture by applying a high voltage in part of the simulation domain [1]. The simulation domain is a cartesian two-dimensional region [2]. In the macroscopic perspective, the effects of transport, i.e. heat transfer and mass, are considered [3], microscopically, effects of heat generation due to electronic collisions, chemical effects among others are considered [4]. Reaction rate and transport coefficients depending upon the electron energy distribution function are calculated from collision cross-section data by solving the electron Boltzmann equation (BE). The application of a technique of separation of operators in the mathematical model, provides to two sub-models, a global for macroscopic effects and another site containing microscopic effects of the plasma. A discrete sub-model for the electron-species and species-species collisions [5, 6] is solved in ZDPlasKin, a zero dimensional plasma analysis tool [7], while BE solver BOLSIG+ [8] required for solved electron energy distribution function. Argon is used as an initial gaseous mixture in the simulation. Due to the high computational cost, a domain decomposition with Message Passing Interface (MPI) is used for parallelization of the calculations [9]. Spatio-temporal profiles for the gas temperature and species density are here calculated and reported.

Applications - MCF

P:11 Edge Localised Mode Simulations of MAST Plasmas

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Edge localised modes (ELMs) are instabilities that occur in tokamak plasmas when high confinement mode (H-mode) is accessed [1]. Experimentally ELMs appear as filamentary structures that erupt transporting heat and particles from the core of the plasma onto plasma facing surfaces, especially the divertor region. ITER, a future tokamak, will operate in H-mode. From extrapolations of experimental scaling laws it has been shown that the peak heat fluxes from uncontrolled type-I ELMs could damage the Tungsten divertor plates [2]. In order to advance the control, mitigation and suppression of these ELMs, there needs to be an improved understanding of ELM physics. It is widely accepted that the ELM onset is driven by magnetohydrodynamic (MHD) instabilities - ballooning modes caused by the pressure pedestal and peeling/kink modes driven by the large edge current density [3]. Among other codes, JOREK [4], a numerical 3D nonlinear MHD code is being developed for ELM simulations. Quantitative validation of the model to current experiments is being established [5]. The objective of this research is to produce ELM simulations of Mega Ampere Spherical Tokamak Upgrade (MAST-U) plasmas, targeting first predictions of ELMs before H-mode operation. This tokamak is currently under construction and will have the first super-X divertor, allowing for extended connection length and increased flux expansion [6]. The new magnetic configuration is thought to reduce the heat flux to the divertor targets but the effect on ELMs is unknown. ELM simulations for MAST plasmas are first carried out to observe the evolution of ELMs and to understand the physics of energy transport at the plasma edge. A neutrals model, similar to that in [7], is used in JOREK for ELM simulations, and an initial benchmark is produced with SOLPS [8]. The model allows observations of neutral transport during an ELM focusing on the divertor conditions, with comparisons to experimental data.

Development of a fully implicit kinetic code for parallel electron transport in the tokamak Scrape-Off Layer

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Modeling of transport in the edge region of tokamaks has relied traditionally on either an hydrodynamic two-fluid approach backed up by transport coefficients calculated by Braginskii[1], or kinetic approaches based on PIC (particle-in-cell) or Monte Carlo methods. These approaches suffer from the inability to easily capture non-local effects (due to varying collisionality in the plasma edge), as well as noise inherent to particle methods. A third approach is to solve kinetic equations using a finite difference method and to obtain particle distribution functions. While codes employing the finite difference method have been used and reported in the Scrape-Off Layer transport literature[2], their use up to now appears to be limited. Kinetic codes capable of capturing non-local effects have been used in simulations of laser-plasma interactions[3,4]. Those codes employ a spherical harmonic decomposition of the electron distribution function (EDF), which allows for efficient treatment of transport and the effects of anisotropy. On the other hand, the same decomposition of the EDF has been used in electron swarm models[5], where electron-neutral interactions are dominant. For simulations involving detached plasmas as well as steep temperature and density gradients (such as those during ELM bursts), a novel combination of these two approaches appears to be natural. This has been the motivation for developing a new fully implicit kinetic 1D3V code using the combination of the above approaches to model plasma of highly varying collisionality. Here we present our new fully implicit 1D3V code for the treatment of parallel electron transport in hydrogen plasmas of varying collisionality and with arbitrary distribution function anisotropy. The code includes models for both Coulomb collisions of charged species, as well as models for several electron-neutral collision processes. Self-consistent fields are calculated using Maxwell’s equations. Present are both the general and novel aspects of the code, along with preliminary benchmarking.

The 3D radiation hydrodynamics code Chimera is used to run simulations aiming to investigate possible yield degradation mechanisms of ICF experiments. Using synthetic diagnostics alongside these simulations could reveal the observable signatures of such features and also provide an additional comparison of simulated and experimental data. Current measurements at NIF include neutron and X-ray spectroscopy as well as gated neutron and X-ray imaging. From simulated datasets, similar synthetic images and spectra can be produced accounting for instrument response and positioning. Neutron transport for attenuated unscattered and singly scattered neutron flux can be performed expediently via an inverse ray trace method [1]. This can be used to create 2D images at a detector. Fluence compensation [2] can be used to decouple the effect of neutron fluence on the shape of the scattered image in order to produce an image more accurately imaging the $\rho R$. Full neutron spectrum information is computationally expensive to transport in 3D in both the ray trace and Monte-Carlo methods. We developed a 1D spherical multigroup discrete-ordinates neutron transport code to analyze possible spectral signatures available to 1D implosions. This allows synthetic measurements of the Down Scattered Ratio (DSR) and the shape of the back-scatter edge from the DT reaction neutron source. Other neutron sources such as DD reactions can also be included, allowing for yield ratio measurements. The unscattered and n-th scattered fluxes can be isolated and the scattering kernel is handled without Legendre polynomial expansion [3].

Numerical Approaches - Computational Fluid Dynamics (CFD)

P:14 Three-dimensional multi-material methods for diffusion

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For high speed flows with large material distortions the Arbitrary Lagrangian Eulerian (ALE) or Eulerian techniques can be used [1]. For Inertial Confinement Fusion (ICF) simulations the evolution of material surfaces become distorted and non-aligned with the computational mesh. In particular, for ALE or Eulerian simulations the mesh alignment cannot be guaranteed, and sub-cell physics models for energy diffusion in multi-material cells must be considered. For this a volume of fluid (VoF) approach is adopted for interface reconstruction. In this paper we will present three different three-dimensional multi-material methods based on improved physical accuracy and associated increase in complexity. The first will be based on simple homogenisation. For the second will be describe a method based on static condensation or hybridisation [2] where local representations of the multi-material cells are included. For the third, and most general, we will describe an approach based on the construction of an unstructured polyhedral supermesh from the underlying base mesh. We present results for a series of test problems that are simple and relevant for code verification. It will be shown that the most general approach produces superior results over the simpler homogenised scheme and that its numerical convergence properties are optimal, while the simpler approach performs poorly [3]. As illustrated in Figure 1, results will be shown for a cylindrical test problem where it is clear that within multi-material cells the diffusion of energy does not propagate correctly near the surfaces when the homogenised scheme is used.

Figure 1: Correct profile (left) and poor behaviour using homogenisation (right).

Numerical computation of microtearing modes in slab geometry

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Microtearing modes are fine-scale tearing modes with large toroidal and poloidal mode numbers [1]. They are one kind of resistivity-driven instabilities tending to be driven in the vicinity of rational flux surfaces and forming a chain of magnetic islands. These modes can increase anomalous electron thermal transport in tokamaks [1,2,3], and can cause loss of confinement in the high pressure gradient edge pedestal region [3,4]. The stability of microtearing modes has previously been shown to be influenced by trapped electron dissipation, ion magnetisation and collisional broadening of passing electron Landau resonance [5] and in some cases can be extremely unstable [6]. Previous research has shown that microtearing modes can be driven by an electron temperature gradient and the energy dependence of the collision operator plays a key role in a slab geometry [2,6,7]. However some recent toroidal gyrokinetic simulations have suggested a collisionless branch exists [3,8]. So far the mechanism of collisionality in driving microtearing modes in toroidal geometry is not yet fully understood. My research begins by reviewing the results of Gladd et al [2] in the slab model, which does not capture the collisionless mechanism. This is the first stage of my research plan, which is to understand the mechanisms governing micro-tearing modes in collisional, semi-collisional and collisionless plasma regimes, ultimately in toroidal geometry. My poster in this conference will review the theory in slab geometry, make initial comparisons of my numerical results with the slab results of Gladd, and discuss the development of a new code that will solve a toroidal extension this system in different collisionality regimes.

Mesh-free Hamiltonian implementation of two dimensional Darwin model

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A new approach to Darwin [1] or magnetoinductive plasma simulation is presented which combines a mesh-free field solver with a robust time-integration scheme avoiding numerical divergence errors in the solenoidal field components. This approach achieves the compromise to model low-frequency electromagnetic phenomena, by neglecting the light waves, which are often source of numerical noise and thus removing the strong computational efforts due to the CFL constrain. The mesh-free formulation is implemented within the PEPC framework [2] and it employs an efficient parallel Barnes-Hut tree algorithm to speed up the computation of fields summed directly from the particles, avoiding the necessity of divergence cleaning procedures typically required by particle-in-cell (PIC) methods. The time-integration scheme employs a Hamiltonian formulation of the Lorentz force, circumventing the development of violent numerical instabilities associated with time differentiation of the vector potential. It is shown that a semi-implicit scheme converges rapidly and is robust to further numerical instabilities which can develop from a dominant contribution of the vector potential to the canonical momenta. The model is validated with various static and dynamic benchmark tests, including a simulation of the Weibel-like filamentation instability in beam-plasma interactions. This work was supported by the Helmholtz Association Grant HIRG-0048.


On secondary contributions to the formation of an Internal Transport Barrier

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In many experiments (especially the Reversed Magnetic Shear), as a result of the combined effect of NBI and ICRH an internal transport barrier is generated, with substantial improvement of confinement in the core. It has been noted that the layer of poloidal rotation is relatively narrow on the minor radius. For the generation of the ITB and its strong localisation (i.e. narrow radial extension) two possible explanations can be formulated, to be added to the usual Reynolds stress origin. One relies on the additional torque due to a local Stringer mechanism [1]-[2]. At counter injection a large fraction of NBI ions is lost from plasma. A NBI ion that remains in the plasma starts from the point of ionization and has a transitory phase in its travel, till it occupies the large, periodic motion on the banana orbit. Both these currents (direct loss and expansion up to banana) are not radial but are directed almost along the equatorial plane, due to up-down symmetry. Therefore they produce an additional poloidal nonuniformity (besides the neoclassical transport one), which leads to a new torque through the Stringer mechanism. We will examine quantitatively this processes, i.e. the loss to the edge (and the return current) and the transitory phase when they occupy their large banana orbits. Like for Reynolds stress, where the sheared poloidal rotation acts against the turbulence, i.e. its cause, for the Stringer mechanism the poloidal rotation smooths out the nonuniformity of the fluxes and reduces the torque. This acts like an intrinsic saturation mechanism. The second hypothesis involves the conversion of the profile of the shock associated to poloidal rotation from a radially extended "line" to a pair of close magnetic surfaces, when the poloidal rotation velocity becomes comparable to the poloidally
projected sound speed. We will try to examine qualitatively the aspects related to the numerical implementation [3].


**P:18 Coupled radiation–hydrocode and VFP code modelling of non-local transport effects in hohlraum energetics**

R Kingham¹, M Marinak², C Ridgers³ and J Brodrick³

¹Imperial College London, UK, ²Lawrence Livermore National Laboratory, USA, ³University of York, UK

The current ‘state of the art’ rad-hydrocode calculations of x-ray drive generation in indirect-drive modelling of NIF hohlraums employ a combination of the Schurtz- Nicolaï-Busquet (SNB) reduced non-local electron transport model [1] and the DCA atomic physics package. SNB removes the need for phenomenological flux-limiters and provides a description of pre-heat. Nevertheless, time dependent multipliers on the x-ray drive are still need to match implosion dynamics for hohlraums with higher density gas-fills [2], which may indicate the need to further improve these packages [3]. In an attempt to validate the SNB model in this context, we are developing the capability to couple together the rad-hydrocode HYDRA and the electron Vlasov-Fokker-Planck (VFP) code IMPACT [4], so that IMPACT can provide a more detailed non-local electron transport capability to HYDRA, particularly in the gas-fill and the wall plasma undergoing heating and ablation. We will describe the coupling approach and present preliminary calculations from a 1D surrogate hohlraum. The goal is to compare the temperature evolution and X-ray emission from this method with the standard modelling approach.

This builds upon our recent work where we compared non-local heat-flow determined by IMPACT and SNB from instantaneous Te, ne and Z* profiles from a 1D surrogate gadolinium hohlraum. There we found discrepancies between the VFP and SNB heat-flow profiles, even after tuning the SNB model [5]. The aim here is to understand the effect of such discrepancies on an integrated calculation of X-ray drive in indirect drive ICF.

Implementing Anisotropic Thermal Conduction on the ALE Grid for the Odin Radiation-Hydrodynamics Code

M Read¹, C Ridgers¹, R Kingham², T Goffrey ³, ⁴, K Bennett³ and T Arber³

¹University of York, UK, ²Imperial College London, UK, ³University of Warwick, UK, ⁴University of Exeter, UK

Electron heat-flow in laser-plasmas is important on nanosecond timescales, for example in the context of inertial confinement fusion (ICF) schemes. Such heat-fluxes are modified in the presence of a magnetic field i.e., as the electron transport becomes magnetised. It is well known that heat-flow is suppressed perpendicular to a B-field as electrons orbit around fieldlines due to the Lorentz force. Accurate simulation of such effects is especially important for understanding the many recent experimental schemes involving the application of B-fields to improve both direct- and indirect-drive ICF [1, 2] and due to the prevalence of strong self-generated ($\mathbf{\nabla} n \times \mathbf{\nabla} T$) fields in laser-plasmas. Additionally, the direction of heat-flow can be rotated perpendicular to temperature gradients as in Righi-Leduc heat-flow, an effect which has recently [3] been shown to be important during fuel capsule implosions. Electron transport in the presence of a B-field is described (in the local case) by the equations of classical transport [4]. Here we discuss the implementation of magnetised heat-flow into Odin – a 2D radiation-hydrodynamics code which is currently being developed as a tool for the UK laser-plasma community. Odin uses an Arbitrary Lagrangian Euler (ALE) scheme, meaning that grid cells can be deformed and non-orthogonal. Odin now includes an isotropic thermal conduction module on the ALE grid which uses super time-stepping [5] and is based on the Pert [6] 9-point difference stencil (a 2D finite-difference scheme for non-orthogonal grids).

Here we present an extension to the Pert scheme accounting for anisotropic thermal conduction using a tensor conductivity coefficient i.e., $q = -\kappa \cdot \mathbf{\nabla} T$. This provides a simple implementation of magnetised heat-flow in Cartesian geometry in the presence of B-fields ($\mathbf{B} = (B_1, B_0, B_1)$). The advantages and potential drawbacks of this scheme are presented along with the results of a number of known test cases and future plans for application.

Scientific software development - Data handling and IO

P:20 Python Script in the processing of electrochemical impedance spectroscopy and current transient measurements for the determination of the chemical capacitance

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Universidad Industrial de Santander CMN, Spain

Big Data is defined in a variety of ways, including a) the search and retrieval of information to make decisions [1, 2], and b) the science behind the data when these are used to respond any question [3, 4]. On other hand, chemical capacitance (a fundamental thermodynamic quantity related to charge accumulation at an electronic conductor/ionic conductor interface), is conventionally obtained by electrochemical impedance spectroscopy (EIS) [5]. Herein, current transients (CT) are proposed as an alternative measurement to determine the chemical capacitance. Thus, we describe a Python script to evaluate whether chemical capacitance can be obtained by CT collected at multiple potentials. The experimental procedure was performed with the redox pair Fe(CN)$_6^{3-}$/Fe(CN)$_6^{4-}$, a model one electron outer sphere process, and applied to the derivation of the chemical capacitance of the redox-active species on a Pt electrode. To validate the methodology here proposed is necessary to organize, process, and matching between these two different types of measurements, like so display information in the form of mathematical models, plots and files. Hence, we develop a protocol to analyze and compare a large amount of data irrespective of time scale. Usually, the experimental data for CT and EIS are analyzed independently and in different ways by computational programs, for instance, repeating the sampling process for different times yields a family of curves named "sampled current-voltammograms", one for each time scale. In addition, EIS data may be presented in several types of plots (e.g., Bode or Nyquist), which increase the volume of information obtainable from these measurements. Therefore, a getData class was created to get and process the experimental data from CT and EIS measurements. To process the experimental data a Python script was used to instantiate two objects: input and data objects. An input object is a JSON-like object where the file name and the potential for experiment data are defined, thereby JSON object was implemented as a Python dictionary. A data object is the instantiated getData object with the information contained in the data files referenced in the input object. A Python script containing the input and data objects was created to process experimental data of Fe(III)/Fe(II) redox pair in solution. A total of 64 data files were obtained with NOVA 2.0 software for electrochemistry. Each CT data file contains approximately 15000 experiment numbers, and EIS, 305. With instantiate getData object the capacitance curves against potential from EIS and CT was constructed and compared in an easier way than process data with traditional tools used in electrochemistry. It is concluded that at a specific condition of time scale, the integral of CT and EIS measurements give similar results of capacitance.

Using GPGPU Hardware In An Integrated Modelling Framework To Forecast Fast Ion Distributions In 3D Fields In ITER

S H Ward¹, R Vann¹, R Akers² and S Pinches³

¹University of York, UK, ²Culham Science Centre, UK, ³ITER Organization, France

If ITER is to achieve its aim of $Q=10$, suprathermal ions must be sufficiently confined to provide a dominant source of heating without damaging plasma-facing components (PFCs). However, waves within the plasma, such as toroidal Alfvén eigenmodes, and 3D field features, such as toroidal ripple or resonant magnetic perturbations, are likely to degrade fast ion confinement in ITER [1]. Studies conclude [2] that higher-order interactions must be included if modern physics simulations are to accurately reproduce this fast ion-wave coupling.

Until recently, resolving these higher-order effects had been computationally intractable for desktop hardware. The LOCUST (the Lorentz Orbit Code for Use in Stellarators and Tokamaks) Monte Carlo code alleviates this problem by utilising highly extensible and parallelisable General-Purpose Graphics Processing Units with OpenMP CPU threads. Over a matter of hours, millions of fast ions are tracked in the presence of 3D fields and a tokamak mesh to produce smooth phase space distribution functions and high fidelity PFC heat loads. This makes LOCUST ideal for routinely including key physics in reactor design workflows.

This work describes the LOCUST code and its application in future ITER fast ion studies whilst outlining the current status of development. Specifically, the testing of LOCUST against experimental measurements, such as the fast ion D- diagnostics on MAST-U and ASDEXU, and the benchmarking against other well established codes, such as ASCOT [3], will be detailed. Finally, LOCUST's inclusion as a synergistic module in ITER's Integrated Modelling and Analysis Suite will be described. A focus of the ITPA energetic particle physics topical group, this software framework will supplement experimental campaigns by combining physics codes to virtually reconstruct aspects of proposed ITER operating scenarios. Synthetic diagnostics and control can then be included to forecast fast ion measurements with associated errors in a standardised ITER data model for direct comparison with experiment.

The views and opinions expressed herein do not necessarily reflect those of the ITER Organization.


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