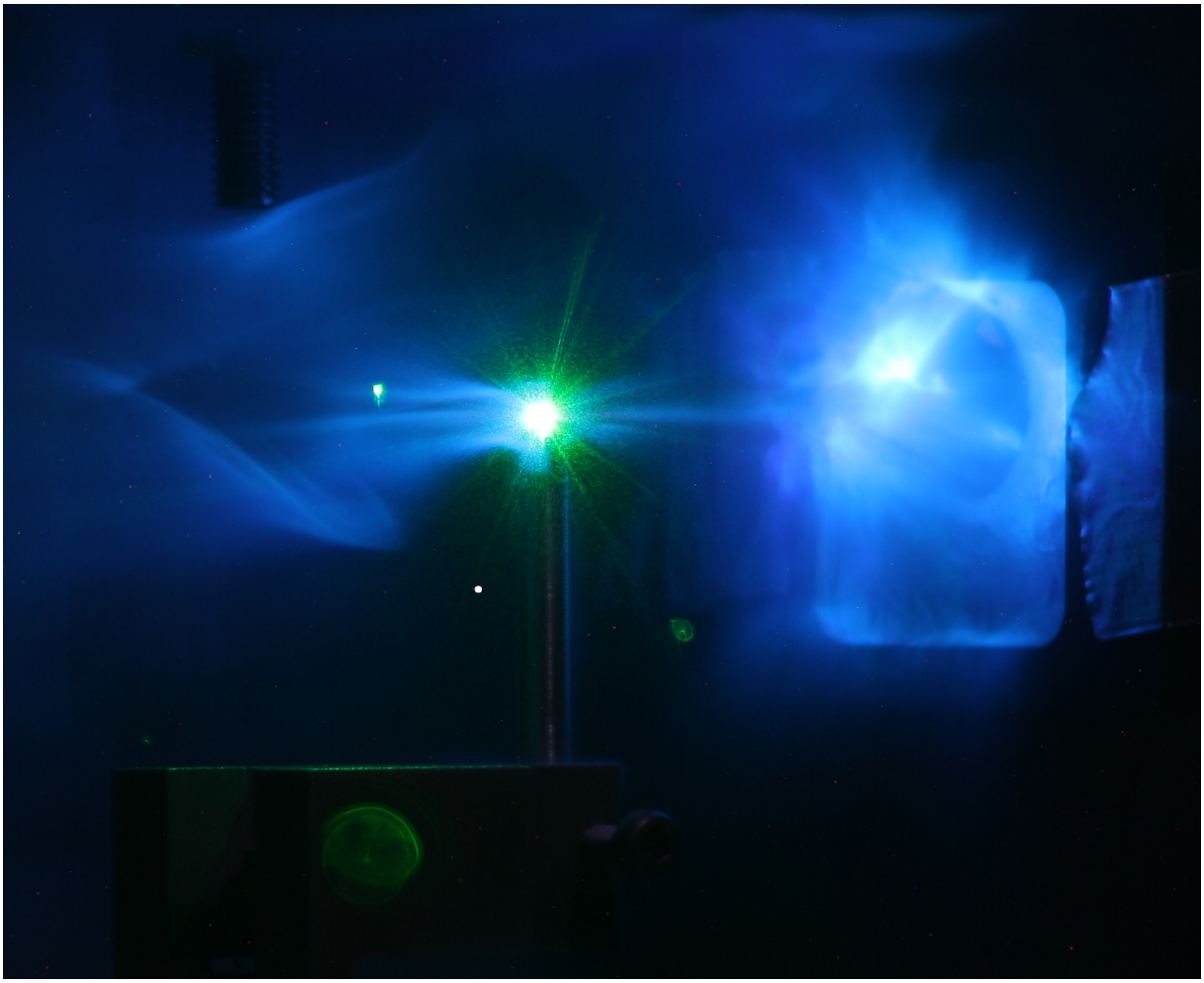
SUMMER 2014

IOP | Institute of Physics
Computational Physics Group

Newsletter



The creation of a dense, non-ideal plasma in the laboratory using a high power laser.
(image courtesy of James Mithen)

Newsletter Contents

This Newsletter... **3**

Molecular dynamics simulations of non-ideal plasmas **4**

Writing parallel programs with Fortran 2008 coarrays **12**

New EPSRC Centres for Doctoral Training **20**
CDT in Next Generation Computational Modelling 20
CDT in Theory and Modelling in Chemical Sciences 21
CDT in Computational Methods for Materials Science 22
CDT on Theory and Simulation of Materials 23

Computational Physics Group News **24**
The Computational Physics Annual PhD Thesis Prize 24
IoP Computational Physics Group - Research Student Conference Fund 24

Conference and Workshop reports **25**
UK Monte Carlo User Group Meeting (MCNEG 2014) 25
Recent Appointees in Materials Modelling (RAMM) Conference 2014 29

Upcoming Events of Interest **30**

Computational Physics Group Committee **31**

Related Newsletters and Useful Websites **31**

This Newsletter...

Dear Readers,

The feature article for this bumper edition of the newsletter is an invited contribution by James Mithen from the University of Surrey, our runner-up of the 2012 IoP Computational Physics Group PhD Prize, on *'Molecular dynamics simulations of non-ideal plasmas'*. We also have an a second feature article entitled *'Writing parallel programs with Fortran 2008 coarrays'* kindly provided by Anton Shterenlikht, an IoP CPG member from the University of Bristol. Thanks again to James and Anton for their contributions.

In addition, we have a series of short articles that describe the new EPSRC Centres for Doctoral Training (CDTs) that have a strong connection with computational physics. We also have two comprehensive reports from the recent MCNEG 2014 and RAMM 2014 meetings.

If any CPG member would like to provide similar articles for future editions of the newsletter that they feel would be of interest to the rest of our readership then please contact the Editor.

Most URLs in the newsletter have web hyperlinks and clicking on them should take you to the corresponding page. The current edition of the newsletter can be found online at:

`www.iop.org/activity/groups/subject/comp/news/page_40572.html`

with previous editions at:

`www.iop.org/activity/groups/subject/comp/news/archive/page_53142.html`
`www.soton.ac.uk/~fangohr/iop_cpg.html`

As always, we value your feedback and suggestions. Enjoy this edition!

David Shipley, Newsletter Editor ✉ david.shipley@npl.co.uk)

(on behalf of the The Computational Physics Group Committee).

Molecular dynamics simulations of non-ideal plasmas

Dr James P. Mithen
Department of Physics, University of Surrey, Guildford, GU2 7XH, UK
✉ j.mithen@surrey.ac.uk)

Introduction

Matter under extreme conditions, for example matter at high temperature and/or pressure, is of fundamental interest in physics.
A plasma, which consists of positively charged ions and negatively charged electrons, is typically thought of as an example of matter under extreme conditions. The relatively high energy required to ionise atoms means that plasmas exist at high temperatures, usually measured in units of electron-volts ($1eV \approx 11,000K$). Plasmas are therefore rather uncommon in our everyday experience on earth. But they are certainly prevalent elsewhere, by some estimates forming 99% of the visible universe [1].
Although often thought of as hot ionised gases, plasmas in fact span a vast range of densities and temperatures. Many found in nature and studied in the laboratory are indeed akin to hot gases. For example, the ITER tokamak, a device designed to prove the viability of magnetic confinement fusion, will aim to confine a plasma with ion density $n \approx 1 \times 10^{14} cm^{-3}$ (which is essentially 'vacuum' density) and temperature $k_B T = 8keV (\approx 10^8 K)$ [2]. But compared to this, many plasmas are relatively 'dense and cold'. For example, the interior of the planet Jupiter consists mainly of a hydrogen plasma, with $n \approx 6 \times 10^{24} cm^{-3}$ (approximately solid density) and $T \approx 1eV$ $(10^4 K)$ [3, 4].
As might be expected, these dense and cold plasmas exhibit very different physical properties from gaseous and hot plasmas. Most notably, as temperature decreases or density increases, the ions in the plasma start to exhibit short range structural order, not unlike that in a normal liquid. This structural order has a profound influence on the physics of the plasma. But it is completely neglected by conventional plasma physics [1, 5], which is concerned with the high temperature, gaseous plasmas only, and is therefore inapplicable. We call the gaseous and hot plasmas for which conventional plasma physics applies 'ideal' plasmas, and the dense and cold plasmas for which it does not apply 'non-ideal' plasmas.
In the last decades, it has become possible to create and study non-ideal plasmas in the laboratory using high power lasers. In particular, X-ray scattering experiments have been able to probe the fundamental physics of these complex states of matter [6]. A recent development is that the X-ray source is provided by a Free Electron Laser (FEL) [7]. These so-called 'fourth-generation' light sources promise to reveal unprecedented details of the microscopic dynamics of non-ideal plasmas. To motivate, inspire, and assist with modelling and interpretation of forthcoming experiments, theoretical insight into the physics of non-ideal plasmas is needed.
But alas, a non-ideal plasma is a rather complex state of matter. In principle an accurate description needs to take into account detailed atomic physics, including the quantum mechanics of partial electron degeneracy, ionisation and recombination processes, and so forth [8]. This is a heady task. Here, an alternative approach is taken, an approach articulated in the pioneering work of Brush, Sahlin and Teller [9], in which the authors suggest:

> "... it seems appropriate to ... study the properties of some simple models which share at least some of the essential features of real physical systems."

Here, simple model systems of non-ideal plasmas are studied, where the single most important 'essential feature' shared with real physical systems is the presence of liquid-like structural order between the ions. Two model systems are studied: the Coulomb one-component plasma (OCP) and the Yukawa one-component plasma (YOCP). The main focus is on the equilibrium properties of these systems, since these can in principle be measured in the X-ray scattering experiments. In addition, when calculated 'exactly' using computer simulations, the equilibrium properties can be compared to theoretical models, leading to

a more comprehensive understanding of the physics of the OCP and YOCP, and hence of non-ideal plasmas in general.

Model systems for non-ideal plasmas

When can we call a plasma 'non-ideal'? A simple quantitative criterion is provided by the dimensionless Coulomb coupling parameter [3, 10],

$$\Gamma = \frac{(Ze)^2}{4\pi\epsilon_0}\frac{1}{ak_BT}\,. \tag{1}$$

Here Ze is the ion charge (Z is a positive integer), $a = (3/4\pi n)^{1/3}$ is a measure of the average spacing between the ions (n is the ion number density), and T is the temperature.
The coupling parameter Γ is the ratio of the average potential energy between two ions, $(Ze)^2/4\pi\epsilon_0 a$, to the average thermal (kinetic) energy of an ion, k_BT. When Γ is small, the potential energy effects are small and the dynamics are dominated by the thermal energy; this is an ideal plasma, which can in principle be adequately described by conventional plasma physics. As Γ increases, a plasma changes from this nearly collisionless, gaseous regime (ideal) into an increasingly correlated, dense, liquid-like regime (non-ideal). Conventionally (and, of course, slightly arbitrarily), a non-ideal plasma is taken to be a plasma for which $\Gamma \geq 1$ [3, 10]. For the tokamak plasma mentioned previously, $\Gamma \approx 1 \times 10^{-6}$, but for the interior of Jupiter, $\Gamma \approx 50$.
Here we restrict our interest to the dynamics of the *ions* in a non-ideal plasma. We therefore model a non-ideal plasma as a single-component fluid of ions with 'effective' interactions. In the simplest model of a non-ideal plasma, two ions separated by a distance r interact via the Coulomb potential

$$v(r) = \frac{(Ze)^2}{4\pi\epsilon_0 r}\,. \tag{2}$$

In this approximation, the electrons are assumed to form a uniform background of charge [10, 11]. This model is known as the one-component plasma (OCP). It can only be expected to be at all realistic in the high density limit, in which the electrons are highly degenerate [3].
A more realistic model is the Yukawa one-component plasma (YOCP). In this case, the ions are taken to interact via the Yukawa or screened-Coulomb potential,

$$v(r) = \frac{(Ze)^2\exp(-r/\lambda_s)}{4\pi\epsilon_0 r}\,. \tag{3}$$

Physically, the faster decay of the ion-ion interactions due to the $\exp(-r/\lambda_s)$ term not present in Equation (2) is due to 'screening' by the electrons; λ_s is the electronic screening length. The electrons in the plasma form a 'cloud' around each ion, thus shielding the ionic charge from distant ions. For an ideal plasma this phenomenon is known as Debye screening, and λ_s is the Debye length, which can be related to the density and temperature of the plasma. For a non-ideal plasma, the Debye length is not necessarily the most sensible choice for λ_s, and so we treat it here as a variable parameter in the potential. The YOCP is a reasonable model system of a non-ideal plasma: although the electron dynamics are not included, these are irrelevant on the much longer time scale of the ion dynamics that are of interest here.
In equilibrium at temperature T, the OCP can be completely characterised by the dimensionless coupling parameter Γ defined in Equation (1). The YOCP can be characterised by two dimensionless parameters, the coupling parameter Γ and the screening parameter κ, defined as

$$\kappa = \frac{a}{\lambda_s}\,, \tag{4}$$

where again $a = (3/4\pi n)^{1/3}$.

Here we study the equilibrium properties of the OCP and YOCP systems for a wide range of Γ and κ values. We focus on the equilibrium dynamics, and in particular on a quantity known as the dynamical structure factor (DSF), defined as

$$S(k,\omega) = \frac{1}{2\pi N}\int_{-\infty}^{\infty}\langle n(\boldsymbol{k},t)n(-\boldsymbol{k},0)\rangle e^{i\omega t}dt \tag{5}$$

where $n(\boldsymbol{k},t)$ is the spatial Fourier transform of the microscopic particle density and $\langle\cdots\rangle$ denotes an ensemble average. When determined from computer simulations, the ensemble average is approximated as a time average [12].

It can be shown that the DSF in Equation (5) is proportional to the scattered intensity measured in an inelastic x-ray scattering experiment, with the wave number $k = |\boldsymbol{k}|$ determined by the experimental geometry, and $\hbar\omega$ the energy shift of the scattered x-ray photons [11]. Therefore, by studying the DSF, we are able to make predictions and give insight into x-ray scattering experiments on real non-ideal plasmas.

Computational Methods

The main technique we use here is well known—classical molecular dynamics (MD) in a box with periodic boundary conditions [13]. Despite this, the simulations are extremely challenging for two reasons. Firstly, we look to elucidate the dynamics of both the YOCP and the OCP *at long length scales*. This requires a large box, and therefore a large number of particles. Simulating a large number of particles is particularly costly in this case, due to the long range interactions in the YOCP and OCP. The simulations require an advanced code with an efficient parallel implementation of the Ewald summation technique for dealing with long range interactions, the so-called Particle-particle-particle-mesh algorithm [14].

Secondly, to compute time correlation functions—such as the density-density correlation function $\langle n(\boldsymbol{k},t)n(-\boldsymbol{k},0)\rangle$ that appears in Equation (5)—accurately, extremely long simulations are needed, particularly at long length scales where the time correlation functions decay slowly. The combination of a large number of particles and long times, along with the desire to conduct a comprehensive investigation of the dynamics of both systems (i.e. to simulate a wide range of (Γ,κ) pairs), make the computational work an ambitious undertaking.

In the remaining sections, we briefly summarise the main results of the work. The results have been presented previously in journal articles [15, 16, 17, 18, 19], and a thesis [20]. The interested reader should consult these references for a more detailed presentation.

Hydrodynamic Models

Naviér-Stokes Hydrodynamics

One of the main contributions of this work is to recognise that hydrodynamic approaches that have been used previously to describe the dynamics of dense liquids [21, 22] can also be applied to non-ideal plasmas. One such hydrodynamic approach is provided by the Naviér-Stokes equations, which are widely used for investigating the dynamics of fluids in general, including gases, liquids, plasmas and nuclear matter. The Naviér-Stokes equations give a simple three peak description of the DSF in terms of familiar transport and thermodynamic coefficients [11, 20, 21]

$$\frac{S^H(k,\omega)}{S(k)/2\pi} = \frac{\gamma-1}{\gamma}\frac{2D_Tk^2}{\omega^2+(D_Tk^2)^2} + \frac{1}{\gamma}\left[\frac{\sigma k^2}{(\omega+c_sk)^2+(\sigma k^2)^2} + \frac{\sigma k^2}{(\omega-c_sk)^2+(\sigma k^2)^2}\right]. \tag{6}$$

Here γ is the ratio of specific heats, D_T is the thermal diffusivity, c_s is the speed of sound, and σ is the 'sound attenuation coefficient', which is related to the shear and bulk viscosities [11]. These quantities are all reasonably well known for the OCP and YOCP systems.

Investigating the applicability of Equation (6) is certainly worthwhile from the perspective of X-ray scattering experiments. For the experiments one usually needs to model the DSF for a wide range of densities and temperatures. There already exist a number of rather involved approaches to doing this, some of which have proven to be successful in certain regimes [8, 10]. But compared to these approaches, the Naviér-Stokes description of Equation (6) retains a rather simple physical picture in terms of fundamental transport and thermodynamic properties of the plasma.

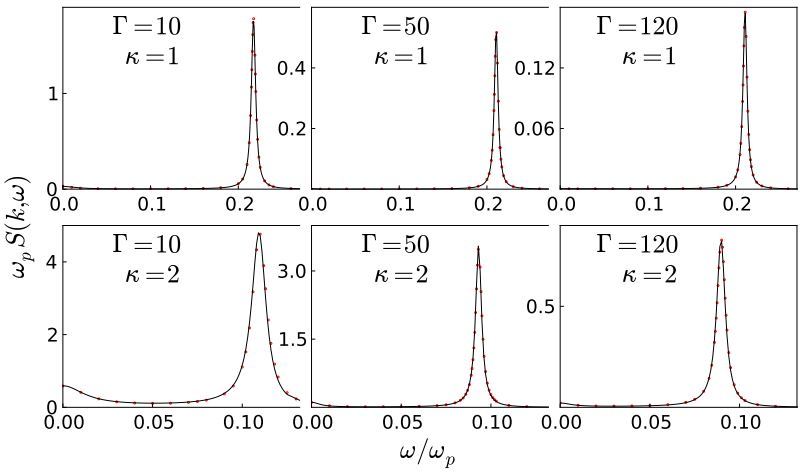


Figure 1: MD results for the DSF $S(k,\omega)$ (dots) at the smallest reduced wave number accessible to the simulations ($ka = 0.23$), plotted alongside the hydrodynamic DSF $S^H(k,\omega)$ given in Equation (6) (solid lines) for six different (Γ,κ) pairs.

To asses the applicability of the Naviér-Stokes description, we compare the DSF of the YOCP for a wide range of (Γ,κ) pairs as computed using MD simulations to the Naviér-Stokes DSF in Equation (6). To reach the long length scales that are relevant to this continuum hydrodynamic description requires up to 10^6 particles—a very large number for systems with long range interactions.

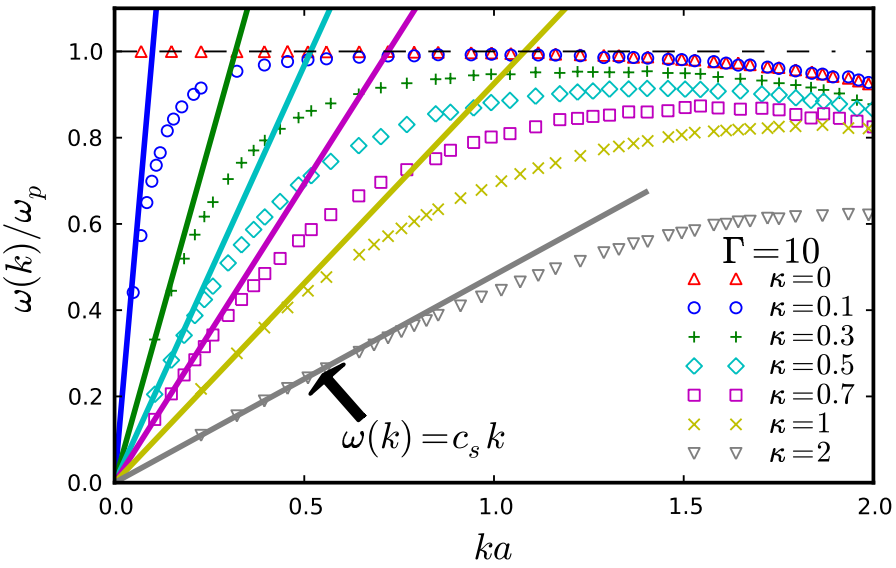


Figure 2: Position of ion-acoustic peak in DSF (this is the peak shown in Figure 1) as obtained from MD simulations (open symbols), showing the breakdown of the Naviér-Stokes dispersion relation $\omega(k) = c_s k$ (solid lines, c_s is the sound speed).

As expected, the Naviér-Stokes description is found to be applicable at long length scales (small wave

numbers k), as shown in Figure 1. But it is also found to remain applicable up to surprisingly short length scales (see Figure 2, and Ref. [15] for further details). A quantitative criterion for the breakdown of hydrodynamics can be given in terms of the maximum wave number k_{max} at which the hydrodynamic description applies, $k_{max}\lambda_s \simeq 0.43$. That this criterion is found to be independent of the level of non-ideality of the system Γ is rather surprising—intuitively one might expect the range of length scales for which hydrodynamics is applicable to increase (and thus k_{max} to increase) with increasing Γ, since this corresponds to the system becoming more 'collisional'. But this is not found to be the case.
These results indicate that by resolving the ion dynamics in small angle X-ray scattering experiments, transport coefficients such as viscosity and thermal conductivity of non-ideal plasmas can in principle be measured. Indeed, it is expected that these measurements will soon be possible by taking advantage of the low bandwidth and high brightness characteristics offered by 'fourth generation' light sources, and X-ray scattering experiments to measure these properties at the LCLS facility are currently underway.

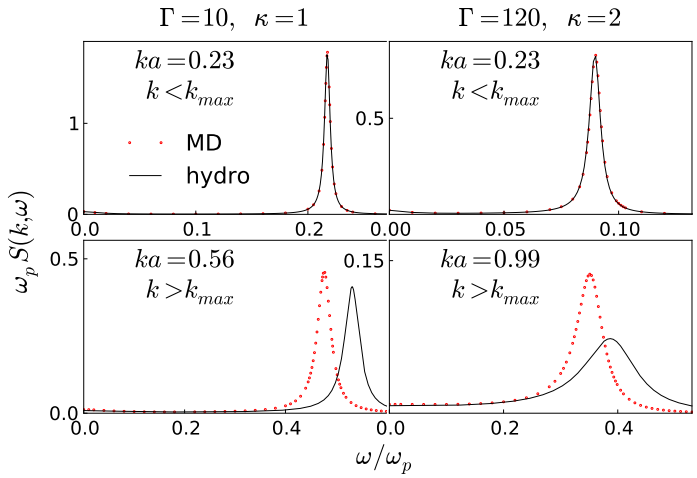


Figure 3: MD results for $S(k,\omega)$ (dots), plotted alongside the hydrodynamic DSF $S^H(k,\omega)$ given in Equation (6) (solid line). For the two (Γ,κ) pairs, examples are shown for wave numbers within the Naviér-Stokes regime $k < k_{max}$, and wave numbers outwith this regime $k > k_{max}$.

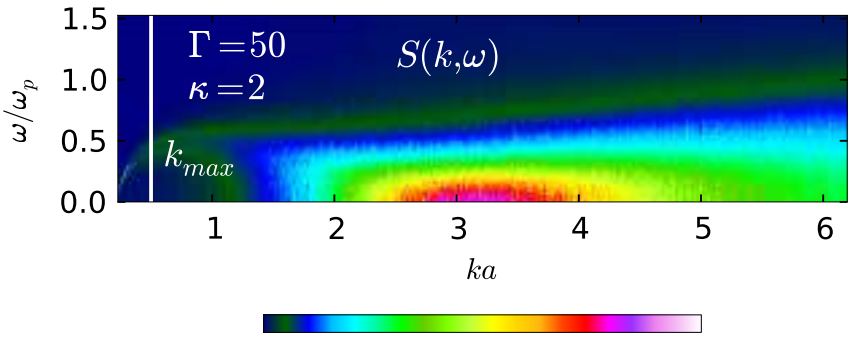


Figure 4: DSF of the YOCP. The entire region to the right of the line marked k_{max} requires models beyond Naviér-Stokes hydrodynamics.

Generalised Hydrodynamics

Despite the success of the Naviér-Stokes hydrodynamic description, for wave numbers $k > k_{max}$ all bets are off (see Figure 3) , unless k is very large, since then the DSF reduces to that of an ideal plasma, which can be

calculated analytically. The intermediate regime is rather large (see Figure 4), and it often encompasses the range of length scales that can be accessed by experiments (in experiments, larger k corresponds to higher momentum transfer of scattered photons). Therefore it is worthwhile searching for a theoretical model of the DSF of the YOCP that works for these higher k values (shorter length scales). The analogous problem for ordinary fluids is the central topic of a number of monographs on liquid-state theory [21, 22, 23].
Again, we compare the results of MD simulations to theoretical models of the DSF. We find that a simple model of so-called generalised hydrodynamics (a formalism in which the familiar transport and thermodynamic quantities are extended in a physically intuitive manner [22]) shows excellent agreement with the DSF obtained from MD (e.g. Figure 5). Remarkably, this is found to be the case for essentially all (Γ,κ) pairs, i.e. for all densities and temperatures, and all k values.

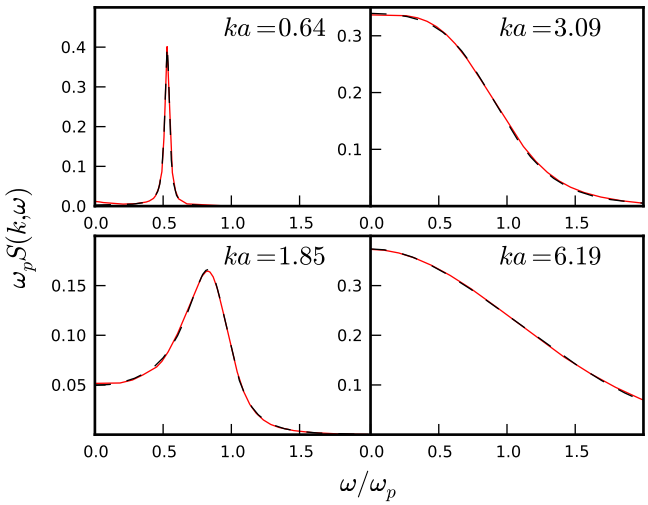


Figure 5: Results of MD simulations for the DSF of the YOCP (solid lines) and a simple model of generalised hydrodynamics (dashed lines) for a few k values. Here $\Gamma = 10$, $\kappa = 1$.

These results indicate that experiments can be interpreted as measuring 'generalised' transport coefficients of non-ideal plasmas. Furthermore, they emphasise the increasing effectiveness of the computational approach in physics: the highly accurate simulations that are possible with modern computing facilities allow for a conclusive comparison between competing theoretical models.

The OCP and the analogy between liquids and non-ideal plasmas

The inapplicability of the Naviér-Stokes description

The hydrodynamic description given by the Naviér-Stokes equations is ubiquitous; in principle it emerges in systems of particles with any interaction potential (i.e., in all monatomic fluids). However, there is one important exception to this: the Coulomb potential. To be sure, the peculiarity of the Coulomb potential is very well known—the longitudinal excitations in this case are not low-frequency sound waves (or ion-acoustic waves in the plasma case) as for the YOCP, but instead high-frequency plasma waves ($\omega = \omega_p$), even at $k = 0$ (see red triangles in Figure 2). In fact, one can wonder why hydrodynamics should describe plasma waves at all.
Baus and Hansen did indeed wonder exactly this some time ago [3]. Furthermore, they were able to show that a hydrodynamic description of the OCP would only be possible if the 'collisionality' dominates the mean field effects that lead to plasma oscillations. They predicted this would occur at some sufficiently high coupling parameter Γ.
By using large scale molecular dynamics simulations, we in fact find that the hydrodynamic description of

the OCP is never valid, even at large Γ values where the OCP behaves similarly to a dense liquid in many other respects (see [15] for more details).
This study highlights the fact that there are outstanding—some might say 'fundamental'—questions in physics that can now be resolved with the help of modern computing facilities. Tackling the question of the validity of the hydrodynamic description of the OCP, as posed by Baus and Hansen, would not have been possible (at least with the computational approach used here) at the when time this intriguing problem was first formulated (1980).

The analogy between liquids and non-ideal plasmas

The results discussed in the previous section highlight the peculiarity of the OCP: due to the long range Coulomb interactions, the OCP exhibits certain dynamical features not shared by ordinary liquids. Other features of the OCP however *are* shared by ordinary liquids. For example, it has been found that, for $\Gamma > 50$, the transport coefficients (self diffusion, viscosity, etc.) of the OCP obey universal laws satisfied by dense ordinary liquids [24]. It is the fact that the OCP shares some, but not all, properties with ordinary liquids that makes it a challenging yet fascinating system to study.
We investigate the complementarity of the liquid and plasma descriptions of the OCP by studying two approaches to modelling its dynamics: the memory function approach of generalised hydrodynamics and the so-called 'dynamic local field correction' (LFC) approach, which is more common to Coulomb systems such as the electron gas [10] (this is the plasma description).
To compare these approaches we compute both the memory function and the LFC; as an input this requires highly accurate MD simulations. High quality MD data is particularly important for computing the LFC, a quantity that has apparently never been computed in simulations previously.
We find that, at any given value of k, the memory function is very well approximated by a simple Gaussian function. The LFC, on the other hand, exhibits a rather more complicated functional form, and one that changes significantly with k (see [19] for further details). Experimentalists commonly use the LFC approach to incorporate non-ideality corrections, but these results suggest that this should be done with caution.

Discussion and Outlook

A thorough investigation of the equilibrium dynamics of two simple systems that can be used to represent a non-ideal plasma, the YOCP and the OCP, has been conducted. This centred around challenging, state of the art molecular dynamics computer simulations. For all of the research, the computational power needed was far beyond what was in reach of the theoretical research groups that looked at these systems in the 1970s (Hansen and co-workers) and 1980s (Ichimaru and co-workers).
The results contribute to the theoretical understanding of the YOCP and OCP systems, particularly of their dynamical properties. Despite recent trends moving towards the study of more complicated, i.e., more 'realistic' systems, the OCP and YOCP will no doubt be studied for years to come. It is hoped that the work summarised here can guide and inspire some of these future investigations. On a more mundane level, the MD data for the DSF of these systems that was produced for this thesis should certainly replace that of Hansen and co-workers [25, 26, 27], which—although a remarkable feat of computational physics at that time—is now more than thirty years old.
As well as contributing to the theoretical understanding of non-ideal plasmas, the research should find some application in the planning, understanding, and analysis of x-ray scattering experiments using high power lasers. This is particularly true for the studies of the YOCP, which is a system that can provide a reasonable representation of the ion dynamics in a non-ideal plasma. Although more sophisticated modelling will no doubt be necessary to capture the details of the expected experimental scattering profile, the fairly comprehensive analysis of the DSF of the YOCP summarised here is a useful first step. This work will help to at least guide future experimental efforts. In fact, some of the results are serving to assist with the planning of forthcoming experiments at high power laser facilities at the time of writing.

As for the discipline of plasma physics as a whole, it seems inevitable that molecular dynamics simulations of the type performed for this work will become more commonplace, and not only for studying 'cold and dense' non-ideal plasmas. These simulations can complement more coarse grained methods such as Particle-in-cell (PIC) that are currently widely used in plasma physics.

References

[1] F. F. Chen. *Introduction to Plasma Physics and Controlled Fusion: Vol. 1 (second edition)*. Springer, New York, 2006.

[2] B. McCracken and P. Stott. *Fusion: the Energy of the Universe*. Elsevier, London, 2005.

[3] M. Baus and J. P. Hansen. Statistical mechanics of simple coulomb systems. *Phys. Rep.*, 59:1–94, 1980.

[4] S. Ichimaru, H. Iyetomi, and S. Tanaka. Statistical physics of dense plasmas: Thermodynamics, transport coefficients and dynamic correlations. *Physics Reports*, 149(2âĂŞ3):91 – 205, 1987.

[5] N. A. Krall and A. W. Trivelpiece. *Principles of Plasma Physics*. McGraw-Hill, New York, 1973.

[6] S. H. Glenzer and R. Redmer. X-ray thomson scattering in high energy density plasmas. *Rev. Mod. Phys.*, 81:1625–1663, Dec 2009.

[7] R. R. Fäustlin, Th. Bornath, T. Döppner, S. Düsterer, E. Förster, C. Fortmann, S. H. Glenzer, S. Göde, G. Gregori, R. Irsig, T. Laarmann, H. J. Lee, B. Li, K.-H. Meiwes-Broer, J. Mithen, B. Nagler, A. Przystawik, H. Redlin, R. Redmer, H. Reinholz, G. Röpke, F. Tavella, R. Thiele, J. Tiggesbäumker, S. Toleikis, I. Uschmann, S. M. Vinko, T. Whitcher, U. Zastrau, B. Ziaja, and Th. Tschentscher. Observation of ultrafast nonequilibrium collective dynamics in warm dense hydrogen. *Phys. Rev. Lett.*, 104:125002, Mar 2010.

[8] D. Kremp, M. Schlanges, and W. D. Kraeft. *Quantum statistics of Nonideal Plasmas*. Springer-Verlag, Berlin, 2005.

[9] S. G. Brush, H. L. Sahlin, and E. Teller. Monte carlo study of a one-component plasma .i. *J. Chem. Phys.*, 45(6):2102–2118, 1966.

[10] S. Ichimaru. *Statistical Plasma Physics: v. 1: Basic Principles*. Westview Press, London, 2004.

[11] J. P. Hansen and I. R. McDonald. *Theory of Simple Liquids (third edition)*. Academic Press, London, 2006.

[12] D. Frenkel and B. Smit. *Understanding Molecular Simulation (second edition)*. Academic Press, London, 2001.

[13] M. P. Allen and D. J. Tildesley. *Computer Simulation of Liquids*. OUP, New York, 1988.

[14] R. Hockney and J. Eastwood. *Computer Simulations Using Particles*. McGraw-Hill, New York, 1981.

[15] J. P. Mithen, J. Daligault, and G. Gregori. Extent of validity of the hydrodynamic description of ions in dense plasmas. *Phys. Rev. E*, 83:015401, Jan 2011.

[16] J. P. Mithen, J. Daligault, B. J. B. Crowley, and G. Gregori. Density fluctuations in the yukawa one-component plasma: An accurate model for the dynamical structure factor. *Phys. Rev. E*, 84:046401, Oct 2011.

[17] J. P. Mithen, J. Daligault, and G. Gregori. Molecular dynamics simulations for the shear viscosity of the one-component plasma. *Contrib. Plasma Phys.*, 52:58–61, Jan 2012.

[18] J. P. Mithen, J. Daligault, and G. Gregori. Onset of negative dispersion in the one-component plasma. *AIP Conference Proceedings*, 1421(1):68–72, Feb 2012.

[19] J. P. Mithen, J. Daligault, and G. Gregori. Comparative merits of the memory function and dynamic local-field correction of the classical one-component plasma. *Phys. Rev. E*, 85:056407, May 2012.

[20] J. P. Mithen. *DPhil thesis*. University of Oxford, 2012.

[21] J.P. Boon and S. Yip. *Molecular Hydrodynamics*. Dover, New York, 1991.

[22] U. Balucani and M. Zoppi. *Dynamics of the Liquid State*. OUP, Oxford, 2002.

[23] N. H. March. *Liquid Metals: Concept and Theory*. Cambridge University Press, New York, 2005.

[24] J. Daligault. Liquid-state properties of a one-component plasma. *Phys. Rev. Lett.*, 96:065003, Feb 2006.

[25] J. P. Hansen. Statistical mechanics of dense ionized matter. i. equilibrium properties of the classical one-component plasma. *Phys. Rev. A*, 8:3096–3109, Dec 1973.

[26] J. P. Hansen, I. R. McDonald, and E. L. Pollock. Statistical mechanics of dense ionized matter. iii. dynamical properties of the classical one-component plasma. *Phys. Rev. A*, 11(3):1025–1039, Mar 1975.

[27] P. Vieillefosse and J. P. Hansen. Statistical mechanics of dense ionized matter. v. hydrodynamic limit and transport coefficients of the classical one-component plasma. *Phys. Rev. A*, 12:1106–1116, Sep 1975.

Writing parallel programs with Fortran 2008 coarrays

Dr Anton Shterenlikht
Mech Eng Dept, University of Bristol, University Walk, Bristol BS8 1TR, UK
✉ mexas@bris.ac.uk

Abstract

Coarrays are Fortran 2008 standard feature for parallel programming. This tutorial describes coarray syntax, efficient usage and synchronisation. A distinguishing feature of coarrays is simplicity, especially compared with MPI. But coarrays are also very flexible and powerful. Several complete coarray programs and code fragments are given. Speed-up of up to 3 orders of magnitude is demonstrated.

Basic coarray syntax

A major new feature of the Fortran 2008 standard [1] are coarrays, a native Fortran way to write SPMD (single program - multiple data) parallel programs. The best introduction to coarrays is given in [2]. Several coarray examples are given in [3, 4] and a single example in [5]. At this time coarrays are fully supported only by the Cray compiler. The Intel coarray support is good, but incomplete. G95 and GCC compilers provide partial coarray support (e.g. GCC supports only single image execution) [6].
So what are coarrays? Fortran 2008 standard introduced the square bracket notation, `[]`, to denote a coarray. For example, `integer :: i[*]` declares a *scalar integer coarray* and `real :: r(2,3)[*]` declares a *real array coarray* of shape `(2,3)`.
A 2008 compliant compiler is required to compile a program with these declarations. To execute the compiled program the runtime environment will spawn a required number of processes, send a copy of the

executable to each *processor* and direct all processors to execute the program in parallel. Each copy of the executable is called an *image*. The square bracket notation tells the compiler that all images have read and write access to this object on any image. The asterisk, `[*]`, means that the number of images is never hard coded in the program, and will be specified at compile or run time.
With this basic notation remote read and write operations are easy. Whenever a reference to a coarray object is made with the square brackets, a remote call is used. If the square brackets are omitted, the reference is made to the *local* variable, held on this image. For example, statement `i = i[3]` executed by every image will copy the value held in variable `i` in image 3 into the local copy of `i` on each image. This is a remote read. A remote write example is the statement `r(:,:)[5] = r`, which, executed by any image, will copy the local value of array `r` into the copy on image 5. Note that the semicolons are required when coarray notation is in use. Clearly this is an example of the race condition, because multiple writes are made to the same memory location. Fortran 2008 provides *image control* statements which help avoid the race conditions. These are described later.
The standard introduced two new intrinsic functions: `num_images`, which returns the total number of images created at runtime, and `this_image` which, when invoked with no arguments, returns the number of the invoking image. Note that, in accordance with the Fortran tradition, image numbers start from 1, not from 0, as in MPI.
With this we can write our first coarray program.

First coarray program

```
1 implicit none
2  integer :: img, nimgs
3  img = this_image()
4  nimgs = num_images()
5  write (*,"(2(a,i2))") "image: ", img, " of ", nimgs
6 end
```

Using Intel compiler, versions 12 to 14, this code is compiled with `ifort -coarray`. By default this will allow only the use of shared memory, i.e. the executable can be run only within a single node. Also by default, the runtime will spawn as many images as there are cores on the node, which are processors in the Fortran standard terminology. In this example we use a node with 16 cores. The program outputs:

```
$ ./a.out
image:  1 of 16
image:  2 of 16
image:  5 of 16
image:  3 of 16
image:  7 of 16
image:  6 of 16
image: 12 of 16
image:  4 of 16
image:  8 of 16
image: 10 of 16
image: 11 of 16
image: 14 of 16
image: 15 of 16
image: 13 of 16
image:  9 of 16
image: 16 of 16
$
```

With Intel runtime, the number of images can be set with `FOR_COARRAY_NUM_IMAGES` environment variable. So, without recompilation, we can run the same program on any number of images:

```
$ export FOR_COARRAY_NUM_IMAGES=2
$ ./a.out
image:  1 of  2
image:  2 of  2
$
```

Note that in this example we haven't actually used coarray objects. However, because we compiled the program with `-coarray` switch, the image control statements are understood and the executable will we linked against the relevant parallel libraries.

Coarray speed-up example

In the first coarray program there was no communication between images. In this example we calculate π using the Gregory – Leibniz series. Given the series upper limit, each image sums the terms beginning with its image number and with a stride equal to the number of images. Image 1 then sums the contributions from all images. To avoid the race condition, image 1 must make sure that all images have completed their calculations, before attempting to read the values from them. Hence some synchronisation between the images is required. The simplest coarray *image control* statement is `sync all`. This statement must be executed on all images. Its effect is that all images wait for each other at this point (line 15) and then proceed further.

```
 1 implicit none
 2 integer, parameter :: ik = selected_int_kind(10),   &
 3                       rk = selected_real_kind(15,3)
 4 integer(kind=ik), parameter :: limit = 2**32
 5 integer(kind=ik) :: i
 6 integer :: img, nimgs
 7 real(kind=rk), parameter :: one = 1.0_rk,           &
 8  piref = 3.14159265358979323846264338327950288_rk
 9 real(kind=rk) :: pi[*] = 0.0_rk
10 img = this_image()
11 nimgs = num_images()
12 do i=img,limit,nimgs
13  pi = pi + (-1)**(i+1) / real(2*i-1,kind=rk)
14 end do
15 sync all
16 if (img .eq. 1) then
17  do i=2,nimgs
18   pi = pi + pi[i]
19  end do
20  pi = pi * 4.0_rk
21  write (*,*) "Calculated  pi=", pi
22  write (*,*) "Absolute error=", pi-piref
23 end if
24 end
```

The program is compiled with `ifort -coarray` and timed with linux `time`:

```
$ setenv FOR_COARRAY_NUM_IMAGES 16
$ /usr/bin/time -f %E ./a.out
 Calculated  pi=   3.14159265335699
 Absolute error= -2.327986692307604E-010
0:01.76
$ setenv FOR_COARRAY_NUM_IMAGES 1
$ /usr/bin/time -f %E ./a.out
 Calculated  pi=   3.14159265335876
 Absolute error= -2.310365232460754E-010
0:18.40
```

By going from 1 to 16 cores a speed-up of over 10 was achieved, which is good. Several further points about this π code deserve a mention.
As with MPI, different strategies can be used to split the work between images. In this example we used strides greater that 1 in the `do` loop. A possible alternative would be to set a chunk size: `cs=limit/nimgs` and then use loops `do i=(img-1)*cs+1,img*cs`.
If the series limit is a multiple of the number of images, then the load balance is achieved, which is the key to high performance.
Coarray syntax usage should be minimised. This is because remote read/write operations are always much slower than local memory access. The only remote operation is in line 18.
Lines 16-23 are executed only on image 1. Note that image 1 always exists, so it makes sense to delegate all single image operations to it. Loop 17-19 involves a remote read operation - image 1 uses its own `pi` to sum the values from all other images. This is an example of a collective global reduction. Although there are no intrinsic collectives in the 2008 standard, technical specification TS 18508 [7] defines them. These are described briefly in section “Problems and future”.

Further coarray syntax and data structures

Coarrays can be allocatable objects. For example, specification statement `real :: r(:,:)[:,:]` declares an allocatable real array coarray with two *codimensions*. The values in brackets are array subscripts. By analogy the 2008 standard calls the values in square brackets *cosubscripts*. Cosubscripts can take values between the lower and the upper *cobound*. Intrinsic functions `lcobound` and `ucobound` return the lower and the upper cobounds respectively. This coarray can be allocated similarly to ordinary array allocation, e.g. `allocate(r(3,2)[2,*])`. Note that the upper cobound of the last codimension is never specified, i.e. asterisk is always used in its place. If the program with this statement is run on 8 images, then `lcobound` would return (1,1) and `ucobound` would return (2,4). Elements of this coarray can be referenced as e.g. `r(1,2)[1,4]`, which is element (1,2) on image [1,4]. `this_image` can take a coarray as an argument. In that case it returns the cosubscripts identifying the invoking image.
We already seen `sync all` image control statement, the effect of which is that all images wait for each other at that point. The standard provides also a more flexible image control statement, `sync images`, which provides synchronisation only between some images.
Fig. 6 illustrates all these concepts with three programs, all run on 4 images, manipulating a `real :: r(3,2)[2,*]` coarray. Colours highlight remote read/write calls.
Program 1 copies `r(1,2)` from image 1 into `r(1,1)` on image 3. The remote read call is issued on image 3. Because image 3 must wait until the data is ready on image 1, synchronisation is required between images 1 and 3. No synchronisation is required for images 2 and 4. Hence selected synchronisation, `sync images` is used here. Image 3 executes `sync images (1)` and waits until image 1 executes the *corresponding* image control statement: `sync images (3)`. The exact rules for corresponding image control statements are given in [1, 2].

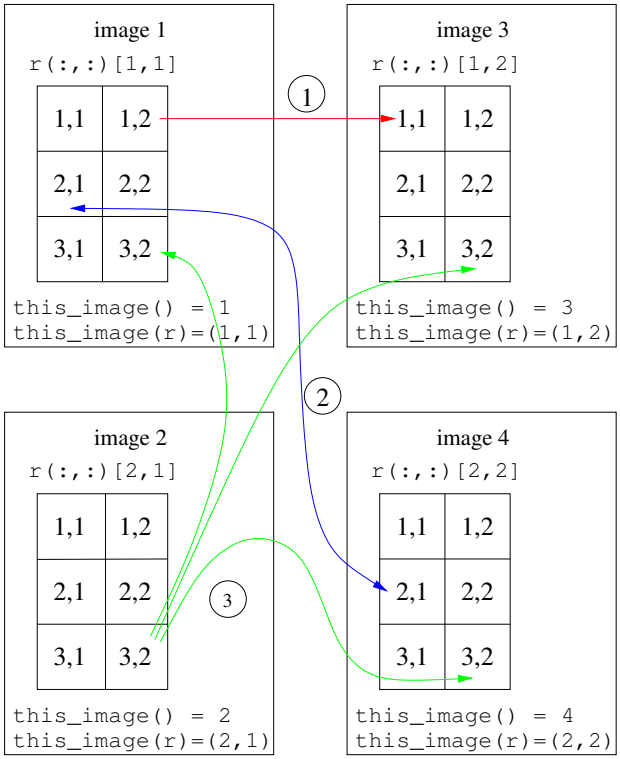
Program 2 swaps `r(2,1)` between images 1 and 4. Images 1 and 4 must first wait for each other until the data is ready to be read. This is the purpose of the first pair of the corresponding `sync images (1)` and `sync images (4)`. After images 1 and 4 synchronised, both images copy remote coarray value into the local, non-coarray variable `tmp`. Again, both images must wait for each other to make sure each has managed to read the other's value. This is the purpose of the second pair of the corresponding `sync images (1)` and `sync images (4)`. Only after that can both images overwrite their local value of `r(2,1)` with `tmp`.
In program 3 image 2 broadcasts its `r(3,2)` to all images. That includes itself, which is, of course, a wasted effort. However, adding checks to avoid this is likely to add more overhead. Image 2 must wait for all other images to set their `r(3,2)` before broadcasting its own. Hence `sync all` is used.
Note that `sync all`, the global barrier, is the easiest and least error prone image control statement. However, in the presence of load imbalance, global synchronisation is very inefficient, because all processor would be waiting for the slowest, thus wasting resources. This is particularly important for high processor counts.
In contrast, `sync images` is more flexible, allowing the programmer to synchronise only selected processors, thus potentially freeing all other processors to do useful work in the meantime. However, there is always a danger of deadlocks, which is notoriously hard to debug.

3D cellular automata simulation of trans-granular cleavage

This is a larger coarray program [8, 9]. A 3D space is partitioned into cubic cells, representing volumes of material at some user-defined scale. A cluster of cells represents a single crystal, a grain, and a collection of grains is a polycrystal. A cell has a 26-cell nearest neighbourhood, i.e. $3 \times 3 \times 3$ cells minus the central cell. The state of the central cell is determined by states of the neighbouring cells, and by some predefined field functions. Part of the neighbourhood of a boundary cell resides in an array on another image, hence halo exchange between neighbouring images is required. The model is defined as a coarray `integer, allocatable :: space(:,:,:)[:,:,:]`. The 3D image grid is chosen because it minimises the amount of internal halo exchange information. To store the halos, coarray `space` is allocated with size increased by 2 cells in each direction. Each image exchanges halos with 26 neighbouring images, except for images on the boundary of the coarray grid, for which halo exchange is more complex. Below is a code fragment, showing a halo exchange in direction 1 across a common face. The code is run on n^3 images.

```
allocate( space(0:11,0:11,0:11) [n,n,*] )
integer :: imgpos(3), lcob(3), ucob(3)
imgpos = this_image( space )             ! Image location in the coarray grid
lcob = lcobound( space )                 ! Lower cobound of space coarray
ucob = ucobound( space )                 ! Upper cobound of space coarray
if ( imgpos(1) .ne. lcob(1) ) &          ! For all images but the leftmost
 space(0, 1:10,1:10) =        &          ! copy the upper boundary cell states
 space(10,1:10,1:10)          &          ! into the lower halo array
  [imgpos(1)-1,imgpos(2),imgpos(3)]
if ( imgpos(1) .ne. ucob(1) ) &          ! For all images but the rightmost
 space(11,1:10,1:10) =        &          ! copy the lower boundary cell states
 space(1, 1:10,1:10)          &          ! into the upper halo array
  [imgpos(1)+1,imgpos(2),imgpos(3)]
```

Fig. 7(a) (from [9]) shows the predicted *equiaxed* microstructure typically found in normalised steels. This was obtained with `space(200,200,200)[8,8,8]` i.e. using 4.1×10^9 cells and 40,960 grains. On HECToR phase 3, which is a Cray XE6 computer the run took 5m 36s wall time using 512 processors (16 nodes, 32 processors per node). The resulting output file was 16GB. Fig. 7(b) shows 2 (100) cleavage cracks propagated across a grain boundary into another grain, thus starting another 2 (100) cracks. This is the effect of the grain boundary mis-orientation.



Program 1.

```
implicit none
real :: r(3,2)[2,*]
r = this_image() * &
 reshape((/ 1,2,3,4,5,6 /),(/ 3,2 /))
if ( this_image() .eq. 1 ) &
 sync images (3)
if ( this_image() .eq. 3) then
 sync images (1)
 r(1,1) = r(1,2)[1,1]
end if
write (*,"(a,i0,a,6f4.0)") "image ",&
 this_image(), ": r=", r
end
```

Output from program 1:

```
image 1: r=  1.  2.  3.  4.  5.  6.
image 2: r=  2.  4.  6.  8. 10. 12.
image 4: r=  4.  8. 12. 16. 20. 24.
image 3: r=  4.  6.  9. 12. 15. 18.
```

Program 2.

```
implicit none
real :: r(3,2)[2,*], tmp
r = this_image() * &
 reshape((/ 1,2,3,4,5,6 /),(/ 3,2 /))
if ( this_image() .eq. 4) then
 sync images (1)
 tmp = r(2,1)[1,1]
 sync images (1)
 r(2,1) = tmp
end if
if ( this_image() .eq. 1) then
 sync images (4)
 tmp = r(2,1)[2,2]
 sync images (4)
 r(2,1) = tmp
end if
write (*,"(a,i0,a,6f4.0)") "image ",&
 this_image(), ": r=", r
end
```

Output from program 2:

```
image 1: r=  1.  8.  3.  4.  5.  6.
image 2: r=  2.  4.  6.  8. 10. 12.
image 4: r=  4.  2. 12. 16. 20. 24.
image 3: r=  3.  6.  9. 12. 15. 18.
```

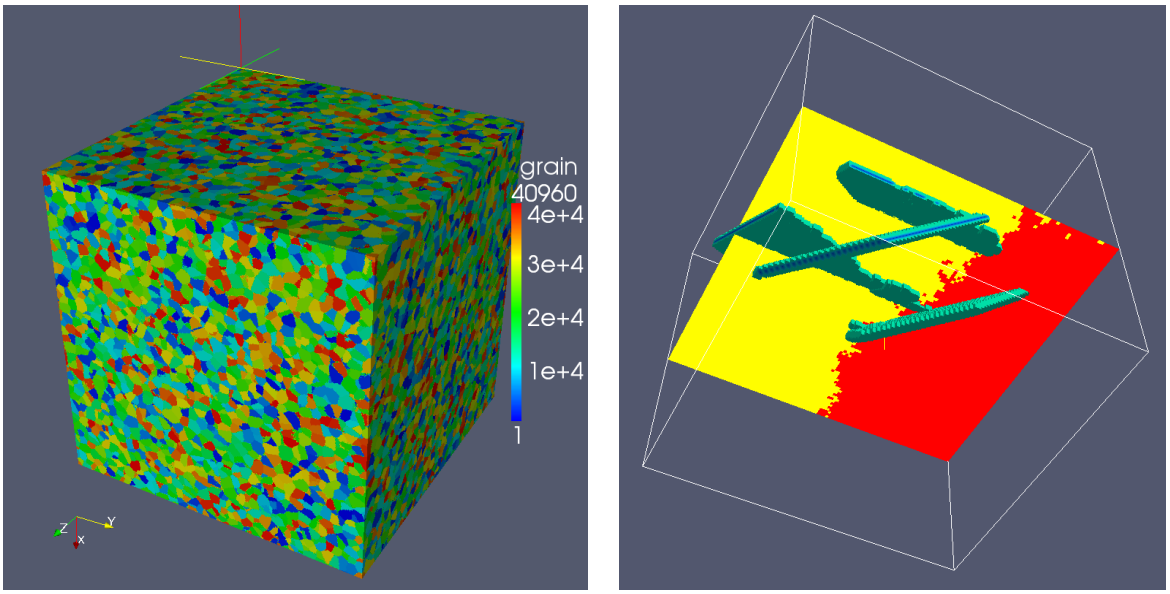
Program 3.

```
implicit none
real :: r(3,2)[2,*], tmp
r = this_image() * &
 reshape((/ 1,2,3,4,5,6 /),(/ 3,2 /))
sync all
r(3,2) = r(3,2)[2,1]
write (*,"(a,i0,a,6f4.0)") "image ",&
 this_image(), ": r=", r
end
```

Output from program 3:

```
image 2: r=  2.  4.  6.  8. 10. 12.
image 1: r=  1.  2.  3.  4.  5. 12.
image 3: r=  3.  6.  9. 12. 15. 12.
image 4: r=  4.  8. 12. 16. 20. 12.
```

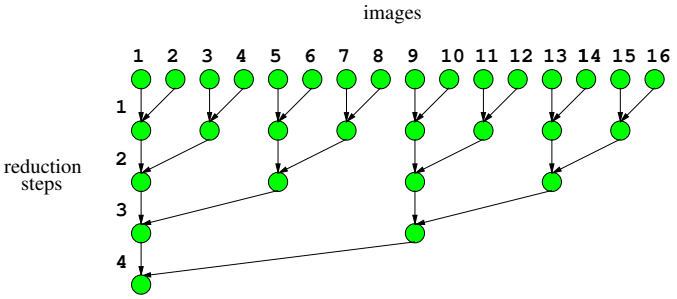
Figure 6: Illustrating remote coarray calls and associated image control statements.



(a) (b)

Figure 7: (a) A 4.1×10^9 cell, 40,960 grain equiaxed microstructure model, showing grain arrangement with colour denoting orientation, and (b) cleavage cracks propagating across a grain boundary.

As we mentioned earlier, Fortran 2008 standard has no intrinsic collective operations. Fig. 8 (from [9]) shows a *divide & conquer* algorithm (or a binary search), that can be used to perform a collective operation, a sum in this example. This example algorithm works only when the number of images is a power of 2, i.e. `num_images()`$= 2^p$. The loop takes only p iterations. On the first loop iteration all even images add their values to lower odd images. On each following iteration the step between the images in each pair increases by a factor of 2. On the last iteration image `num_images()/2+1` adds its total value to that of image 1. Synchronisation is done with a pair of matching `sync images` image control statements.
Fig. 9 (from [9]) shows scaling of the solidification routine for a model with 2^{30} cells, using from $2^3 = 8$ to $2^{15} = 32768$ cores, i.e. with the model coarray defined from `(512,512,512)[2,2,2]` to `(32,32,32)[32,32,32]`. The speed-up of nearly 3 orders of magnitude (!) was achieved for the core count raising by a factor of 2^{12}, from 2^3 to 2^{15}. Note that D&C reduction and Cray `co_sum` collective deliver the best performance. The serial reduction algorithms become increasingly inefficient at high processor counts. At this time `co_sum` collective is a Cray compiler extension to the Fortran 2008 standard. Hopefully, it will become an intrinsic




```
integer :: fin[*]
step    = 2
stepold = 1
```

```
do i = 1,p
 if ( mod(img,step) - 1 .eq. 0 ) then
  sync images ( img + stepold )
  fin = fin + fin[ img + stepold ]
 else if (mod(img+stepold,step)-1 .eq. 0)&
  then
   sync images ( img - stepold )
end if
stepold = step
step = step * 2
end do
```

Figure 8: Divide & conquer reduction, showing the diagram and the coarray program.

procedure when TS 18508 [7] is adopted into the standard.
The cellular automata microstructure code is freely available from http://eis.bris.ac.uk/∼mexas/cgpack.

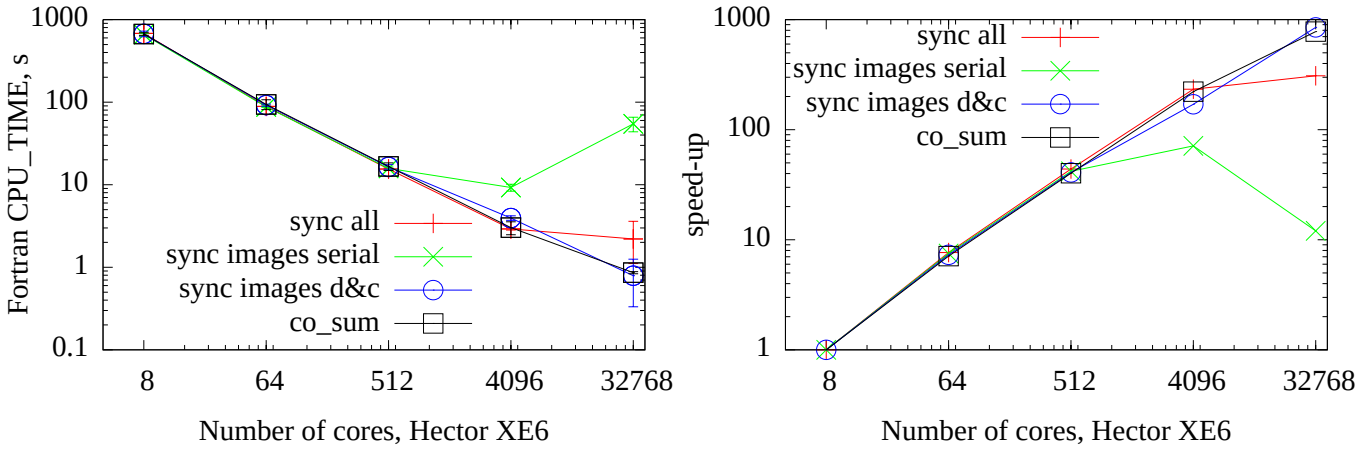


Figure 9: Timing and speed-up of the solidification routine with different implementations of the collective operation and corresponding synchronisation.

Problems and future

Coarray I/O is a major problem. The 2008 standard does not allow a file to be connected to more than one image. Hence there is no standard Fortran parallel I/O method for coarrays. The programmer has 3 routes. First: each images does its own I/O. This incurs a lot of OS overhead, to do with opening multiple files, particularly for large numbers of processors. Moreover, some post-processing of data will be required, as typically the data output from each image forms a chunk of a larger dataset. Second: a single image does all I/O in required order. This is essentially a serial I/O with added overhead of putting the data from all images in correct order. It is possible to design a method which is somewhere between 1 and 2, i.e. several writers (or readers), each communicating with a subset of all images. Third: MPI/IO [10, Chapter 13, I/O]. This will give by far the best performance. However, this means the coarray program must be linked with MPI, which at present is only supported by the Cray compiler.
Technical specification TS 18508 [7] contains several proposed new coarray intrinsics, most importantly collectives (`co_broadcast`, `co_max`, `co_min`, `co_reduce` and `co_sum`) and those manipulating *teams of images*. If approved, TS 18508 will be included in the next revision of the Fortran standard, expected about 2015. However, at present, Cray Fortran compiler provides coarray collectives as an extension to the standard, with syntax and function very close to the technical specification.

Acknowledgments

This work made use of the facilities of HECToR, the UK's national high-performance computing service, which is provided by UoE HPCx Ltd at the University of Edinburgh, Cray Inc and NAG Ltd, and funded by the Office of Science and Technology through EPSRC's High End Computing Programme. This work also used the computational facilities of the Advanced Computing Research Centre, University of Bristol - http://www.bris.ac.uk/acrc/.

Coarray references

[1] ISO/IEC 1539-1:2010. *Fortran – Part 1: Base language, International Standard*. 2010. http://j3-fortran.org/doc/year/10/10-007r1.pdf.

[2] M. Metcalf, J. Reid, and M. Cohen. *Modern Fortran explained*. Oxford, 7 edition, 2011.

[3] A. Markus. *Modern Fortran in practice*. Cambridge, 2012.

[4] I. Chivers and J. Sleightholme. *Introduction to Programming with Fortran*. Springer, 2 edition, 2012.

[5] N. S. Clerman and W. Spector. *Modern Fortran: style and usage*. Cambridge, 2012.

[6] I. D. Chivers and J. Sleightholme. Compiler support for the fortran 2003 and 2008 standards, revision 13. *ACM Fortran Forum*, 32(2):14–26, 2013. http://www.fortranplus.co.uk/resources/fortran_2003_2008_compiler_support.pdf.

[7] ISO/IEC JTC1/SC22/WG5 N1983. *Additional Parallel Features in Fortran*. 2013. ftp://ftp.nag.co.uk/sc22wg5/N1951-N2000/N1983.pdf.

[8] J. Phillips, A. Shterenlikht, and M. J. Pavier. Cellular automata modelling of nano-crystalline instability. In *Proc. 20th UK ACME Conf.*, 2012. http://eis.bris.ac.uk/∼mexas/cgpack/acme2012paper.pdf.

[9] A. Shterenlikht. Fortran coarray library for 3D cellular automata microstructure simulation. In M. Weiland, A. Jackson, and N. Johnson, editors, *Proc. 7th PGAS Conf. Edinburgh, Scotland, UK*, pages 16–24. The University of Edinburgh, 2014. http://www.pgas2013.org.uk/sites/default/files/pgas2013proceedings.pdf.

[10] Message Passing Interface Forum. *MPI: A Message-Passing Interface Standard, ver. 3.0*, 2012. http://www.mpi-forum.org/docs/.

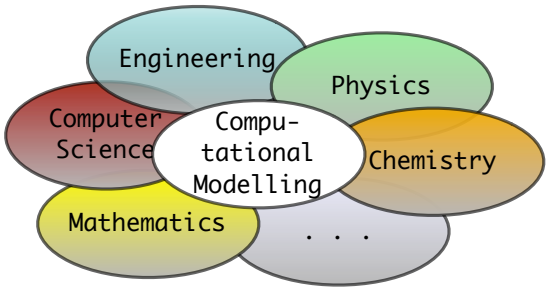
New EPSRC Centres for Doctoral Training

Centres for Doctoral Training (CDTs) are one of the three main ways by which Engineering and Physical Sciences Research Council (EPSRC) provides support for Doctoral Training. The other routes are the Doctoral Training Partnerships (DTP) and Industrial CASE Studentships. EPSRC-funded centres bring together diverse areas of expertise to train engineers and scientists with the skills, knowledge and confidence to tackle today's evolving issues, and future challenges. They also provide a supportive and exciting environment for students, create new working cultures, build relationships between teams in universities and forge lasting links with industry. An overview of the CDTs that have strong connection with computational physics are described in a series of short articles below.

- ## CDT in Next Generation Computational Modelling

  The EPSRC Centre for Doctoral Training in Next Generation Computational Modelling brings together world-class simulation modelling research activities from across the University of Southampton and hosts a 4-year doctoral training programme that is the first of its kind in the UK.

  There are PhD studentships available for at least 11 students to start every year in the middle of September (from September 2014 onwards).



Computational modelling is emerging as a "third pillar" of science and engineering alongside theory and experimentation. Computer simulations bridge between theory and experiment, generate hypotheses, forecasts and predictions about real-world systems. This reduces the number of experiments that need to be carried out in the real world and the number of design prototypes that have to be built, thereby reducing cost, encouraging innovation, optimising system design and enabling the study of systems for which experimental work is infeasible (for example due to prohibitive cost or risk of endangering lives, the environment, etc).

The £10m EPSRC Centre for Doctoral Training in Next Generation Computational Modelling is a 4-year PhD programme (first year similar to a taught Masters with some research components, followed by 3 years of full-time research) that provides comprehensive training in state-of-the art computational modelling methodologies, including programming and software engineering for computational science and engineering, simulation methods and numerical techniques, and high performance computing; combined with additional transferrable skills training. The taught programme starts with a one week intensive course teaching the Python programming language which is embedded throughout the course, and which is complemented with compiled languages (such as C) and parallel programming (such as OpenMP, MPI) where performance is key.

The research component of the CDT programme will push forward and innovate computational methodology, such as exploitation of emerging parallel hardware, new multi-physics, multi-scale and multi-paradigm simulation methods, and tools and methods to apply computer simulation in an effective and reproducible way. This will happen in the context of applied real-world research problems, generally in collaboration with a diverse set of partners.

For more information about the program please visit `ngcm.soton.ac.uk` or contact the Director Hans Fangohr (✉ ngcm@soton.ac.uk).

Article kindly provided by Hans Fangohr, Director, CDT in Next Generation Computational Modelling

- ## CDT in Theory and Modelling in Chemical Sciences

Theory and modelling play a central role in the chemical sciences and related disciplines, complementing experiment in the effort to understand and predict properties of new molecules and materials, and devise new processes. The importance of chemical simulation is increasing not only in academia, but also in a host of high-tech industrial sectors, including energy, healthcare and pharmaceuticals.

Theory and Modelling in Chemical Sciences is a newly founded EPSRC CDT built on a consortium of researchers at the Universities of Oxford, Bristol and Southampton. Our interests span almost the entire range of research activity in computational chemistry, with internationally leading groups in electronic structure of molecules and materials, quantum dynamics, chemical reactivity, and simulation of soft-matter and biomolecular systems. The CDT is supported through strong links with around 20 industrial partner organizations, and through collaboration with chemists, materials scientists, physicists and biological scientists from around the world.

We formed the CDT because of demand in industry and academia for researchers with a wider set of skills than are typically gained through the standard route of an undergraduate degree in chemistry or physics and a PhD in one particular subdiscipline. In creating our centre we have sought to identify the common themes and research practices that unify the whole spectrum of methods and applications in our field. Our students will receive integrated, in-depth training in the core activities of fundamental theory, software development, and application to contemporary research challenges. Students will study in Oxford in year one with training from academics at each site, then progress to a DPhil or PhD research project in Oxford, Bristol or Southampton.

We are the country's only CDT dedicated to computational and theoretical chemistry, and from the start it was part of our ambition to make TMCS a resource for graduate training throughout the UK. To that end we have embedded the highly successful UK Summerschool in Theoretical Chemistry in the CDT, and are using some of the money awarded by EPSRC to open our year-one taught programme for PhD students from other universities.

We have completed a very successful recruitment round for our first year, and are looking forward to welcoming our first cohort of students to TMCS in October. General information about TMCS can be found at `www.tmcs.ac.uk`, and students can find out how to apply for the 2015 cohort at `www.tmcs.ac.uk/how-to-apply.aspx`.For further information please email info@tmcs.ac.uk).

Article kindly provided by Fred Manby, Co-Director, CDT in Theory and Modelling in Chemical Sciences

• CDT in Computational Methods for Materials Science

The development of new materials lies at the heart of many of the technological challenges we currently face as identified in a recent Government review. Our CDT will train a critical mass of more than 80 young scientists over a period of 5 years, not only in the use of existing software but also in the underlying computational and mathematical methods, so that they can develop and enhance the software and introduce new capabilities and functionalities. This training, and the extensive input and contact with our numerous industrial partners, will also provide them with an understanding of the developments, needs and inter-relationships in this field from which they will be able to identify opportunities for developing completely novel software for materials modelling and for combining methodologies into robust and easy-to-use multiscale methodologies.

The CDT in Computational Methods for Materials Science is founded on partnership and engagement with our industrial partners. This combined focus on cutting-edge science and industrial requirements is reflected in the decision to house this CDT in the new Maxwell Centre – a building that is, at its heart, dedicated to "bringing together frontier (physics) research and the needs of industry". The vision of the CDT is to create a large cohort of highly skilled computational scientists who will drive forward the existing strength of UK physical science to support and strengthen industry, creating new business opportunities over the next decade, and who will develop software codes that achieve transformational impact in both academic and economic terms.

Rather than the current *ad hoc* approach to graduate education in modelling methods, the Centre makes it possible to assemble *a priori* large numbers of students who have been systematically trained in a wide range of techniques, and in the theory behind them. Furthermore, our strong links with our industrial partners will provide almost immediate benefit through placements during the

initial training period, with longer lasting returns as graduating students move their skills into the job market, both within and beyond academia. The CDT will bring a close engagement between our students and both industrial software-development companies and industrial end users of materials modelling technologies, and it will also provide formal training in entrepreneurship and technology transfer. Furthermore, a Centre for training and sharing of expertise allows us to carry out novel, student-led programmes or activities. For example, the Centre will support groups of CDT students who may wish to develop entire new simulation codes for academic and/or industrial use by providing both academic and commercial expertise and support for their efforts.

The CDT is led by the Director, Professor Mike Payne FRS (Physics), and two Deputy Directors who carry the largest executive roles – Dr Nikos Nikiforakis (Physics) in coordinating the teaching and Dr James Elliott (Materials) in management of the CDT, including administration of research-project allocation and mentoring of cohorts. The CDT is closely associated with the Lennard-Jones (LJ) Centre for Computational Material Science, established in 2011 via a strategic investment from the University. Through the LJ Centre, the CDT students can readily access an existing community of researchers across the physical sciences throughout the University in a seamless and efficient way.

For further information, including details of how to apply for studentships, please visit our website at `www.csc.cam.ac.uk/academic/cdtcompmat`

Article kindly provided by James Elliott, Deputy Director, CDT for Computational Methods for Materials Science

• CDT on Theory and Simulation of Materials

The mission of the EPSRC CDT on Theory and Simulation of Materials (TSM) at Imperial College London is to create a generation of scientists and engineers with the theoretical and computational abilities to model properties and processes within materials across a range of length and/or time scales.

The impact of materials on our economy is significant, since it is materials that place practical limits on the efficiency, reliability and cost of almost all modern technologies, including: energy generation from nuclear and renewable sources; energy storage and supply; land-based and air transportation; electronic and optical devices; defence and security; healthcare; the environment. The Government has identified Advanced Materials as one of the 'eight great technologies' that will propel future growth of the UK economy, and the capability to predict materials properties and understand fundamental mechanisms using computational tools based on physical principles makes TSM as an indispensable pillar of modern research on materials.

First established in 2009, the TSM-CDT has admitted 50 students so far. The four-year programme is highly multidisciplinary, with the involvement of over 80 academic staff across nine departments as well as industrial partners with whom we collaborate closely. There is a rigorous training in theoretical methods, computational methods and algorithms, and simulation techniques. All PhD research projects have two supervisors working at complementary scales, normally from different departments, bringing together the perspectives of two disciplines on a common problem.

The experience of students in the TSM-CDT is strongly cohort based. A member of academic staff is assigned as the mentor for the cohort of students starting the programme in a given year and he/she stays with the cohort throughout the four years of training. The role of the cohort mentor has a number of facets, including welfare and pastoral care, receiving evaluation of the course, providing feedback to the students, and encouraging peer-to-peer learning.

There are over 50 studentships to be awarded over the next 5 years. For more information and how to apply, please see `www.tsmcdt.org` or contact the Senior Administrator Miranda Smith (✉ Miranda.Smith@imperial.ac.uk).

Article kindly provided by Arash Mostofi, Assistant Director, CDT on Theory and Simulation of Materials

Computational Physics Group News

• The Computational Physics Annual PhD Thesis Prize

Each year, the IoP Computational Physics Group awards a Thesis Prize to the author of the PhD thesis that, in the opinion of the Committee, contributes most strongly to the advancement of computational physics.

The winner of the 2013 Thesis Prize is Dr Joydeep Pal for his thesis entitled *'Exploiting nonlinear piezoelectricity in novel semiconductor-based electronic devices'*, carried out at the University of Manchester. A feature article describing his work will appear in a forthcoming edition of the CPG Newsletter.

Thanks to the generosity of the IoP and AMEC (`www.amec.com`), Dr Pal receives £500 for his achievement.

Applications are now being accepted for the 2014 Thesis Prize. Eligibility and deadline are as follows:

- Applications are encouraged across the entire spectrum of computational physics.
- Entry is open to all students from an institution in the UK or Ireland, whose PhD examination has taken place since 1st January 2014 and up to the submission deadline.
- The submission deadline is **30th April 2015** (though early submissions are encouraged).

Submission format:

- A four page (A4) abstract.
- A one page (A4) citation from the PhD supervisor.
- A one page (A4) confidential report from the external thesis examiner.

Entries (PDF documents preferred) and any questions relating to the Prize should be sent by email, with "IoP CPG Thesis Prize" as the subject header, to Dr Arash Mostofi (✉ a.mostofi@imperial.ac.uk).

• IoP Computational Physics Group - Research Student Conference Fund

The Institute of Physics Computational Physics Group is pleased to invite requests for partial financial support towards the cost of attending scientific meetings relevant to the Group's scope of activity.

The aim of the scheme is to help stimulate the career development of young scientists working in computational physics to become future leaders in the field.

Further details on this award can be found at:

`www.iop.org/about/grants/research student/page_38808.html`

Conference and Workshop reports

• UK Monte Carlo User Group Meeting (MCNEG 2014)

28-29 April 2014 : The Foresight Centre, University of Liverpool, UK.
Website: `www.mcneg.org.uk/mcneg14.html`

The nineteenth meeting of the UK Monte Carlo Use Group (MCNEG) was held on 28th to 29th April 2014 at the Foresight Centre, University of Liverpool on applications of Monte Carlo technique in medical physics and industry and was enthusiastically attended by scientists and research students, mainly from UK, and two invited speakers from CERN and Finland. There were 23 participants who presented 14 oral contributions.

The meeting was followed by a 3 day first FLUKA Monte Carlo Code course/tutorial in the UK, held on 30th April to 2nd May 2014 with some applications on medical physics. It was attended by 9 scientists and research students. Three lecturers from CERN kindly accepted the invitation of the MCNEG group and contributed 10 lectures followed by examples and discussions. The lecturers were: Alessio Mereghetti and Luigi Salvatore Esposito from CERN, Geneva (CH), and Andrea Mairani from CNAO, Pavia (IT). The FLUKA Code calculates the interaction and transport of various particles including photons, electrons and positrons via the Monte Carlo method. FLUKA is widely applied in various areas ranging from shielding, dosimetry and proton therapy, to description of high energy detector, radiation damage, calorimetry, isotope transmutation, maze design for medical accelerators, etc. Today FLUKA can be regarded as a general purpose tool for several applications.

MCNEG Meeting Day 1 : 28th April 2014

- **Stephen Monk from Lancaster University presented his work on *'The comparison of three Monte Carlo based codes when evaluating a complex real world nuclear environment'*** He

presented a comparison of the simulation codes MCNPX, FLUKA and GEANT4 for the high-energy neutron field at the Tri Universities Meson Facility (TRUIMF) in Vancouver, British Columbia. A cyclotron produces around 10^{15} 500 MeV protons per second. The Thermal Neutron Facility (TNF) which is the final beam-dump and is used for testing in environments, such as that on board an aircraft where instrumentation and crew can be subject to neutrons of cosmic origin. 1 hour exposed to the output of the TNF is comparable to 1,000,000 hours of actual flying at typical altitudes. Particle transport simulation codes MCNPX, FLUKA and GEANT4 have been used to model the facility. This information was further compared to the neutron spectrum calculated to be due to neutron radiation of cosmic origin at typical aircraft altitudes. As a means to explain differences between the results obtained, 4 models were compared in the MCNPX environment (BERTINI, ISABEL, CEM03 and INCL4).

– **The first invited speaker Jaakko Leppänen from VTT Technical Research Center of Finland gave a presentation entitled *'Current status and new features in the Serpent code'*.** He gave an overview on the development of an entirely new Monte Carlo neutron transport code, specifically intended for reactor physics calculations at the fuel assembly level. Development started at VTT Technical Research Centre of Finland in 2004 under the working title 'Probabilistic Scattering Game', PSG. Calculations involving high burn-up fuels, advanced MOX technology and next-generation reactor systems are likely to cause problems in the future, if code development cannot keep up with the applications. A potential solution is the use of Monte Carlo based lattice transport codes, which brings all the advantages of the calculation method. The PSG main application is the generation of homogenised group constants for deterministic reactor simulator codes. He discussed the theoretical background on general transport theory, nodal diffusion calculation and the Monte Carlo method. The basic methodology used in the PSG code was introduced and previous studies related to the topic were briefly reviewed. PSG is validated by comparison to reference results produced by MCNP4C and CASMO-4E in infinite two-dimensional LWR lattice calculations. He gave a few Examples of typical Serpent applications from the user community such as: Royal Institute of Technology (KTH), Sweden, has been using Serpent extensively in their European Lead Cooled Training Reactor (ELECTRA) project, as a design and analysis tool, involving the work of several PhD students. Work has been in progress since 2010 to develop a new code version (Serpent 2) is described at the discussion forum: `ttuki.vtt.fi/serpent`.

– **Antony Carver from The Clatterbridge Cancer Centre presented a research on*'Independent Monte Carlo dose calculation for radiotherapy'*.** He gave an introduction about an ideal system which calculates patient dose independent of the planning system calculation. This would help to detect gross errors such as the Panama incident where 28 patients received up to twice the intended dose due to an error in planning system use and would also detect errors such as the New York incident where a plan was inadvertently changed between planning and treatment. BEAM (EGSnrc) was used for modelling the linac : this creates a specified number of photons heading into the patient. A Graphical User Interface (GUI) would control the link between EGS and the Dicom server. Only one calibration per energy is required and that would be field-size independent. Commissioning and testing of the proposal would be based on comparing relative beam profiles and depth dose curves with experimental beam data, determining energy dependent dose-MU calibration factors, verifying calibration factors for different field sizes and testing on patient plans. Initial results from testing are reasonable. The main issue is the time required for the calculation. He concluded that Monte Carlo will provide an independent dose-check tool which would be suitable for the most complex plans.

– **Jenny Richardson from the Christie Hospital talked about *'Developing a beam model for a proton therapy spot scanning Monte-Carlo verification system'*.** The aim of her research was to develop an accurate model of a Spot Scanning Proton Beam (SSPB) so that the spatial distribution of dose deposition can be predicted and implement the model into an automated

MC based treatment verification system. The reason was to reduce the amount of machine-based patient specific QA so that more patients can be treated and physicists would be freed up for other duties. Hence it is planned to be a cost effective method.

- **Turki Almatani from Swansea University presented interesting work on *'Adaptive Treatment Planning in Prostate Radiotherapy'*.** External beam radiation therapy (EBRT) remains one of the primary treatment modalities for patients with localized or locally advanced prostate cancer. It is commonly used in the treatment of patients who have a greater likelihood of non-organ-confined disease. In 2003, prostate cancer affected 28,870 men and caused about 9,000 deaths. The aim of EBRT is to maximize the dose to target volume, as defined by the tumour control probability (TCP) and to spare dose to normal tissue, the normal tissue complication probability (NTCP).
- **Colin Baker from The Clatterbridge Cancer Centre presented *'VisualMC: Teaching the principles of Monte Carlo simulation for radiation dose calculation'***. The motivation for this work was to improve the teaching of radiation interactions and to provide in-depth knowledge to students, and to support self-investigation for the student by trying to distinguish between particle types and interaction mechanisms. Visual display of incident and out-going particles is likely to assist in the retention of knowledge through student investigation and 'practical experiments' to determine interaction characteristics through 'observation'. He gave an example of the investigation of the attenuation coefficient, looking at interactions at certain points and particle tracking. He also gave a demonstration of electron and photon tracks at the end of his presentation. He is hoping to extend the work to include additional particles such as protons and improved geometry and transport options.
- **Rick Tanner from Public Health England gave a presentation on *'EURADOS Working Group 6: Computational Dosimetry'*.** WG6 promotes scientific research and development activities in the field of Monte Carlo Modelling for Radiation Dosimetry and Protection. The core of the WG6 expertise is radiation transport Monte Carlo modelling which has high relevance and impact on all dosimetric applications of ionizing radiation fields. This motivation implies a transverse role among the other EURADOS Working Groups, covering a large number of up-to-date topics in radiation dosimetry. Special attention is also devoted to training and tutorial actions on the competent use of Monte Carlo codes. Exercises are proposed and made available on EURADOS website for MC codes users and the analysis of the results and of the codes performances are discussed in dedicated workshops or at conferences. The WG assists in the dissemination of such knowledge to a larger number of Monte Carlo users.

MCNEG Meeting Day 2: 29th April 2014

- **Ana Lourenco from the National Physical Laboratory talked about *'Water and tissue equivalent phantom materials for clinical proton beam dosimetry'*.** The use of proton therapy provides the highest dose to the tumour while keeping the radiation dose to the surrounding tissues to a minimum. Proton therapy has also the advantage over photons for the treatment of tumours located near a critical organ. She explained why phantoms are not water equivalent for protons because nuclear interactions are different depending on the medium and differing production rates of secondary particles at equivalent depths. Also there is difference in the particle fluence between water and a target material at an equivalent depth (which requires a fluence correction factor). The FLUKA code was used to find suitable tissue-equivalent materials and was validated using water against graphite from ICRU Report 49. Preliminary results show for an energy range of 60-200 MeV, the simulated compositions showed a water-equivalency of between 0.993 and 0.97 independent of depth (with a 0.2% variation).
- **David Shipley from the National Physical Laboratory talked about *'Fluence correction factors for graphite calorimetry in clinical proton beams using Geant4'*.** He stated that the

quantity of interest in clinical proton beams is absorbed dose-to-water, and no primary standards currently exist to measure this quantity in these beams. Water calorimeters have been successfully used and prototype graphite calorimeters also developed and demonstrated. There are lots of benefits with graphite calorimetry. However the conversion from absorbed dose-to-graphite to dose-to-water requires accurate determination of water-to-graphite stopping power ratios and fluence correction factors. Fluence correction factors have been determined initially for 60 and 200 MeV proton beams using Geant4.

- **Amina Patel from Liverpool University gave a presentation on *'ProSPECTus: A Compton camera for medical imaging'*.** The principle of the Compton camera allows the accurate localisation of a gamma-ray source through the reconstruction of interaction sequences in position and energy-sensitive detectors. The Liverpool imaging group are investigating the feasibility of a Compton imaging system for applications in diagnostic nuclear medicine. Monte-Carlo simulations have been conducted with the Geant4 Architecture for Medicine Oriented Simulations (GAMOS) in order to devise a detector configuration which maximises the number of gamma-ray interactions. Gamma rays interact with the scatterer and absorber detectors after passing through a patient/phantom. The energy deposited is used to find out the scattering angle via the Compton scattering formula. Conic sections represent all possible source locations. Many events lead to an overlap of conics, revealing the source location. GAMOS was validated against experiments and found to have a good agreement for Cs-137 and Co-60. This rise in imaging efficiency using GAMOS holds the potential to reduce scan-time thus minimising patient dose.
- **Rick Tanner Public Health England presented initial research on *'Modelling skin doses from microparticles'*.** Rick reviewed the various types of radiation which can affect the skin. This included alpha particles from radon and its decay products.
- **Richard Hugtenburg of Swansea University presented work resulting from a collaboration with Bristol University and Bristol University Hospitals, entitled *'Event-by-event transmission dosimetry with a MAPS detector'*.** Transmission detectors can be used to determine the dose to the patient at the time of treatment without the perturbing influence of the patient. MAPS detectors are sufficiently thin to attenuate the beam by less than 1%. He described their attempts to model the photon and contaminant electrons components of the beam and of methods of separation.
- **Ihsan Al-Affan, from Swansea University presented a recent research on *'The use of FLUKA Monte Code in the re-design of the maze shape and size of the radiotherapy room at Singleton Hospital'*.** He presented a pilot study of an existing radiotherapy room at Singleton Hospital in Swansea to pioneer the use of lead cladding in maze walls to absorb scattered low energy photons reaching the entrance of the maze. FLUKA computations have shown that there is up to a 90
- **Alessio Mereghetti, from CERN gave his invited talk on *'Monte Carlo Radiation Transport at the CERN Accelerators'*.** His presentation included the use of FLUKA at CERN with various examples, including the comparison of FLUKA results against monitor readouts; dealing with large accelerator geometries and coupling FLUKA to a single particle tracking code for beam physics (a new feature). Examples of regular use of FLUKA at CERN include machine protection issues (prompt radiation) and also insertion devices, such as collimators, sensitive equipment such as super-conducting magnets, control electronics and monitors. Radiation protection issues are also treated, such as delayed radiation and activation. A large variety of scenarios have been simulated with FLUKA, involving the whole life-cycle of an accelerator such its design, commissioning, operation, intervention and upgrade, and disposal. Amongst quantities calculated by FLUKA are the particle fluence, dose, activation and residual dose rate, with an accuracy reflecting the quality of the critical processes implemented. He gave examples about the use and range of each accelerator in CERN which are all simulated by FLUKA which involved hadron-nucleus

interactions, nucleus-nucleus interactions, electron interactions, photon interactions, muon interactions (inc. photonuclear), neutrino interactions, decay and low-energy neutrons (less than 20 MeV). Alessio concluded his presentation by confirming that FLUKA is a powerful simulation tool for any kind of study involving interaction of radiation with matter, spanning over several order of magnitudes in energy of the interacting particles and it is extensively used at CERN, in support to the operation of the present accelerators and the design of new components, for both operational and failure scenarios.

Finally, we would like to extend our thanks to the staff at the Foresight Centre and all staff at the computer Department for their hospitality and their continuous support during the meeting.

Report kindly provided by Richard Hugtenburg, Colin Baker and Ihsan Al-Affan, MCNEG committee

• Recent Appointees in Materials Modelling (RAMM) Conference 2014

31 July -1 August 2014 : Imperial College, London, UK
Website: `www.rammconference.org/`

Recent Appointees in Materials Modelling *2014*

The first ever Recent Appointees in Materials Modelling meeting was held on 31st July to 1st August 2014 in the Chemistry Department at Imperial College London. The event was co-organised by Dr. Kim Jelfs (Chemistry, Imperial), Dr. Michail Stamatakis (Chemical Engineering, UCL) and Dr. Cedric Weber (Physics, King's College London). Our initial aim was to have between 20-30 attendees, a number we exceeded with the 34 attendees who registered and attended the event. Although organised through members of the London-based Thomas Young Centre for Materials Modelling in London, there were attendees from across the UK, with more than half being based outside London. The attendees ranged from senior post-docs to those in the first few years of an independent fellowship or lectureship.

The programme included three plenary talks - Prof. Nicola Marzari (EPFL) on *'Soggy, Swampy and Sometimes Steamy: Quantum Mechanics in Watery Environments'*, from Prof. Alberto Striolo (UCL) on

'Simulating Soft Materials at Interfaces: Progress, Challenges and Perspectives' and Prof. Jenny Nelson FRS (Imperial) on *'The relationship between Molecular Packing and Electronic Transport Properties of Organic Semiconductor Films'*. In addition there were two talks from our industrial sponsors - Dr. Jacob Gavartin (Schrödinger PLC) and Dr. Victor Milman (BIOVIA), both of whom stayed for more of the meeting and made interesting comments during the discussions. We also had Dr. Nigel Birch from the EPSRC who spoke on *'How to try and extract money from EPSRC'*, his talk was full of information and 'top tips' for getting funding for those starting to get funding in their own right for the first time. A key point was, that 'no matter the odds, if you don't submit a grant you'll have zero percent chance of getting one!'. Whilst particularly valuable for new appointees from overseas, it was great that Nigel was able to stay for the poster session and conference dinner to allow people to ask questions on a one-to-one basis. In addition to these invited talks, there were 14 contributed talks of 20 minutes from the attendees, together with a dozen or so posters for the poster session. These all highlighted the broad range of materials modelling research being undertaken in the UK, from surfactant proteins, to crystallisation, battery materials and photocatalysis. As many of the applied methods are applicable to different systems, it was a great forum at which ideas could be shared.

The conference dinner at a nearby restaurant in the evening was a great success and a further opportunity for everyone to network in a more relaxed setting. The event was highly successful in its initial aim of bringing together recent appointees in this area and helping them begin to build networks with others at the same stage of their career. It was particularly valuable for those from outside the UK, who have a small UK network and much to learn about the UK research system, in particular funding opportunities. From the vastly positive feedback from the event we are hopeful that the event can now become a regular occurrence over the coming years and make a real difference in helping young materials modellers establish their research.

Report kindly provided by Kim Jelfs, Department of Chemistry, Imperial College.

Upcoming Events of Interest

Upcoming events of interest to our readers can now be found via the following web links.

- NGCM Summer Academy at Southampton in June 2015. A one-week intensive workshop aimed at UK PhD students providing training in Python, Version control, IPython, VTK and Paraview, CUDA, Intel Phi Programming, Pandas and FEniCS/dolfin and Azure Cloud Computing taking place at Southampton University. There will be opportunity to exchange research results and ideas in an informal environment. Details at:

  `ngcm.soton.ac.uk/summer-academy.html`

- IOP's index page for scientific meetings, including conferences, group events and international workshops:

  `www.iop.org/events/scientific/index.html`

- IOP Conferences page for conference information, calendar and noticeboard:

  `www.iop.org/events/scientific/conferences/index.html`

- All events being run or supported by IOP Groups including calendar and links to event web pages:

  `www.iop.org/events/scientific/group/index.html`

- Thomas Young Centre: The London Centre for Theory and Simulation of Materials organises many different kinds of scientific events on the theory and simulation of materials, including Highlight Seminars, Soirees and Workshops. For further details of upcoming events please visit:

  www.thomasyoungcentre.org/events/

- CECAM is a European organization devoted to the promotion of fundamental research on advanced computational methods for atomistic and molecular simulation and their application to important problems in science and technology. CECAM organises a series of scientific workshops, tutorials and meetings. For further details please visit:

  www.cecam.org

Computational Physics Group Committee

The current members of the IoP Computational Physics Group committee with their contact details are as follows:

Hans Fangohr	h.fangohr@soton.ac.uk
Vera Hazelwood (Chair)	Vera.Hazelwood@smithinst.co.uk
Stephen Hughes	Stephen.Hughes@awe.co.uk
Paul Hulse	paul.hulse@sellafieldsites.com
Arash Mostofi (Thesis prize)	a.mostofi@imperial.ac.uk
John Pelan	j.pelan@gatsby.ucl.ac.uk
Marco Pinna	mpinna@uclan.ac.uk
David Quigley	d.quigley@warwick.ac.uk
Simon Richards	s.richards@physics.org
Jesus Rogel (Secretary)	j.rogel@physics.org
David Shipley (Newsletter)	david.shipley@npl.co.uk
Nathan Sircombe (Treasurer)	Nathan.Sircombe@awe.co.uk

Some useful web links related to the Computational Physics Group are:

- CPG webpages
  comp.iop.org
- CPG Newsletters
  Current issue:
  www.iop.org/activity/groups/subject/comp/news/page_40572.html
  Previous issues:
  www.iop.org/activity/groups/subject/comp/news/archive/page_53142.html
  www.soton.ac.uk/∼fangohr/iop_cpg.html

Related Newsletters and Useful Websites

The Computational Physics Group works together with other UK and overseas computational physics groups. We list their newsletter locations and other useful websites here:

- Newsletter of the Computational Physics Division of the American Physical Society:

  www.aps.org/units/dcomp/newsletters/index.cfm

- Europhysicsnews newsletter of the European Physical Society (EPS):
  `www.europhysicsnews.org/`
- Newsletter of the Psi-k (Ψ_k) network:
  `www.psi-k.org/newsletters.shtml`