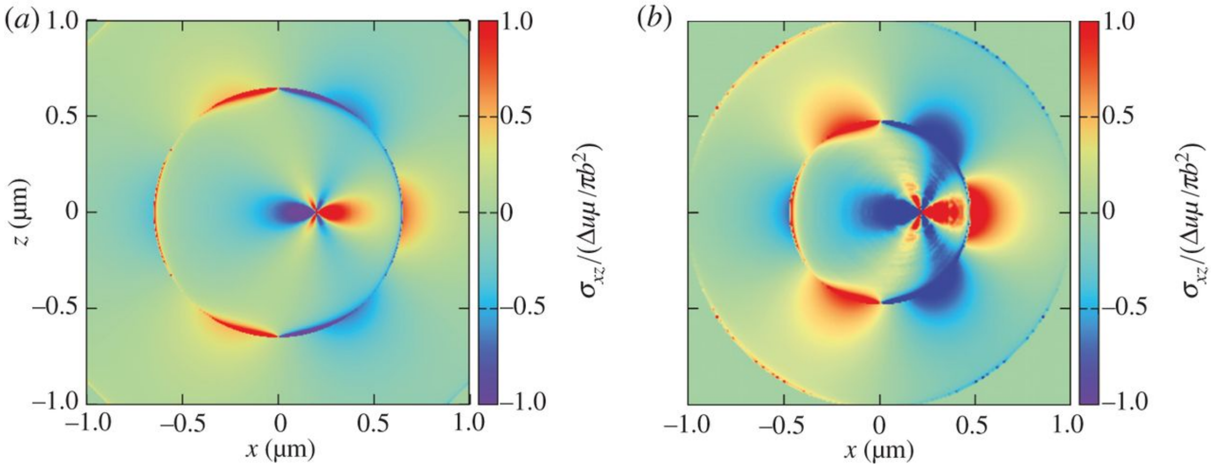
IOP Institute of Physics
Computational Physics Group

Newsletter



Shear stress field component for the injection of a (a) uniformly moving and (b) non-uniformly moving edge dislocation.
(image courtesy of Dr Beat Gurrutxaga Lerma)

Newsletter Contents

This Newsletter... **3**

A Dynamic Discrete Dislocation Plasticity Model for the Study of Plastic Relaxation under Shock Loading **4**
- Introduction . . . 4
- Dynamic Discrete Dislocation Plasticity . . . 5
  - Static and dynamic elastic fields . . . 5
  - The dynamic fields of dislocations . . . 7
  - A Dynamic Discrete Dislocation Plasticity model . . . 11
- Applications of D3P: the decay of the elastic precursor . . . 12
- Conclusions and Outlook . . . 13

Computational Physics Group News **15**
- The Computational Physics Annual PhD Thesis Prize . . . 15
- IoP Computational Physics Group - Research Student Conference Fund . . . 16

Conference and Workshop reports **16**
- Optical Waveguide Theory and Numerical Modelling workshop (OWTNM 2015) . . . 16
- 15^{th} European Turbulence Conference 2015 . . . 17

Upcoming Events of Interest **18**

Computational Physics Group Committee **19**

Related Newsletters and Useful Websites **19**

This Newsletter...

Dear Readers,

The feature article for this bumper edition of the newsletter is an invited contribution by Dr Beat Gurrutxaga Lerma from the Imperial College London, our winner of the 2014 IoP Computational Physics Group PhD Prize, on *'A Dynamic Discrete Dislocation Plasticity Model for the Study of Plastic Relaxation under Shock Loading'*.
Dr Beat also kindly provided the cover image for this edition.

In addition, we have a comprehensive report from the OWTNM (Optical Waveguide Theory and Numerical Modelling) 2015 workshop by Dr Arti Agrawal.

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!

Marco Pinna, Newsletter Editor ✉ mpinna@lincoln.ac.uk)

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

A Dynamic Discrete Dislocation Plasticity Model for the Study of Plastic Relaxation under Shock Loading

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Introduction

Shock loading refers to the sudden application of a strong compressive load on a material. The ensuing shock wave propagates through the medium at a speed that is representative of the magnitude of the initial disturbance, and displays characteristics specific to the shocked material. In that sense, the macroscopic shock response of any medium can be very revealing of both the medium's microstructure and of the underlying microscopic processes governing the latter. Although this alone would justify the study of shock loading from the perspective of fundamental science, one must not forget that shocks and *impact* loads are a very real feature of many engineering applications, particularly in the aerospace, automotive, manufacturing and defence industries. In these applications, engineers often have to design large scale structures that must be able to withstand shock loads; under those circumstances, a detailed knowledge of the shock response of a material can be decisive in the success or failure of both the design and the company.

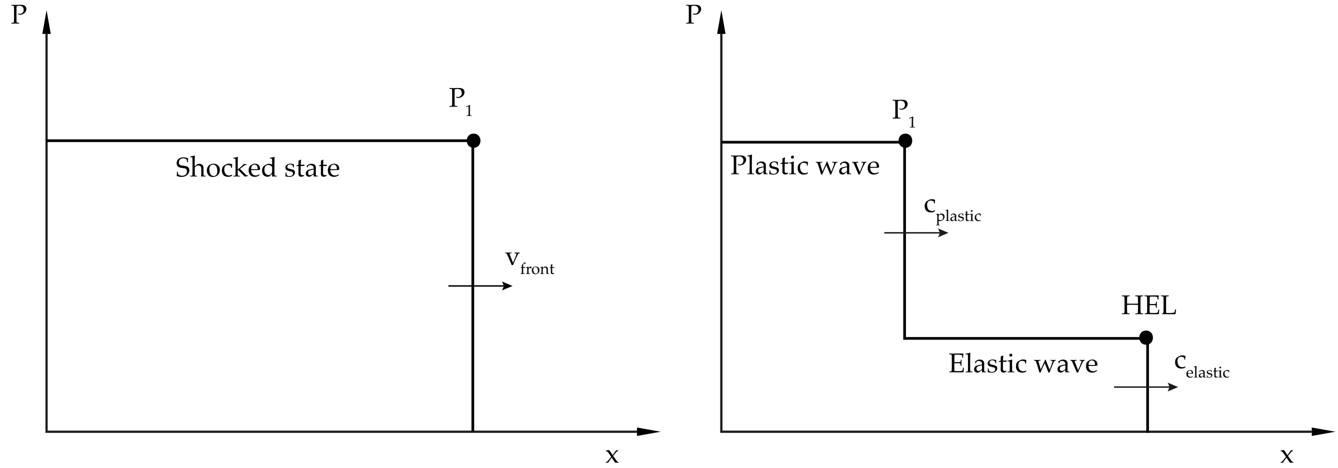
For both practical and historical reasons, the traditional picture of a shock wave that both physicists and engineers hold is that of shock waves in fluid media; after all, the earliest examples of shock waves, such as the sound of thunder or the cracking of a whip, are typically caused by shock waves in fluids. Shock waves in fluid media are characterised by an atomic-thin discontinuous surface that separates a strongly compressed region (the shocked region) from the undisturbed fluid. In 1887, Pierre-Henri Hugoniot [1] showed that the intensive variables defining the thermodynamic state of the shocked state (often called the *Hugoniot state* in his honour) can be related to the undisturbed region's via a set of four equations, comprising the conservation of energy, mass and linear momentum across the shock wave's interface, and a closure equation of state which characterises the medium's thermodynamic evolution.

Shock waves in crystalline solids allow for a similar treatment, and one can indeed define the Hugoniot shocked state invoking the aforementioned thermodynamic considerations. However, because of the inherent symmetries, anisotropy and structural defects present in crystalline solids, the shock wave itself stops resembling a pure discontinuity. Instead, and depending on the magnitude of the initial compression, it displays features such as the wave-splitting phenomenon, whereby the shock wave dissociates into a weak *elastic precursor* propagating at the longitudinal speed of sound, and a subsequent, slower, *plastic front* which carries the lattice all the way to the actual Hugoniot shocked state [2]. This is shown in fig.1.

Shock waves are inherently dynamic (i.e., time-dependent) phenomena. It is therefore slightly perplexing that shock loading has traditionally been studied with a theory—thermodynamics—where time is not a variable. Hugoniot's thermodynamic approach is very successful at describing the shocked state, particularly with aims at producing empirical equations of state. However, it does not provide much physical insight as to how the shocked state is reached, nor can properly study the time-dependent features that one observes in shock waves in solids.

One of the features that thermodynamics fail to capture is the so-called *elastic precursor decay*. The elastic precursor decay is the empirically observed attenuation of the amplitude of the elastic precursor wave as a shock wave propagates through a solid. The amplitude of the elastic precursor marks the onset of plastic deformation in a crystalline solid, i.e. it is the dynamic *yield point*.

Plastic yielding and the subsequent plastic wave are commonly ascribed to the generation and motion of dislocations [3]. Dislocations are linear crystalline defects well-known to be the carriers of plasticity in crystalline solids. The attenuation of the dynamic yield point can therefore be associated with dislocation activity; however, with the current and quasi-static understanding of plastic yielding, one would expect the dynamic yield point to take a unique, time independent value, instead of displaying the attenuation



(a) An idealised shock waves in a fluid. (b) An idealised shock waves in a crystalline solid.

Figure 1: Idealised shock waves.

described above. It would therefore seem that the dynamics of dislocation activity at the onset of the plastic wave differ from current understanding provided by classical Dislocation Theory. In fact, although it has been consistently reported since at least 1953 [4], six decades of study have failed to explain the elastic precursor decay.

Dynamic Discrete Dislocation Plasticity

The study of dynamic yielding from a microscopic perspective has received little attention so far, beyond a few molecular dynamics studies focusing on the microscopic processes leading to the shocked state (cf.[5, 6]), and a few attempts to study the macroscopic response of the material by means of discrete dislocation dynamics (DDD) methods ([7, 8]).
DDD attempts to simulate plastic deformation as the result of the collective motion of individual dislocations. Dislocations are modelled as individual Volterra singularities in an elastic continuum, and plasticity arises as a result of their generation and motion. Long range interactions between dislocations are accounted for through the overlapping elastic fields of individual dislocations. Short range interactions such as annihilations, pinning by obstacles, or collisions between dislocations are modelled through constitutive rules that are applied when the dislocations involved meet a series of specific criteria (e.g., coming within a certain distance of one another, reaching a threshold value of stress, etc.). Mobility laws are defined to describe the motion of the dislocations as a result of an applied external stimulus.
Dynamic Discrete Dislocation Plasticity (D3P), the main contribution of my doctoral work, is one of such DDD methods. However, it represents a radical departure from the paradigm set by current DDD and the classical Theory of Dislocations. In either of those, long-range interactions of dislocations are modelled via time independent, *static*, elastic fields. This means that the fields of dislocations are instantaneously propagated everywhere. D3P is the first methodology where time is included as an explicit field variable, making all long-range interactions propagate at finite speed.

Static and dynamic elastic fields

The motivation for introducing D3P is made clear when one considers the kind of problems DDD deals with. The underlaying equation governing traditional DDD methods is the conservation of linear momentum, which adapted for homogeneous, isotropic media, which in cartesian tensor form can be written as

$$\sigma_{ij,j} = 0 \tag{1}$$

where repeated index denotes summation, $a_{i,j} = \partial_j a_i$, and σ_{ij} is Cauchy's stress tensor. This equation is applied to a problem consisting of the fields of each individual dislocation subject to external boundary conditions.

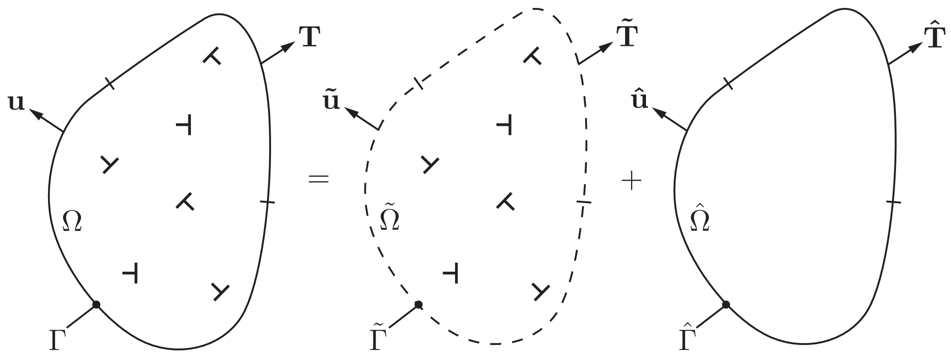


Figure 2: The principle of linear superposition: the original problem Ω is subdivided into an infinite field $\tilde{\Omega}$ and a finite field $\hat{\Omega}$. Closure is achieved by requiring that $\hat{T} = T - \tilde{T}$ and $\hat{u} = u - \tilde{u}$, where T denotes tractions over the surface, and u displacements. The $\tilde{\Omega}$ field can be solved analytically, and the $\hat{\Omega}$ field employing numerical methods such as the finite element method.

The dislocations are modelled as Burgers-vector wide displacement discontinuities along specific directions (the slip planes), so the resulting problem is heavily incompatible. Furthermore, dislocations are atomic-wide discontinuities, so their numerical treatment in micron-size or larger systems would entail a numerical method able to keep its accuracy across 4 to 5 orders of magnitude while remaining computationally inexpensive.

In 1995, Van der Giessen and Needleman [9] proposed a way around. Their solution consists on invoking the *linear superposition principle*. As shown in fig.2, the problem, commonly a finite system Ω, is subdivided into an infinite domain $\tilde{\Omega}$ where all dislocations are placed; and a finite sized domain $\hat{\Omega}$ where the boundary conditions are applied, alongside (for closure) the tractions and displacements exerted over the mapped boundaries in the infinite domain by the dislocation's fields. The infinite plane can be solved analytically, as the fields of dislocations in an infinite plane have well-known analytic solutions (vid.[3]); the finite sized problem is usually solved employing numerical methods such as boundary elemenents or the finite element method.

This approach offers the best of both worlds: an accurate description of the interactions between dislocations and an inexpensive numerical method for treating complex boundary conditions at larger scales. However, it is clear that it is ill-suited for the treatment of plasticity under shock loading, for the simple reason that there is no way $\sigma_{ij,j} = 0$, a time-independent equation, can generate a shock wave.

One can still attempt to amend this shortcoming in the way proposed by Shehadeh et al. in 2005 [10], which consisted in making the finite sized $\hat{\Omega}$ problem elastodynamic, i.e., in solving $\sigma_{ij,j} = \rho \frac{\partial^2 u_i}{\partial t^2}$ instead, where u_i is the displacement vector, ρ the medium's density and $\rho \frac{\partial^2 u_i}{\partial t^2}$ the inertial force. This correctly generates a shock wave when the material is subjected to appropriate boundary conditions.

There remains a blunder to overcome: in this hybrid approach, the fields of the dislocations themselves remain time independent, elastostatic. As a result, the fields of the static dislocations exist immediately everywhere, whilst shock wave fronts propagate at the longitudinal speed of sound. Depending on the application, this might not be problematic, but for the case of shock loads, Gurrutxaga-Lerma et al. (2013) [11] showed that this invariably leads to behaviour that violates causality: as shown in fig.3, the fields of dislocations generated behind the shock wave are able to influence the medium ahead of the front, to the point they trigger spurious dislocation generation and motion, which is absurd.

This violation of causation can only be avoided if one introduces time as a field variable, both for the $\hat{\Omega}$ problem and the dislocations. This is the essence of D3P.

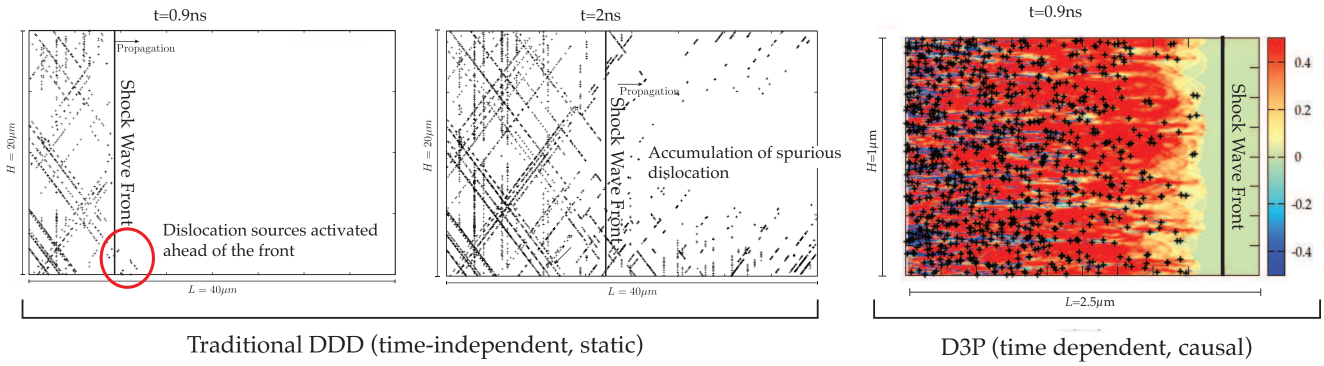


Figure 3: Violation of causality as a result of instantaneous propagation of the fields of dislocations; D3P corrects this behaviour by making their fields time dependent.

The dynamic fields of dislocations

One must therefore provided a fully time-dependent, elastodynamic and analytic treatment of the fields of dislocations that are injected (generated) and move non-uniformly thereafter. This had never been attempted before, perhaps due to the inherent complexity of elastodynamics, which are explored in this section.

In elastodynamics, the governing equation of an isotropic, homogeneous system is called the Navier-Lamé equation, itself an adaption of the equation of conservation of linear momentum:

$$(\Lambda + \mu)\, u_{j,ji} + \mu u_{i,jj} = \rho \frac{\partial^2 u_i}{\partial t^2} \tag{2}$$

where Λ and μ are Lamé's first and second elastic constants, and ρ is the density of the medium, u_i is the i'th component of the elastic displacement vector, a function of position and time; $u_{i,j}$ denotes the first partial derivative of u_i with respect to x_j, where $x_1 \equiv x, x_2 \equiv y, x_3 \equiv z$ are Cartesian coordinates.

The Navier-Lamé equation is reminiscent, and indeed very similar to, the famous Navier-Stokes equation governing fluid motion. However, unlike fluids, solids do have a shear resistance, which fortunately allows for the Navier-Lamé equation to be solved analytically. Focusing on a planar system where the y-axis is out of plane, it is possible to divide eqn.2 into two wave equations (vid.[12]):

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial z^2} = a^2 \frac{\partial^2 \phi}{\partial t^2} \tag{3}$$

and

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial z^2} = b^2 \frac{\partial^2 \psi}{\partial t^2} \tag{4}$$

where $a = 1/c_l$ and $b = 1/c_l$ are the longitudinal and transverse slownesses of sound (c_l and c_t the speeds), and where ϕ and ψ are the Kelving-Helmholtz potentials, defined such that

$$u_x = \frac{\partial \phi}{\partial x} - \frac{\partial \psi}{\partial z} \tag{5}$$

$$u_z = \frac{\partial \phi}{\partial z} + \frac{\partial \psi}{\partial x} \tag{6}$$

are the two in-plane displacement components.

The problem at hand here is that of the generation and subsequent non-uniform motion of a straight edge dislocation. This corresponds to the following boundary conditions:

1. A *mobile contribution*, describing the injection and motion a dipole, one of the components of which moves along the x-axis whilst the other remains quiescent:

$$u_x(x,0,t) = B\left[H(x-l(t)) - H(x)\right] H(t) \tag{7}$$

2. A *static contribution*, describing the injection of a quiescent (non-moving) dislocation,

$$u_x(x,0,t) = B\mathrm{H}(-x)\mathrm{H}(t) \tag{8}$$

Here B is the magnitude of the Burgers vector, and $l(t)$ the past history function, i.e., the function that returns the position of the dislocation line at time t. The solution to the first condition was originally obtained by [13], whilst the second was found by [11].

The analytic solution to this problem is perhaps one of the simplest solutions to *Lamb's problem*, because the boundary conditions are applied over the displacement fields [14]. Define the following transforms:

$$\hat{f}(x,z,s) = \mathcal{L}_t\{f(x,z,t)\} = \int_0^\infty f(x,z,t)e^{-st}dt, \quad F(x,\lambda,s) = \mathcal{L}_x\{\hat{f}(x,z,s)\} = \int_{-\infty}^\infty \hat{f}(x,z,s)e^{-\lambda sz}dz \tag{9}$$

Notice that the bilateral Laplace transform is defined with respect to z here; as before s is a scaling factor. Apply them successively to the governing equations to obtain

$$\frac{\partial^2\Phi}{\partial x^2} = \alpha^2 s^2\Phi, \qquad \frac{\partial^2\Psi}{\partial x^2} = \beta^2 s^2\Psi \tag{10}$$

where $\alpha^2 = a^2 - \lambda^2$, and $\beta^2 = b^2 - \lambda^2$.

The solution to these equations are

$$\Phi(x,\lambda,s) = C_\phi(\lambda,s)e^{-s\alpha x}, \qquad \Psi(x,\lambda,s) = C_\psi(\lambda,s)e^{-s\beta x} \tag{11}$$

Here, $C_\phi(\lambda,s)$ and $C_\psi(\lambda,s)$ are integration constants, to be found from applying the boundary conditions. Since the solution procedure is analogous for each problem, consider solely the case of the static contribution (eqn.8). Upon applying the transforms described above over the said boundary condition, one finds that the transformed potentials are

$$\Psi(\lambda,z,s) = \frac{\Delta u(b^2-2\lambda^2)}{s^3\lambda b^2\beta}e^{-\beta sz}, \quad \Phi(\lambda,z,s) = \frac{2\lambda\Delta u}{b^2 s^3\lambda}e^{-\alpha sz} \tag{12}$$

The inversion of this potentials can then be achieved employing the method of Cagniard-de Hoop [15, 16]. Here, the procedure is illustrated for the shear component of stress, σ_{xz}:

$$\sigma_{xz} = \mu\left(2\frac{\partial^2\phi}{\partial x\partial z} + \frac{\partial^2\psi}{\partial x^2} - \frac{\partial^2\psi}{\partial z^2}\right) \implies \Sigma_{xz} = \mu\left[2s\lambda\frac{\partial\Phi}{\partial z} + s^2\lambda^2\Psi - \frac{\partial^2\Psi}{\partial z^2}\right] \tag{13}$$

The transformed potentials are given by eqns. 12, so substituting above

$$\Sigma_{xz} = \mu\left[-\frac{4\alpha\lambda\Delta u}{sb^2}e^{-s\alpha z} - \frac{\Delta u}{s\beta\lambda b^2}\left(b^2-2\lambda^2\right)^2 e^{-\beta sz}\right] \tag{14}$$

There are clearly two separate components, one depending on Ψ representing transverse excitations, and one depending on Φ representing longitudinal excitations. Each term must be inverted separately. Consider for instance the longitudinal term in eqn. 14:

$$I_1 = \frac{-4\alpha\lambda\Delta u}{sb^2}e^{-s\alpha z} \tag{15}$$

In the Cagniard–de Hoop technique, the inversion is performed by applying the inverse Laplace transforms in time and space described above in reverse order. The inverse bilateral Laplace transform is defined by the Bromwich integral

$$\mathcal{L}_x^{-1}\{F(\lambda,z,s)\} = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} F(\lambda,z,s)e^{\lambda sx}s\, d\lambda \tag{16}$$

The scaling factor 's' in the integrand is necessary for consistence with the definition of the bilateral Laplace transform in time, that bears it in the kernel of the transformation.
Apply this integral to eqn. 15

$$\mathcal{L}_x^{-1}\{I_1\} = \hat{i}_1 = \frac{-2\Delta u}{\pi i b^2}\int_{-i\infty}^{i\infty} \alpha\lambda e^{-s(\alpha z-\lambda x)}d\lambda \tag{17}$$

This inversion can be rewritten in the form of a forward Laplace transform by distorting the integration path. Accordingly, the following change of integration variable can be introduced

$$\alpha z - \lambda x = \tau \tag{18}$$

where $\tau \geq 0$. It follows that λ and α are, with respect to τ:

$$\lambda_\pm = \frac{-\tau x \pm iz\sqrt{\tau^2 - r^2a^2}}{r^2} \quad \text{and} \quad \alpha(\lambda_\pm) = \frac{\tau z \pm ix\sqrt{\tau^2 - r^2a^2}}{r^2} \tag{19}$$

where $r^2 = x^2 + z^2$.

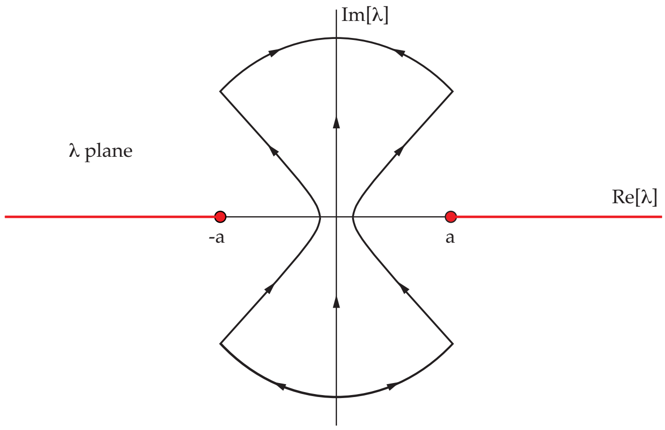


Figure 4: Cagniard-de Hoop integration contour: the integral along the Bromwhich contour (imaginary axis) has the same value as that along either of the branches of the hyperbola, which is described by eqn.19.

Now enter Cagniard and de Hoop's method. From eqn.19, it is clear that the value of the integral along Bromwich contour in λ is the same as that along the hyperbola branch that λ describes in terms of τ (eqn.19), by invoking Cauchy's theorem and Jordan's lemma as shown in fig.4. Crucially, the hyperbola branch in λ describes a line in τ, so that the inversion integral can be rewritten, after some manipulations, as

$$\begin{aligned}\hat{I}_1 &= \frac{-4\Delta u}{\pi b^2}\int_{ra}^{\infty} \mathrm{Im}\left[\alpha(\lambda_+)\lambda_+\frac{\partial\lambda_+}{\partial\tau}\right]e^{-s\tau}d\tau \\ &= \frac{-4\Delta u}{\pi b^2}\int_{0}^{\infty} \mathrm{Im}\left[\alpha(\lambda_+)\lambda_+\frac{\partial\lambda_+}{\partial\tau}\right]\mathrm{H}(\tau - ra)e^{-s\tau}d\tau\end{aligned}$$

Now, upon applying the inverse Laplace transform in time,

$$i_1 = \frac{1}{2\pi i}\int_{Br}\left[\frac{-4\Delta u}{\pi b^2}\int_{0}^{\infty} \mathrm{Im}\left[\alpha(\lambda_+)\lambda_+\frac{\partial\lambda_+}{\partial\tau}\right]\mathrm{H}(\tau - ra)e^{-s\tau}d\tau\right]e^{st}dt \tag{20}$$

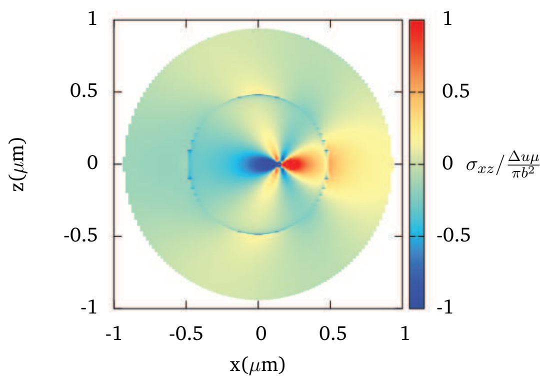
it becomes clear that the solution can be obtained by mere inspection as

$$i_1 = \frac{-4\Delta u}{\pi b^2}\text{Im}\left[\alpha(\lambda_+)\lambda_+\frac{\partial\lambda_+}{\partial\tau}\right]\text{H}(t-ra) \tag{21}$$

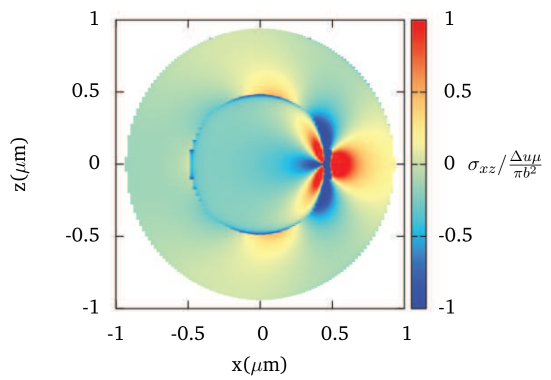
Following this procedure for all other terms, contributions and boundary conditions, one can achieve an analytic solution to the elastodynamic fields of a non-uniformly moving dislocation. For instance, for σ_{xz} it is the following ([11]):

$$\begin{aligned}\sigma_{xz}(x,z,t) = &-\frac{4B\mu}{\pi b^2}\frac{tx\left[t^2(x^2-3z^2)+a^2(2z^4-x^4+x^2z^2)\right]}{r^6\sqrt{t^2-r^2a^2}}\text{H}(t-ra)\\ &-\frac{B\mu}{\pi b^2}\frac{tx\left[-4t^4(x^2-3z^2)+4b^2t^2(x^4-5z^4)\right]}{r^6(t^2-b^2z^2)\sqrt{t^2-b^2r^2}}\text{H}(t-rb)\\ &-\frac{B\mu}{\pi b^2}\frac{tx\left[b^4(7z^6+x^2z^4-7x^4z^2-x^6)\right]}{r^6(t^2-b^2z^2)\sqrt{t^2-b^2r^2}}\text{H}(t-rb)+\\ &+\mu\frac{4B}{\pi b^2}\frac{\partial}{\partial t}\int_0^\infty \text{H}\left(\tilde{t}-\tilde{r}a\right)\frac{a^4\tilde{x}^2z^2\tilde{r}^4-T_a^2\left(8\tilde{t}^2\tilde{x}^2z^2-\tilde{r}^4\tilde{t}^2\right)}{T_a\tilde{r}^8}d\xi-\\ &-\mu\frac{\Delta u}{\pi b^2}\frac{\partial}{\partial t}\int_0^\infty \text{H}\left(\tilde{t}-\tilde{r}b\right)\frac{b^4\left(\tilde{x}^4-z^4\right)^2+T_b^2\left(8\tilde{t}^2\tilde{x}^2z^2-\tilde{r}^4\tilde{t}^2\right)}{T_b\tilde{r}^8}d\xi\end{aligned} \tag{22}$$

where $\tilde{x} = x-\xi$, $\tilde{r} = \sqrt{\tilde{x}^2+z^2}$, $\tilde{t} = t-\eta(\xi)$, $\eta(\xi) = l^{-1}(t)$, $T_a = \sqrt{\tilde{t}^2-\tilde{r}^2a^2}$, $T_b = \sqrt{\tilde{t}^2-\tilde{r}^2b^2}$.



(a) 1000m/s.



(b) 3000m/s

Figure 5: σ_{xz} stress field for a uniformly moving injected edge dislocation at 1000m/s and 3000m/s, showing clear Doppler-like contractions at the latter speed.

Despite the mathematical complexity, the solution opens a new perspective into the dynamics of dislocations. The fields are shown in fig.5. As can be seen, the field description is entirely causal, and expressed in terms of two independent, monochromatic waves: a longitudinal wave (outer ring in fig.5) and a transverse wave (inner ring in fig.5), propagating respectively at the longitudinal and transverse speeds of sound.
The fields of dislocations are expressed in terms of wavelets emitted by the moving dislocation's core. As is shown in fig.5, the fields can display strong Doppler effects (i.e., contractions and dilations) as the dislocation's speed approaches the shear speed of sound. The field contractions experienced as a dislocation approaches the speed of sound is akin to the *Fitzgerald contractions* in relativistic electric charges—they too entail that the potential energy of the dislocation diverges at that speed.

The fields depend heavily on the kinematic state of the dislocation at prior locations, and are entirely causal: the wavelets propagate at the speeds of sound, and whether they contract or expand depends on the dislocation's kinematic state when they were emitted. Mathematically, this is captured via $\eta(\xi) = l^{-1}(t)$, the past history function. This entails that the elastic fields of the dislocations at some point in space and instant in time will depend not only on the current position of the dislocation, but also on each past position. Furthermore, because the elastic fields do not travel instantaneously, all the interactions of dislocations with one another and with the boundaries are now based on a retardation principle akin to that experienced by relativistic electric charges: dislocations will not interact with the current position of others, but with their past history up to a certain past instant in time.
All this constitutes a radical departure point from the traditional Dislocation Theory perspective of dislocations as static charge-like entities that interact instantaneously with each other and with the medium.

A Dynamic Discrete Dislocation Plasticity model

These solutions were used to extend the plane strain formalism of DD to include time as a true field variable. The resulting method is dubbed *Dynamic Discrete Dislocation Plasticity* (D3P) after Discrete Dislocation Plasticity (DDP), the DD method [9] of which D3P is its dynamic counterpart. D3P still relies in the linear superposition principle too (fig.2), as the latter remains exact for each instant in time. Thus, the analytic solutions above are combined with a numerical solution procedure for the associated $\hat{\Omega}$ finite size problem (solved numerically employing the Finite Element Method).
The definition of D3P requires some accessory work in the definition of the mobility laws of dislocations, which can be extracted from relevant molecular dynamics simulations of dislocations moving up to the transverse speed of sound [17]. Typically, these mobility laws will relate the resolved shear stress applied over each dislocation (obtained from summing the contributions of each other dislocation's elastodynamic fields, and that of the boundary conditions) with a kinematic variable of the dislocation (usually its speed or acceleration). Thus, pairwise interactions must be computed. Upon finding all dislocations' speed, their positions can be updated for a given increment in time, and their fields re-computed; thus the system is allowed to react and evolve.
The usual mechanism through which dislocation density is allowed to increase is Frank–Read sources. By introducing analytical models of the line tension involved in the bowling out of such sources, one can show that even for the lower bound, unarrested case where no elastodynamic effects are considered, the activation rate of Frank–Read sources would be insufficient to generate a new dislocation loop within the rise time of a shock front [18]. An alternative, fast paced mechanism is often needed, and can be found in homogeneous nucleation of dislocations, long proposed to be the only viable dislocation generation mechanism in shock loading [19, 20, 21, 22]. Its modelling as a fully stochastic process, alongside the fields descriptions and mobility laws described above, enables to build the basic planar framework of D3P, the first and so far only method of dislocation dynamics offering a fully time-dependent treatment of dislocation interactions and motion.
Computationally speaking, D3P poses many challenges compared to traditional DDD codes. It is computationally demanding, and requires extensive parallelisation. Two are the main parallelisation schemes employed. On a first level, the computation of the pairwise interactions between dislocations is parallelised by multi-threading (via MPI) the computation of the effect of all other dislocations over a given dislocation. For N dislocations, this entails an N^2 computational complexity, and no cut-offs are allowed because dislocation fields decay slowly ($1/r$)—hence the need to parallelise the problem. This level of parallelisation is all the more important in shock loading, where extremely large dislocation densities (in excess of 1000 dislocations per μm^2) are expected. On a second level of parallelisation, the numerical integration of the fields of each dislocation over their past history are multi-threaded via OpenMP. Otherwise, the computational cost of evaluating each pairwise interaction made D3P exceedingly expensive, particularly because the cost of integration increased with time (as the size of the past history increased). Thus, the D3P code is parallelised (unusually) both in time and in interactions.

Applications of D3P: the decay of the elastic precursor

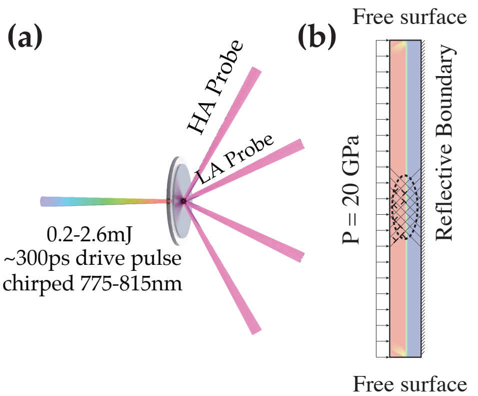
The first application of D3P was the study of the elastic precursor decay in Aluminium, published in [18]. The material was chosen because it displays a very well-defined precursor decay and there exists a wide corpus of empirical studies on the topic.

Fig.6a shows a schematic of a typical shock loading experiment. The target (sample) is a micron-thick material, and the driving force at very high strain rates (above $\approx 10^9 s^{-1}$) is usually a laser pulse. Upon hitting the target's surface, the laser pulse vaporises part of the surface, as a result of which a shock wave is launched towards the material. The shock wave profile is then measured via diagnostic tools at the rear surface (also shown in fig.6a).

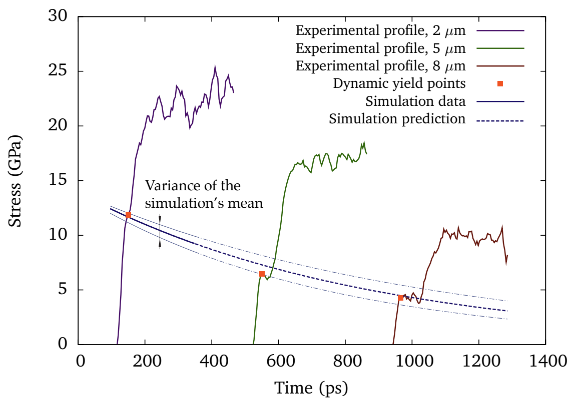
The D3P model simulates this set-up by considering a planar geometry as shown in fig.6a), consisting of a single crystal sample of FCC aluminum at room temperature; the dimensions of the sample, 10μm wide and 1μm thick, reflect experimentally relevant length scales. As shown in fig.6a, the simulations were loaded with an instantaneous 20GPa pressure; due to the loading, a shock front is generated and propagates through the material, triggering dislocation activity. The strain rate is enforced numerically.

The D3P simulations were compared to experiments carried out by Whitley et al. (2011) [23] over the system described in fig.6a. Unlike experiments, that are usually limited to measuring wave profiles at a specific surface (the target's rear), D3P enables the measurement of wave profiles throughout the sample. One can easily transform the inherently planar wave profile into an experimentally relevant unidimensional profile by averaging D3P's wave profile across the transverse section.

The resulting simulations show that the σ_{xx} fields of dislocations destructively interfere with the front's compressive amplitude, leading to an attenuation of the elastic precursor wave that could only be interpreted as the decay of the elastic precursor. As shown in fig.6b, comparison between the decay rates of the simulations and those measured in experiments shows a remarkable agreement, furthering the evidence that the elastic precursor decay is caused by dislocation activity at the shock front.



(a) Shock loaded sample to simulate using D3P, showing a typical experimental set-up and the corresponding D3P model. HA stands for high-angle, and LA for low-angle; both refer to diagnostic tools at the rear surface of the laser-shocked sample. Courtesy of [18].



(b) Comparison between the computed and experimental decay of the elastic precursor. Courtesy of [18].

Figure 6: D3P simulation of the elastic precursor decay in FCC aluminium.

The simulations are also consistent with experimental observation that the rate of decay increases with the strain rate. Moreover, the computed dislocation densities were found to be of the same order of magnitude as that measured experimentally, and comparable to that predicted by analytical models under the same loading conditions.

Aside from reproducing the elastic precursor decay, D3P enables the probing of the specific mechanisms causing the decay. Following the simulations, the following mechanism was found to be the cause behind. When a dipole is generated within the shock front, one dislocation of each dipole has a velocity component anti-parallel to shock front's velocity, and its stress wave is 'anti-shielding' because it constructively interferes with the shock front's compressive amplitude. The other dislocation, with a velocity component parallel to the front's velocity, is a 'shielding' dislocation, as it destructively interferes with (decreases) the front's compressive amplitude. The cumulative effect of the shielding dislocations is greater than the effect of the anti-shielding dislocations, because the former are within the front for much longer. Hence, the cause of the elastic precursor decay is the cumulative and destructive interference of elastic waves emanating from shielding dislocations at the shock front.
Furthermore, the destructive interference is greater at larger strain rates, because the contraction of the dislocation's fields in the direction of motion as v_{dis} increases. The contraction exists only ahead of the dislocation, in the direction of motion; behind the dislocation the magnitude of its fields tends to decrease. Consider the shielding dislocations: with increasing speed, the magnitude of the longitudinal component of σ_{xx} increases ahead of the dislocations, contributing to a greater relaxation of the shock front; this effect persists longer because the dislocations are moving faster towards the shock front. For anti-shielding dislocations, since they move away from the front, increasing their speed results in a relative decrease in the magnitude of the longitudinal component of σ_{xx} influencing the front. Because they move faster away from the front, they influence the shock front for less time. As a result, the amplitude of the shock wave is reduced much more by the shielding dislocations than it is increased by the anti-shielding dislocations, and this effect is magnified by increasing the strain rate.
Thus, it is found that the dynamic yield stress is determined by an interference phenomenon between the elastic precursor wave and the elastic waves of shielding dislocations generated at the front. The increasing attenuation of the dynamic yield point with increasing strain rate is a direct result of the elastodynamic fields of moving dislocations. This insight was achieved by simulating the elastodynamic fields of dislocations nucleated and propagating as a result of the shock, a unique feature of D3P.

Conclusions and Outlook

D3P is the first fully time-dependent, elastodynamic model of dislocation dynamics. This would on its own open new and interesting venues of research, as dislocations has seldom been treated dynamically before. Moreover, D3P has predictive powers, namely in that it can explain the causes of the attenuation of the dynamic yield point, by showing that it is caused by a wave interference phenomenon between the elastic precursor wave and elastic waves of shielding dislocations that are generated at the shock front itself. The explanation of a six decade old phenomenon via D3P places it as a true breakthrough within the materials modelling community.
The mathematical formalism underlaying D3P shows dislocations from a hitherto largely unexplored perspective: as sources of mechanical waves, highlighting the importance time-dependent effects can have in dislocation theory, which had formerly been regarded as a largely exhausted field.
Many of the features observed therein, such as field contractions, past-history effects, etc., have proven to be extremely relevant in explaining the elastic precursor decay. In that sense, D3P is a true step forward. It opens the door to the simulation of all other dislocation-mediated physical phenomena where the time scales are similar to the propagation time of elastic waves, or where the speed of dislocations is expected to approach those speeds. That is the case of crack arrest in dynamic fracture, adiabatic shear banding, fault propagation in geophysics, low cycle fatigue, laser shock peening (thermoelastic effects in shocks) or twinning, amongst many other. These phenomena involve timescales such that they can only be studied with a time-dependent dislocation dynamics method like D3P, and have never been studied in detail due to the limitations of current simulation methodologies. They are also of immediate relevance to society, underpinning some of the most common and catastrophic modes of mechanical failure known to humankind. Hence, the potential applications and impact of D3P are vast.

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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 2014 Thesis Prize is Beñat Gurrutxaga-Lerma for his thesis entitled *A Dynamic Discrete Dislocation Plasticity Model for the Study of Plastic Relaxation under Shock Loading*, which was undertaken at Imperial College London.

  Runner-up prizes are awarded to Tom Goffrey, for his thesis entitled *A Cylindrical Magnetohydrodynamic (MHD) Arbitrary Lagrangian Eulerian (ALE) Code*, carried out at the University of Warwick, and Bartomeu Monserrat, for his thesis entitled *On the vibrational properties of solids*, carried out at the University of Cambridge.

  Thanks to the generosity of the Smith Institute (`www.smithinst.co.uk`) and AWE (`www.awe.co.uk`) Beñat receives £450 and Tom and Bartomeu receive £150 each for their achievements.

  Summaries of their PhD research will appear in forthcoming issues of this newsletter.

  For this year's prize 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 2015 and up to the submission deadline.

  Prize winners will be invited to write a feature article in the Computational Physics Group newsletter.

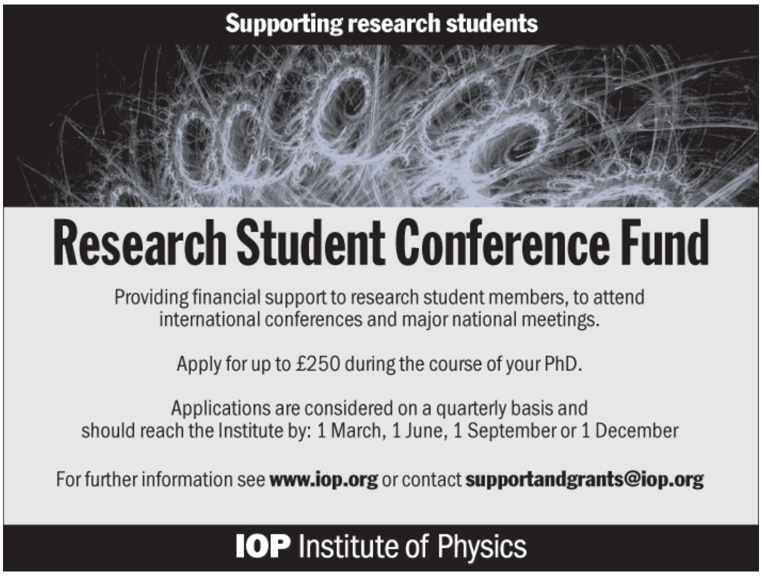
  The submission deadline is **30 April 2016**.

  The submission format is as follows:

  - A four page (A4) abstract describing the background and main achievements of the work
  - A one page (A4) citation from the PhD supervisor
  - A one page (A4) confidential report from the external thesis examiner

  Entries (PDF documents preferred) should be submitted by email, with "IOP CPG Thesis Prize" as the subject header, to Dr Arash Mostofi (a.mostofi@imperial.ac.uk). Any queries should also be directed to Dr Arash Mostofi. A few more details, including a list of past winners, can be found on the group webpage `http://iop.msgfocus.com/c/1sLF2oBZrFBLmzXkAIcKxp` .

- **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

- **Optical Waveguide Theory and Numerical Modelling workshop (OWTNM 2015)**

16-18 April 2015 at City University London.
Website: `http://www.city.ac.uk/owtnm-2015/`

Chaired by Dr. Arti Agrawal City recently hosted the 23rd **Optical Wave and Waveguide Theory and Numerical Modelling Workshop** from 16-18 April 2015. The workshop brought together the leading experts from across the globe on modeling of Photonic components and theory of electromagnetic waves. The Vice Chancellor, Professor Paul Curran gave the opening remarks and inaugurated the conference.

116 participants from 31 countries attended the workshop, with 9 from industry and 79 from academia. In previous years the workshop has had 60-70 participants. The main sponsors were CST Microwave and Lumerical, both leading firms that make simulation software for Photonics. 7 other companies and professional bodies including the Optical Society of America (OSA) and Institute of Physics (Optical Group, Computational Physics Group, Quantum Electronics and Photonics group) were also sponsors.

Highly relevant topics such as how radiative cooling can be achieved through optics to conserve energy, how plasmonics and metamaterials can be used in defence and security applications, how fiber lasers can be scaled up in power were discussed. 91 papers (including 2 keynotes, 8 invited talks, 21 contributed talks and 60 posters) were presented. These papers have been published in a book of abstracts. A special issue of the journal Optical and Quantum Electronics will also result from the conference later in the year. Springer Verlag have approached Dr. Agrawal to publish an edited book related to advances presented in the conference. 3 best student paper prizes were given co-sponsored by Wiley and OSA. There were also representatives from Press: International editor of Nature Photonics attended the conference and gave away the student prizes.

The workshop had several unique features that were much appreciated by delegates:

- free Women in Optics workshop and lunch with industry speakers who spoke about how women can make successful careers in Photonics. This was attended by 45 people
- free training by Lumerical on FDTD technique and software, attended by 25 PhD and postdoctoral students
- Social Programme that included a welcome reception on the 16^{th}, gala dinner at HMS President, a retired Navy warship on Friday, 17^{th} April and a traditional "fish and chips" supper on the 18^{th}. Delegates thoroughly enjoyed the opportunity to mingle in a relaxed and informal atmosphere.

Link to conference video:
`https://www.dropbox.com/s/j7aqcnst1q536zt/City_OWTNM_edit01.mp4?dl=0`

Link to photos:
`http://www.city.ac.uk/owtnm-2015/gallery`

Report kindly provided by Dr. Arti Agrawal, Chair OWTNM.

• 15^{th} European Turbulence Conference 2015

25-28 August 2015 at TU Delft, the Netherlands.
Website: `http://www.etc15.nl/`

Thanks to the IOP Computational Physics Group bursary, I was able to attend the 15th European Turbulence Conference in TU Delft, the Netherlands from the 25th to the 28th of August. During this event, I was also able to present my work in flow control by Direct Numerical Simulation as part of my PhD research project. This meeting as one of the largest focusing on turbulence problems encompasses a wide range of subjects. Therefore it was a very good opportunity for me to learn about subjects beyond those I am more familiar with in my project. The talks given during the guest lectures were particularly interesting. Indeed, the speakers introduced the topic from a very simple viewpoint and kept on developing from there. Three of the talks were particularly enlightening. The first was given by Professor Steve Tobias on Direct Statistical Simulation of turbulent astrophysical flows. He showed how astrophysical flows were able to display remarkable organisation so that non-trivial mean flows and mean magnetic fields became apparent. The jets on Jupiter, the differential rotation of the Sun and the solar activity cycle were presented as examples of global organisation from smaller scale chaotic behaviour. The focus was put on the numerical technique to overcome the difficulty for high Reynolds number computations in such large scale flows and known as Direct Statistical Simulations. This subject was particularly interesting from the point of view of my research as it dealt with one of the issues encountered in Direct Numerical Simulations, i.e. the deadlock imposed by high Reynolds number simulations. In addition the speaker described how one could attempt to apply some of these methods to smaller scale flows. The second talk that I really appreciated was given by Professor Marc Brachet on Quantum turbulence and the Gross-Pitaevskii Equation for turbulence modelling at low temperatures. After describing the fundamentals of superfluidity and the range of applications, the model along with the numerical methods were described. The model is based on a modified version of the Schrödinger equation. This subject was new to me from the viewpoint of turbulence modelling as I studied quantum mechanics applications from another perspective. Finally the talk presented by Professor Bettina Frohnapfel gave an overview on Skin friction drag reduction in turbulent flows. This subject is central to my PhD research project. It was particularly interesting as it was the occasion to consider the concepts related to drag reduction from another perspective than the one generally adopted. As such, it was suggested that drag reduction in itself may not be the ultimate benchmark in flow control studies and that in the future one should address flow control problems using the energy savings. Another issue which was also presented, dealt with the way one has to use scaling in flow control problems in order to extract the relevant information. This second part proved to be very useful for better understanding these problems. I now have a better understanding on how to tackle this issue. I mainly attended the sessions on flow control, vortex dynamics, large eddy simulations and instability/transition. After my presentation on the second day of the conference, I had the occasion to discuss more in details about my work with the chair of the session. This discussion proved to be useful as it was the occasion to explain my work and understand which points should be more emphasised. I definitely think that it is worthwhile attending such a prominent scientific event held every two years, particularly as a PhD student. Indeed, it allows to meet people that are working on the same field as well as to gain knowledge on other subjects that one may not be familiar with. I am grateful to the IOP for giving me the possibility to attend this conference. Besides, this was the occasion to meet other PhD students from TU Delft whom I met in another conference. They showed me their labs and facilities which was really interesting for me as my work focuses mainly on numerical modelling.

Report kindly provided by Sohrab Khosh Aghdam, PhD student, Department of Mechanical Engineering at the University of Sheffield.

Upcoming Events of Interest

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

- 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:

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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`