Integrated calculations of short-pulse laser interactions with matter

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Abstract. A complete description of high energy density physics experiments on laser systems incorporating short, picosecond, beamlines requires a daunting breadth of physics, which cannot reasonably be included in a single model. Modern particle in cell (PIC) codes, Vlasov–Fokker–Planck models and radiation hydrodynamic codes together constitute the tools required to model key aspects of short-pulse laser–plasma interaction in such experiments. A predictive modelling capability in this area requires that all these tools are applied to a given problem. Our approach is to develop an integrated modelling capability in which these detailed models for different aspects of the problem are linked together. We outline our methodology and demonstrate the approach taken to link PIC models of laser–plasma interaction into hybrid models of electron transport within a radiation hydrodynamics code. This integrated model is used to study the absorption and transport of short-pulse delivered energy in a solid diamond target, highlighting distinct differences between the integrated results and modelling which relies on an assumed hot electron spectrum. We extend this work to consider structured targets which show the promise of providing an additional element of control over target heating as well as presenting an opportunity to test the transport models employed. Finally we demonstrate the survivability of such targets to the pressures generated by isochoric heating over the timescales of the laser–plasma interaction.

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1. Motivation

High energy density physics (HEDP) research at AWE is focused on building a detailed understanding of material properties under extreme conditions. The Orion laser recently constructed at AWE’s Aldermaston site is a key component of this research effort. The Orion laser system consists of two petawatt class short-pulse (picosecond-scale) beamlines operating at a wavelength of $\lambda = 1.06 \mu m$, one of which can be frequency doubled to produce second harmonic, or ‘green’, light at a wavelength of $\lambda = 0.53 \mu m$, together with ten third harmonic, or ‘blue’ $\lambda = 0.35 \mu m$, long-pulse (nanosecond-scale) beams. Each beam has a maximum energy of the order of 500 J. Short-pulse lasers allow material, which can be pre-compressed by the action of the long-pulse beams, to be heated to high temperatures before hydrodynamic motion can disassemble the target. Thus material properties can be studied across a range of temperatures and densities in the laboratory.

The inclusion of short-pulse beams greatly enhances the capabilities of the laser system, but also makes modelling the experiment extremely challenging. Not only is this a problem for interpreting HEDP experiments, but it is also an acute issue for the fast ignition (FI) [23, 35] approach to inertial confinement fusion (ICF) [24, 28], a proposed method for achieving high gain laser-driven fusion by separating the compression and ignition phases of ICF, and (in many but not all schemes) using a short-pulse laser to deposit energy, in the form of hot electrons, into a pre-compressed fuel mass to ignite it.

A complete description of the problem, be it for FI or HEDP in general, requires an extensive range of physics: accurate treatment of Maxwell’s equations and kinetic effects where the laser is absorbed; collisional effects for the onward transport of the fast particles generated; return current effects; ionization, equation of state and hydrodynamic response in the dense target. Much of this must also be treated in a relativistically-correct manner.

The natural approaches to numerical modelling in each of these areas are, however, not generally compatible. Modelling laser–plasma interaction (LPI) necessitates a mesh which can capture the dispersion of electromagnetic waves. The plasma in the interaction region must be treated with a kinetic model to resolve the absorption physics which, at high intensities, generates fine scale structure in the distribution function and leads to distinctly non-thermal electron and ion populations. The problem of modelling LPI boils down to the explicit solution of the Vlasov–Maxwell system of equations, typically through a macro-particle (i.e. particle in
cell (PIC) [6]) or continuum (i.e. direct Vlasov [32]) approach. In tackling this problem we have found the PIC code EPOCH [7, 8] to be a reliable and flexible tool, offering a reasonable balance of fidelity and turn-around time.

In the dense material of the bulk target, away from the LPI region, collisional physics dominates. The transport of hot particles generated by the action of the laser is dependent on their slowing and stopping in the dense material and their need to draw a return current to counterbalance the current they themselves carry into the target—and so bypass the Alfvén limit [1, 4]. These effects will heat the target, which in turn influences transport. On longer timescales, the hydrodynamic response of the target will begin to play a role as the pressure generated from isochoric heating begins to take effect. Resolving such densities using an explicit kinetic code would place severe limitations on the spatial and temporal scales which can be modelled, or else make such an approach prohibitively expensive in terms of compute—at least as a target design tool. Since material properties and bulk hydrodynamic motion must also be considered, the natural approach would be to add additional physics to a radiation hydrodynamics model, treating the energetic hot populations separately to the colder bulk material. The transport code THOR seeks to achieve this by applying a Monte-Carlo approach to the solution of the Vlasov–Fokker–Planck equation for the energetic particles, against a background of cold, dense material which provides the return current. This ‘hybrid’ model can then be coupled back into an existing hydro code which provides material properties and hydrodynamic response.

It is clear then that we have available the tools to model key aspects of HEDP experiments. However, these tools, as described above, do not make for a single, self-consistent model of the laser–target interaction problem. What about the effects of hydrodynamic motion, possibly due to the laser pre-pulse, before the arrival of the main pulse? How does the transport model know what the energetic particle spectra should be? To address these issues, we link our kinetic, transport and hydro codes together to provide an integrated modelling capability.

Here, we demonstrate a system for coupling the physical scales in the problem using an integrated code suite. The long-term aim is to prepare a robust, practical, tool for HEDP research that will allow as much of the relevant physics to be modelled as possible. The set of codes and link methods used is outlined in section 2; applied to a solid diamond target in section 3, noting the differences compared to an equivalent functional form for distribution of hot electrons; and extended to more complex ‘structured’ targets in section 4. Section 5 contains a summary and outlines future work required to deliver a flexible predictive capability built on the results described here.

2. The code suite

Our approach to integrated modelling is based on a suite of three codes: the PIC code EPOCH, Monte-Carlo hybrid transport code THOR, and radiation hydrodynamics code CORVUS. These are supported by two link codes: FENRIS and LOKI. This section gives a brief overview of each of the core codes, and outlines the techniques adopted to link them together.

2.1. EPOCH

EPOCH is an explicit, relativistic, PIC code developed in the UK under the auspices of the Collaborative Computational Project in Plasma Physics (CCPP)2. In common with many

2 http://www.ccpp.ac.uk.
such codes, the second order accurate particle push splits the acceleration due to the electric fields from the momentum-space rotation due to the magnetic fields [6] and follows a charge conserving scheme of the form described in [37]. High order particle shapes can also be employed to minimize the effects of numerical heating. Electric and magnetic fields are updated via a finite difference time domain scheme [22] on a fixed Eulerian mesh. The code, including the IO subsystem, is parallelized using the common message passing interface libraries. While not utilized here, EPoCh has a collisions model, and a hybrid algorithm of the form pioneered in [12], and used in HEDP and FI scenarios in [15], is also under development.

2.2. THOR

THOR models the leading order effects of hot electron transport using a hybrid approximation similar to that of [13, 14]. The basic features of the model are Monte-Carlo simulation of energetic (>10 keV) electrons with collisional drag and scattering and self-generated electromagnetic fields induced by the bulk return current. Implicit in this approach is the assumption that the kinetic population is a perturbation to a thermal fluid background.

The advantages of hybrid schemes are that they are fast, robust and scale well on modern parallel systems. It is also relatively straightforward to couple such a code to a radiation-hydrodynamics code. On the other hand, many physical effects such as collective modes are neglected, and the assumption of the fast population as a perturbation restricts application to densities on the order of, or above, solid. Codes such as THOR offer a computationally inexpensive model for the transport of energy from a short-pulse laser interaction region throughout a target. The basic model is as follows:

1. Kinetic electrons are sourced in a defined region. This is a cylinder in real space, a hemisphere in momentum space, and weighted using some form of distribution function. These distributions will be explored in more detail later.

2. The electric fields are derived from a simplified Ohm’s law, and magnetic fields via Maxwell’s equations assuming that a cold return current exactly balances the flux of hot electrons i.e. an electric field is set up to draw this current and a magnetic field induced.

3. The electron population is pushed in response to the electric and magnetic fields over a timestep set by the CFL limit. The collisional (or Coulomb) drag and scatter are operator split, and distinct from the effects of the global field:

\[ d\mathbf{r} = \mathbf{v} \, dt, \]

\[ dp = \langle \Delta p \rangle \, dt = -\frac{Zne^4}{4\pi \epsilon_0^2 m v^2} \ln \Lambda_1 \, dt \]

\[ d\theta = \langle \Delta \theta^2 \rangle^{1/2} \, dW = \left( \frac{Z^2 ne^4 \gamma m}{2\pi \epsilon_0^2 p^3} \ln \Lambda_s \right)^{1/2} \Gamma(t), \]

where \( \mathbf{r} \) is the particle position, \( \mathbf{v} \) is its velocity, \( p \) is its momentum magnitude and \( \gamma \) is the Lorentz factor. The \( \Gamma(t) \) factor is a random number with a Gaussian distribution, a mean of zero and a standard deviation of 1. The terms in \( \Lambda_1 \) and \( \Lambda_s \) are Coulomb logarithm-like terms, detailed in [13]. All other symbols have their usual meaning and are in SI units.

4. The particles are accelerated by the electric field and their direction of motion is altered by the magnetic field analogously to equations (2) and (3).
5. Energy lost by the particles to drag is deposited on the grid. Energy lost to the field stopping equates to Ohmic heating. These two terms are summed and the background is heated according to an estimation of the specific heat.

The background medium is modelled as a single temperature, static fluid. Currently THOR includes numerous material models, further development of these material models (other than for resistivity) is not anticipated, as these can be provided by the hosting hydrodynamics code, which can also handle ion–electron temperature separation.

2.3. CORVUS

CORVUS is a two-dimensional (2D) finite-element arbitrary Lagrangian–Eulerian code for plasma physics simulations, which includes radiation diffusion and an explicit refractive laser ray trace model.

2.3.1. Integrating THOR into CORVUS. THOR is included explicitly in CORVUS. This allows the hot electron transport physics, such as return current heating, to be included consistently with the hydrodynamic modelling. Energy deposition into the background fluid is mapped to the hydrocode mesh, and the evolved density profile is returned to update THOR.

2.4. Link codes

In order to deliver an integrated modelling capability it is necessary to link the disparate physical models together. In some cases the most practical method is to run one model entirely disconnected from the other, using outputs from one as an input for the other. This is the method adopted for linking the PIC code to other models, since the kinetic model adopted in PIC and the timescales of the physics involved make in-line modelling impractical. There are two links which are required.

2.4.1. Linking EPOCH to hydrocode output. This enables the initial density and temperature profiles of a short-pulse LPI simulation to be derived directly from the output of a hydrocode simulation of long-pulse, or pre-pulse, interaction. A link code, FENRIS, has been developed for this purpose. However, here we focus on the physics of absorption and transport in short-pulse experiments, rather than long-pulse effects. This does create some limitations. Assumptions must be made about the plasma conditions the short-pulse encounters, which would be determined by the laser’s pre-pulse or the action of any long-pulse beams present. However, in the context of FI, where the high intensity ignition beams would need to last for tens of picoseconds, the pre-plasma conditions may not be so critical. Recent work [21] demonstrates that over these longer timescales, the ponderomotive force of the laser is able to modify the initial density profile to such an extent that its final state is largely insensitive to its initial state. As we will demonstrate in section 4, while pre-pulse hydrodynamics may not be critical under these conditions, the evolution of the solid target due to the action of the short-pulse delivered energy, is significant over such timescales, and so a transport model which can accurately represent hydrodynamic effects is highly advantageous.

2.4.2. Linking EPOCH to THOR. This means that the energetic electron distributions used in THOR can be derived directly from the particle distributions generated by EPOCH. One approach adopted elsewhere [34] has been to generate a functional fit to the particle distribution, based on
a combination of simple functions of angle and energy. Our approach is to construct, from the PIC particles, a discrete distribution function on a fixed phase-space mesh; the link code LOKI provides this capability. Particle probe diagnostics record particle quantities (i.e. mass, charge, weight, position and momentum) as they pass through a pre-defined plane in the simulation. This data is then included in EPOCH’s output dumps. The result is extremely detailed, time resolved, particle data. However, this data is not suitable for use as a source term in THOR for two main reasons. Firstly, it contains details specific to the macroparticle description adopted in EPOCH, which does not necessarily fit with that of THOR. For example, decisions about the extent of phase space to sample, and the number of macroparticles, as well as the spatial and momentum coordinate systems, need to be independent for each code; THOR should not be bound by choices made by EPOCH when generating particles. Secondly, the quantity of data can be significant. The sum of all particle data for every particle in a species which passes through a given plane, over a complete simulation, can total many hundreds of gigabytes. It is impractical to use such a quantity of data as a source, indeed simply loading the source into memory could easily come to dominate the workload. It may also be impractical to store such quantities of data in the long term.

To avoid these issues, it is necessary to post-process the particle data into a more manageable form. LOKI generates a particle distribution function in position, energy, angle and time from EPOCH probe data, which is stored using the standard HDF5 file format. THOR generates particles from a LOKI source by generating a point in 3D phase space using a Sobol quasi-random number sequence [27], with appropriate limits on the space set by querying the LOKI dataset, in order that the sampling is efficient. The weight of the source particle is then set according to the appropriate phase space bin in the LOKI data.

It is important to note that there are some distinct limitations on this approach. The acceleration of fast electrons in the absorption region can only persist while there is a sufficient supply of electrons from the cold return current. However, there is no link back from THOR to EPOCH; as a result the return current near the absorption region is entirely independent of the return current in the region modelled with THOR. This means that the modelling of the absorption region does not take into account the impact of resistive return current effects, such as magnetic field generation, which may influence the current balance in the absorption region and so influence the hot electron spectra. In addition, the contribution of fast particles reflected by magnetic fields or reflecting boundaries in the hybrid region is not accounted for. Furthermore, it is possible for electrons to be recirculated in the PIC code and pass through the probe plane multiple times. These issues could be addressed, in part, by employing a full collisional model, but at solid densities this is not a practical solution for routine use. As discussed earlier, work is underway to improve the model, by the adoption of a macroparticle description which treats the cold background electrons differently using a simplified Ohm’s law in the higher density regions [12], and thus marginalize the impact of running the absorption and transport models sequentially. In this paper we demonstrate that despite these limitations the integrated modelling capability as outlined here has notable advantages over assuming a functional form for the energetic and angular distribution of hot electrons and represents a step towards a practical predictive modelling capability for HEDP experiments.

3. Heating solid diamond

Plastic, diamond and diamond-like carbon are commonly used target materials in short-pulse HEDP experiments. Material samples, in the form of buried layers, such as the aluminium layers
used in [9, 19] can be held at solid density within the bulk material and heated to 100s of eV, primarily via Ohmic effects. Similar experiments can also be used to help study hot electron absorption and transport [3, 17, 33] providing key data for the evolution of hot electron driven FI ICF point designs.

Here we consider the absorption of short-pulse laser energy, and subsequent hot electron transport, in a solid diamond target. The LPI and hot electron generation is modelled in EPOCH, and the resulting hot electron spectrum passed to THOR as described above. At present we do not include a buried layer in the simulation and focus instead on calculating the temperature of the substrate at depth.

The incident laser is chosen to be comfortably within Orion’s capabilities: a wavelength of $\lambda_0 = 0.53 \, \mu m$, i.e. second harmonic or ‘green’ light; a peak intensity of $I_0 = 6 \times 10^{19} \, \text{W cm}^{-2}$; and a total energy of 83 J. The laser spot is a super-Gaussian of the form $\exp\left(-\left(\frac{r}{r_0}\right)^4\right)$ where $r_0 = 7.5 \, \mu m$, and the temporal profile a simple Gaussian of the form $\exp\left(-\left(t - t_{\text{peak}}/t_0\right)^2\right)$ where $t_0 = 0.5 \, \text{ps}$ and $t_{\text{peak}} = 1.0 \, \text{ps}$, the simulation ends at $t = 2.28 \, \text{ps}$.

In this work we concentrate on the link between the PIC and transport codes, in particular the impact on target heating of using a particle source derived from a PIC code, rather than relying on empirical scaling laws. Therefore, we do not consider the effect of pre-plasma conditions, this will be given greater consideration in future work, using FENRIS to initialize EPOCH from radiation-hydrodynamic simulations, as outlined earlier.

As a result of the nonlinear characteristics of the frequency-doubling KDP crystals used to generate it, the 0.53 $\mu m$ beam from laser systems such as Orion is typically very high contrast, with significantly lower pre-pulse than would be expected from the first harmonic. Hence, we assume the plasma conditions that the main pulse encounters are characterized by an exponential profile with a relatively short scale-length of 1 $\mu m$ up to critical density, and 0.1 $\mu m$ from critical to solid density. The target is angled at $-10^\circ$ to laser normal—since in such experiments it is often the case that perfectly normal incidence is not used, to reduce the potential risk to the final focusing optics. Resolving such a steep density profile, and such a high peak density, is challenging in a PIC code; high order cubic spline particle shape functions are employed to suppress the effects of numerical heating. It is not feasible at this stage to reproduce these conditions in a three-dimensional (3D) model, and so we restrict our modelling to 2D for the present work. The target is treated as fully ionized carbon with a peak density equivalent to solid diamond (approximately $226 n_c$, where $n_c$ is the critical density for the laser) and an initial temperature of 200 eV. The simulation was run with 84 particles per cell on a $5760 \times 4560$ cell mesh measuring 78 $\mu m \times 58 \, \mu m$. It is important to note that the physical extent of the system is not the same in both EPOCH and THOR. The domain in THOR extends from $-50$ to $50 \, \mu m$ parallel to the probe plane in EPOCH and 50 $\mu m$ perpendicular to it. The THOR domain does not include any of the absorption region and pre-plasma. We do not attempt to model the full extent of the target in EPOCH—the solid density portion of the EPOCH simulation corresponds only to a small region of the THOR domain, as shown in figure 1. Open particle boundaries were used in THOR but thermal boundaries were chosen for the EPOCH modelling. Thermal boundaries return exiting particles to the system with their energy re-sampled from a thermal distribution at the initial background temperature. This helps to minimize any impact of hot particles recirculating in the much smaller EPOCH domain.

The electron population is partitioned into ‘hot’ and ‘cold’ electrons. Electrons are migrated between these two populations depending on their velocity relative to the local cold population’s thermal velocity $v_{te}$, with all electrons starting the run in the cold population.
Figure 1. Arrangement of EPOCH (blue) and THOR (red) domains adopted for the integrated simulation, plotted in THOR’s geometry. THOR’s open boundaries are highlighted in magenta, while EPOCH’s thermal boundaries are shown in orange. The location of the particle probe in EPOCH, where particle data is collected and post-processed by LOKI to provide source distributions for THOR, is shown in green.

In the results presented here, electrons are promoted from the background to the hot populations when their velocity exceeds \(4v_{te}\) and demoted if their velocity falls below \(3v_{te}\). A particle probe diagnostic was placed parallel to the target surface a distance of 2.5 \(\mu\)m behind the top of the density ramp. This probe will only record the details of hot electrons which traverse it from the laser direction. This allows us to effectively filter out the numerous, but relatively low energy, cold background electrons which might otherwise dominate the workload of the transport code while adding little to the target heating profile at depth. We used LOKI to generate a source distribution for THOR by integrating the particles onto a 3D \((r, E, \theta)\) mesh over twenty equal 0.114 ps intervals. The radial, \(r\), mesh consisted of 40 equally sized cells from \(r = 0\) to 40 \(\mu\)m. We used a stretched energy, \(E\), mesh consisting of 128 cells from \(E = 0\) to 128 MeV and cell sizes increasing from \(dE = 0.0078\) to 1.9922 MeV to enhance the resolution at lower energies. The angular, \(\theta\), mesh is also stretched, consisting of 50 cells from \(\theta = 0^\circ\) to 100\(^\circ\) with cell sizes increasing from \(d\theta = 0.4183^\circ\) to 2.7888\(^\circ\). We define \(\theta\) to be the angle relative to the average particle direction over an integration interval. Hence if \(\phi\) is the angle that a particle makes with the normal vector of the probe plane then \(\theta = \phi - \langle \phi \rangle\).

Figure 2 summarizes the particle data collected at the probe plane. Fits to the time-integrated energy distribution at low (1–3 MeV), medium (4–12 MeV) and high (15–25 MeV) energies give temperatures of 2.52, 7.58 and 18.94 MeV respectively while the average electron energy at the peak of the pulse is 2.2 MeV. The probe data indicates that the hot electron
Figure 2. A particle probe diagnostic in EPOCH records particle data $2.5 \mu m$ into the solid diamond. Shown here is the normalized time integrated hot electron energy distribution (top left), on a logarithmic scale. Linear fits to the slope of the curve at low (1–3 MeV), medium (4–12 MeV) and high (15–25 MeV) energies give temperatures of 2.52, 7.58 and 18.94 MeV respectively highlighting the inadequacies of characterizing the distribution with a single temperature. The hot electron distribution near the peak of the pulse, in electrons per MeV, per degree, per cubic metre, at spot-centre is plotted with a logarithmic scale (top right). The divergence falls at higher electron energies, an effect which is easily omitted if the hot electron population is characterized by a single divergence angle. The time integrated angular distribution of the entire hot electron population (black curve, bottom left) is well approximated by $f(\theta) \sim e^{-\theta^2 / 2\sigma^2}$, where $\sigma = 40.34$ (dashed red curve, bottom left). The divergence angle is given relative to the average angle of the hot electron population which varies over time (bottom right), averaging $-6.85^\circ$. However, at the peak of the pulse, the average angle is close to $-20^\circ$—which has a clear impact on the target heating profile.

distribution is a function of $E$ and $\theta$ and clearly shows that the divergence of the hot electron population falls at higher electron energies, an effect which is easily omitted if the hot electron population is characterized by a single divergence angle. The time integrated angular
distribution of the entire hot electron population has an average divergence half-angle given by \(\langle \theta \rangle = 28.09^\circ\) but is well approximated by a function of the form \(f(\theta) \sim e^{-\theta^2/\sigma^2}\), where \(\sigma = 40.34\). The average angle of the hot electron population, \(\langle \phi \rangle\), varies over time, averaging \(-6.85^\circ\) relative to the probe (or equivalently, target) normal. However, at the peak of the pulse, the average angle, \(\langle \phi \rangle\), is close to \(-20^\circ\)—which has a clear impact on the target heating profile. The total energy carried through the probe by the hot electrons was equivalent to 38.75% of the incident laser energy, although this does not represent the total absorption which would be higher, as it does not account for effects such as heating of the ion population or the low density pre-plasma.

The variation in direction appears to be a result of the evolution of the pre-plasma in front of the target in response to the laser itself. The impact of this is evident in the target heating profile, shown in figure 3—which is a composite figure constructed from both EPOCH and THOR simulations. There is a clear directionality to the heating profile angled at 15–20\(^\circ\) from target normal and not aligned to the laser axis either.

It is common to assume a Maxwellian form for the hot electron population characterized by a single ‘temperature’, \(T_{\text{hot}}\), which scales with the ponderomotive potential of the laser [38]. We adopt the following form for \(T_{\text{hot}}\):

\[
T_{\text{hot}} \text{ (MeV)} = 0.511 \left\{ \left( 1 + \frac{I \text{ (W cm}^{-2}\text{)} \lambda (\mu m)^2}{1.37 \times 10^{18}} \right)^{1/2} - 1 \right\},
\]

where \(I\) is the laser intensity, \(\lambda\) is the laser wavelength and plane polarized light has been assumed. For the laser conditions detailed above, this gives \(T_{\text{hot}} = 1.343\) MeV—lower than indicated by the probe data summarized in figure 2. We initialized THOR with a Maxwellian energy distribution and fixed the total injected energy to match that observed in the EPOCH simulation. The angular distribution, while not a function of energy, was also chosen to match the time, and energy, integrated distribution shown in figure 2. This permits a fair comparison of the heating profiles from an integrated simulation and a simpler transport simulation using an analytic source.

Figure 4 demonstrates that if the heating profile from our integrated simulations is compared with THOR simulations, which assume a ponderomotive scaling of \(T_{\text{hot}}\) and a Maxwellian energy distribution, clear differences in the material temperature become apparent. It is clear then that there are potential problems basing a predictive modelling capability on assuming a simple functional form for the hot electron energy spectrum characterized by equation (4), even when the total energy and average divergence have been calculated by other means, which would not always be practical. One important feature of the integrated model, which is not captured with an analytic source, is the temporal variation in the average angle of the electron source which acts to increase the apparent spot size at the rear surface.

Further work is needed to refine and validate such models before we are in a position to state with confidence what the expected hot electron flux from a given set of laser and plasma parameters will be, and before it will be possible to model FI point designs with the level of fidelity common in ICF modelling [11, 18, 25]. Well-characterized experiments, on laser systems such as Orion, Vulcan and OMEGA EP, will be critical in building this confidence.

In a similar manner to the probes used in EPOCH, the use of a particle probe plane in THOR permits all of the hot electrons crossing a plane within the simulation to be interrogated. By placing such a probe at the boundary of the simulation it was possible to record all of the hot electrons leaving the target rear surface. As charged particles move between regions of differing
Figure 3. A representation of the complete system modelled with an integrated approach, generated using the background ion density and $B_z$ from the EPOCH simulation of laser absorption in solid density diamond and overplotted with the heating profile from a THOR simulation using a particle source derived from the EPOCH, at $t = 0.456$ ps (top) and 1.026 ps (bottom). The white contour line shows the extent of target heating in excess of 500 eV.
Figure 4. THOR simulation of heating of solid diamond by hot electrons: using a source derived from a 2D EPOCH simulation (left column); and using a Maxwellian distribution with a temperature given by ponderomotive scaling (right column) at \( t = 1.026 \) ps (top row) and \( t = 1.6 \) ps (bottom row). The total energy and average divergence angle in the ponderomotive scaling case is fixed to match that of the EPOCH simulation to allow a fair comparison. There are clear differences in the heating profile and temperatures achieved.

dielectric constant transition radiation is emitted [16]. This phenomenon is sometimes used as a means of diagnosing the hot electron population reaching the rear surface of a short pulse laser target [2, 31]. By employing the following formula [16] for transition radiation, time-integrated optical transition radiation (OTR) intensity profiles across the rear surface can be calculated:

\[
\frac{d^2I}{d\omega d\Omega} = \frac{e^2}{4\pi^3\epsilon_0 c} \frac{\beta^2 \sin^2 \theta}{(1 - \beta^2 \cos^2 \theta)^2},
\]

where \( \beta = v/c \) and \( \theta \) is the angle between the electron’s trajectory and the observer. This allows us to easily generate OTR lineouts from our simulations which provide a qualitative indication of the impact on rear-surface hot electron diagnostics of changes to the source and target parameters without the need to resolve fast timescale effects—as would be required for the generation of, for example, a coherent transition radiation diagnostic. Figure 5 shows OTR lineouts generated from fast particle spectra at the rear surface of THOR simulations of target heating in solid diamond. The emission using the ponderomotive source is stronger in both cases. Where an EPOCH source has been used, there is a distinct increase in the apparent OTR spot size as the thickness of the target increases, while the spot generated with a ponderomotive source remains relatively stable. The divergence half-angle, calculated from the FWHM of these simulated OTR lineouts, is \( \sim 0.5^\circ \) for the ponderomotive source and \( \sim 17.14^\circ \) for the EPOCH source. The EPOCH source is comparable to the reported divergence angles in [17]. This is less than the average half-angle of the source itself, \( \langle \theta \rangle = 28.09^\circ \). However, since the OTR intensity is a function of \( \beta \), and the divergence falls at higher energies (see figure 2) this is consistent
Figure 5. Simulated OTR normal to the target rear surface. Generated from fast particle spectra at the rear surface of THOR simulations of target heating in solid diamond. Blue curves denote a ponderomotive (i.e. Maxwellian) source while red denotes an EPOCH source. Dashed lines show the relative OTR lineouts for a 20 $\mu$m thick target, while solid lines represent a thicker, 50 $\mu$m target. The emission from simulations using the ponderomotive source is stronger in both cases. Where an EPOCH source has been used, there is a distinct increase in the apparent OTR spotsizes as the thickness of the target increase; this is not the case with a ponderomotive source. This could have implications for attempts to characterize the hot electron divergence angle using diagnostics on the hot electron population at the rear surface.

with the measured distribution. This highlights the difficulty in trying to measure a single hot electron divergence angle experimentally. Most importantly, the integrated model demonstrates a spot size which increases with target thickness, as observed experimentally [31], while the simple ponderomotive source does not.

4. Heating structured targets

An important HEDP application for short-pulse lasers is the isochoric heating of material samples, but this is often constrained as the samples are buried in a substrate [19] in an effort to isolate them from the effects of prepulse hydrodynamics and heating. This has the effect of reducing the coupling to the material of interest due to the divergence of the electrons. One way to improve the efficiency is to employ ideas from recent numerical [10, 29] and experimental [20] work highlighting the potential of structured targets for controlling the fast electron flux. Advanced target designs which utilize this mechanism have also been suggested as a possible method to improve hot electron coupling to the compressed fuel in FI [30].

Magnetic fields generated by the fast electron current can provide a collimating effect [5] which has the potential to enhance and direct the flux by careful choice of target materials and structure; for example a higher resistivity material can be embedded within a lower resistivity target. Assuming the material interface remains intact following any prepulse or precursor...
hydrodynamic phase, a different electric field should be generated on either side of the interface
given the approximation of return current neutralization and $\mathbf{E} = -\eta \mathbf{j}_{\text{hot}}$: this change in electric
field drives a magnetic field via Faraday’s Law which acts to confine the hot electrons.

Here we apply the methods detailed above to study hot electron transport in a number
of different structured targets. Following the approach of [29] we choose a target consisting
of an aluminium guide surrounded by lithium. We consider a cylindrical wire and a truncated
cone (figure 6) and contrast against a simple ‘slab’ reference target where the first 20 $\mu$m is
aluminium with the remainder of the target lithium. In each case the aluminium structure extends
only part-way through the target to the depth where a material sample would be placed—the aim
being to enhance the heating at this specific depth.

The THOR calculations were all carried out in 2.5D Cartesian geometry with a resolution of
1 cell per micron. Increasing the resolution to 2 cells per micron had a negligible impact on the
heating, or on the magnetic fields. All of the boundary conditions were set as transmissive: we
are anticipating experiments where the front and rear surfaces have been ablated by prepulse
or long-pulse compressor beams leading to long scale length plasmas that would suppress
refluxing. The code injects a certain number of particles per processor per timestep to sample
the LOK phase space, for these calculations we used 2000 over 16 processing cores i.e. 32,000
particles per timestep. With transmissive boundaries computational particles rapidly leave the
system, so net populations peak at $\sim 2.5 \times 10^6$.

In all cases we use the same electron source as section 3, this allows a fair comparison
between the different structures. In experiment this is equivalent to a thin surface layer of carbon
on the front of the target.

The specific heat of the material was inferred from tabular data, ionization was computed
from a simple Thomas–Fermi model, and the resistivity from a capped Spitzer form
i.e. $\eta(T) = \eta(100 \text{ eV})$ for temperatures below 100 eV. Better analytic forms are available in
THOR e.g. the Milchberg fit for aluminium [26] and matching to the room temperature at low $T$
for lithium [29], but we have sought to be consistent between the two materials and, furthermore,
would need to ensure that the specific heats used were equally adapted for the low temperature
regime to ensure a thorough handling of any resistivity approximation.

Reference results for the simple aluminium/lithium block are shown in figure 7 at 2 ps after
the laser pulse is switched on in EP0Ch. Whilst there is enhanced heating visible in panel (a) at
the interface this is primarily due to the lower specific heat of the lithium. The direction of the
electron beam varies significantly over the duration of the PIC simulation but the bulk of the energy deposition appears to concentrate around 10–20° from the target normal. The magnetic field is principally induced at the edge of the electron beam and at the interface between materials.

Figure 8 shows the results for an aluminium wire embedded in lithium. Superficially some enhancement to heating and collimation is visible in the temperature spatial profile compared with figure 7, however there appears to be little evidence from the heating of change in the directionality of the electrons as they transit the interface. It can be seen from panel (b) that whilst the magnetic field still builds up at the edge of the electron beam, the principle component outlines the shape of the aluminium structure (cf figure 6). The tilt of the beam direction relative to the target normal produces a more complicated field structure at the wire edge (around $x = 10 \mu m$).

With a cone target (figure 9) the heating of the lithium as the beam exits the aluminium appears more pronounced than with a wire, but this is at least partially a result of the shorter stand-off distance between the source and the material interface with the cone geometry. The beam is diverted towards target normal and the heating at depth is also enhanced in comparison to the wire.
As figure 7 but the target is now an aluminium wire embedded in lithium. Whilst there is enhanced heating visible in panel (a) at \( z > 20 \mu m \) this is due to the lower specific heat of lithium. There appears to be little change in the directionality of the electrons through the material interface. It can be seen from panel (b) that whilst magnetic field still surrounds the electron beam, the principle component outlines the shape of the aluminium structure. The tilt of the beam direction relative to the \( z \)-axis appears to produce a more complicated field structure towards \( x = 10 \mu m \) as the fast electron current is much lower at this material interface.

As discussed, we are attempting to demonstrate the potential of structured targets to enhance the heating of material samples at a specific depth \(-20 \mu m\), at the edge of the insert. An improvement in the heating efficiency should manifest as enhanced heating at this point in the target. A comparison of temperature profiles for the wire and cone targets in figure 10 along the target normal demonstrates that the cone insert achieves a higher peak temperature at 20 \( \mu m \) depth. Figure 11 applies the post-processing tools demonstrated in section 3 to these structured targets. The wire insert has little impact, compared to the slab target, but the conical insert generates a marginally smaller, brighter spot, although it fails to significantly alter the direction of propagation of the beam.

The cone target appears to perform well, however because of the source angle, the bulk of the electrons do not pass through the tip. Figure 12 shows results where the cone axis of symmetry has been tilted at 10°, 15° and 20° about the origin; adapting to the direction of the electron beam during the peak of the pulse. At 10° peak heating concentrates in a smaller spot and rises suggesting enhanced collimation of the beam. Increasing the angle further enhances the heating at the tip. A tilt of 20° aligns the cone with the source direction at the peak of the pulse, which appears to give the best heating at the desired depth. There is a clear enhancement

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Figure 9. As figure 7 but with a solid aluminium cone target configuration. The heating of the lithium as the beam exits the aluminium appears more pronounced than in figure 8, but this may partly be due to the shorter stand-off distance between the source and the material interface in the beam propagation direction.

Figure 10. Temperature line profiles from structured targets modelled with Thor. The profiles are taken along target normal and show temperature in eV as a function of distance. Results are shown for: a lithium target with an embedded cylindrical aluminium wire (yellow) and lithium with an embedded truncated aluminium cone (green). In each case the embedded structure terminates at 20 µm. For reference, the red line shows the profile in slab geometry.

of the peak temperature reached at the tip of the cone by a factor of ~2 between the 0° and 20° cases. This suggests there is some merit in considering the angle of the electron beam close to the peak intensity, and it may be particularly worthwhile in attempting to design structured
Figure 11. Simulated OTR lineouts, normal to target rear surface, from structured targets modelled with THOR. Results are shown for: a simple aluminium target (red); a lithium target with an embedded cylindrical aluminium wire (green); lithium with an embedded truncated aluminium cone (blue). All structured targets deflect the hot electron flux back towards target normal and produce a smaller OTR spot that the simple aluminium target.

Figure 12. Temperature lineouts from structured targets modelled with THOR. The target is lithium with an embedded truncated aluminium cone tilted from the z-axis at: 0° (black); 10° (blue); 15° (green); 20° (red). The lineout is taken along the axis of symmetry of the cone. The heating of the tip of the cone, located at 20 µm, is significantly enhanced when the cone is aligned with the electron beam.

collimators that optimize the heating of a target layer. However, in this configuration at least, collimators do not appear to offer a method for freely controlling the particle flux, which is still dominated by the source direction.

To see how the target would respond to the short-pulse heating on longer timescales, the 0° cone case was investigated using THOR in-line in CORVUS. Figure 13 shows the initial
Figure 13. CORVUS calculation of the hydrodynamics phase. Panels are shown at 2, 20 and 50 ps with the electron transport source used in figure 9. The velocity in µm ps$^{-1}$ is plotted over density in g cm$^{-3}$ (velocity is not shown at 2 ps as it is negligible). Material boundaries are indicated in all panels. Little hydrodynamic motion occurs in the first 2 ps of the calculation, justifying an isochoric approximation for the transport. After 20 ps the cone has begun to expand into the lighter lithium. After 50 ps significant motion has occurred. Whilst the evolution of the aluminium cone appears largely symmetrical, the back surface of the lithium has a noticeable asymmetry, reminiscent of the OTR plot in figure 11.
configuration, and subsequent evolution of the target. At late time, whilst the front of the target, including the aluminium cone, evolves symmetrically, the velocity and density profile at the back surface reveal an asymmetry, comparable to that present in figure 11. The target evolves little in the first 2 ps which would appear to justify the isochoric assumption implicit in the earlier simulations—however, it is important to note this might not be true if precursor hydrodynamics had imposed an initial velocity field; if there were a significant pre-pulse or separate long-pulse compression beams present—as would be the case for full-scale Orion experiments. Furthermore, over a timescale of tens of picoseconds there is significant movement in the aluminium/lithium boundary with density features appearing in the lithium, which highlights the potential importance of including hydrodynamic effects when considering longer, high intensity pulses—such as the ignition pulse in FI.

5. Summary

We have shown how an integrated modelling framework can be employed to simulate some simple short-pulse targets with an application to HEDP experiments. The use of explicit PIC sources in a hybrid code indicates that the hot electron population produced in short-pulse laser solid interaction may have a distribution in energy and divergence angle, as well as a spatial and temporal evolution, that is difficult to capture with a parameterized analytic form. While the modelling tools currently available offer invaluable insight into the dominant physical processes in short-pulse laser–matter interaction, a predictive modelling capability will need to be validated against experiment. We have demonstrated, by the use of simulated OTR diagnostics, the use of novel structured targets and the self consistent modelling of the bulk hydrodynamic response to short-pulse deposited energy that there are opportunities to test the modelling suite against experiment. Conversely, the capability outlined here can already be applied to help design and interpret experiments; the efficacy of this approach will improve over time as HEDP campaigns progress.

Structured targets have been shown to offer additional control over the hot electron flux which could be used to enhance the heating of buried layers or microdots. This will require further development as an experimental platform. In particular, equivalent designs with low-Z materials (such as plastics or diamond) will be required to facilitate spectroscopy diagnostics on buried samples. A target incorporating changes in material density, rather than changes in material, is one possibility [10].

Coupling transport and hydrodynamic algorithms also confirmed that, over the time-frame of the short-pulse interaction, an isochoric approximation is often sufficient, as little hydrodynamic motion takes place. This means that a considerable quantity of modelling can be carried out using just THOR, drawing on the same set of EPOCH simulations for the hot electron source—as demonstrated with the structured target simulations. Given the modest computational demands of the Monte-Carlo model, this provides a flexible tool for designing and interpreting experiments which can be refined with further PIC simulations and augmented with bulk hydrodynamic motion as required. The isochoric approximation is less appropriate if pulses get longer and more energetic, as would be the case for many FI concepts and for HEDP experiments which utilize long-pulse beamlines. In such cases an accurate density profile following nanoseconds of hydrodynamic motion is required, it is here that the integration of THOR into CORVUS comes to the fore.
An integrated approach short-pulse modelling does come with limitations. In linking the PIC and transport codes we ensure that each simulation represents a single ‘realization’ of the system. Whilst this relieves us of the need to choose values for parameters such as the divergence angle, hot electron temperature and absorption fraction, it is important to understand the sensitivity of the observable quantities (such as material temperature, OTR emission and the motion of the targets rear surface) to small variations in the PIC simulation parameters.

The interfaces between codes are another area of uncertainty [36]. In particular, in the simulations discussed here there is a ‘transport gap’, between the laser absorption region and the particle probe, of several microns. This region is modelled in the explicit, collisionless, PIC code, but covers densities from $\sim n_c$ to $\sim 200 n_c$. The lower end of this density range is beyond the reach of $\text{THOR}$ and the upper end would be impractical for a collisional PIC code. A model is required to bridge this gap and provide an overlap between the two models. The approach adopted in [12] retains a macroparticle description for all species but treats the cold background electrons differently—replacing the standard Maxwell solver with a simplified Ohm’s law in the higher density regions. This would allow transport effects in the absorption region to be included self-consistently. Such an approach has been successfully incorporated into other PIC codes [15] and will be adapted to $\text{EPOCH}$ in order to provide key hot electron transport physics, namely resistive return current heating and associated magnetic field generation, in the region between laser absorption and solid density.

Continuing development of both the constituent codes and a refinement of the links between them, underwritten with new experimental data from facilities such as Orion will ensure that nascent capabilities such as those outlined here develop into a practical, predictive modelling tool which can help the design and interpretation of ever more ambitious HEDP experiments in the coming years.

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