Self-consistent particle-in-cell modelling of short pulse absorption and transport for high energy density physics experiments

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Abstract. In order for detailed, solid density particle-in-cell (PIC) simulations to run within a reasonable time frame, novel approaches to modelling high density material must be employed. For the purposes of modelling high intensity, short pulse laser-plasma interactions, however, these approaches must be consistent with retaining a full PIC model in the low-density laser interaction region. By replacing the standard Maxwell field solver with an electric field update based on a simplified Ohm’s law in regions of high electron density, it is possible to access densities at and above solid without being subject to the standard grid and time step constraints. Such a model has recently been implemented in the PIC code EPOCH. We present the initial results of a detailed two-dimensional simulation performed to compare the adapted version of the code with recent experimental results from the Orion laser facility.

1. Introduction
To support experimental campaigns on short pulse laser facilities, or develop point designs for fast ignition, laser interaction simulations with peak densities at, or approaching, solid density are required. Simulating high density plasmas places severe constraints on the use of standard particle-in-cell (PIC) techniques to solve Maxwell’s equations and the particle equations of motion, limiting the spatial and temporal scales which can be easily modelled. Due to these constraints, detailed modelling of the hot electron transport resulting from a high intensity, short pulse laser interaction is often only possible by sampling the hot electron population and passing this information to a separate, dedicated code [1]. In order to extend the range of densities which can be feasibly modelled, and thus reinforce the link between PIC and hot electron transport codes, an algorithm, based on that developed by Cohen, Kemp & Divol [2], has been implemented in the PIC code EPOCH [3]. This model utilizes a ‘hybrid’ description for the plasma which replaces the standard Maxwell field solver in regions of high electron density (≥ 100nₑ) with a field update based on a simplified Ohm’s law:

\[ E = \eta \left( J_b + J_i \right) - \frac{J_b \times B + \nabla P_b}{en_b}, \]

where \( J_b \) is the background electron current density, \( J_h \) and \( J_i \) are the hot electron and ion current densities, and an isotropic resistivity, \( \eta \), and background electron...
pressure, $P_b$, have been assumed. This approach relaxes the grid and time step constraints, permitting simulations to be run at a lower resolution while also dramatically reducing numerical self-heating.

In order to distinguish hot electrons from the background, the electron population is partitioned into two electron species. Background electrons are promoted to the hot electron population if their kinetic energy satisfies the condition: $|v_h| > \alpha \sqrt{3 k_B T_b/m_e}$, where $T_b$ is the local background electron temperature and $\alpha$ is a free parameter (typically $\sim 5$).

### 2. Buried layer heating

A detailed 2D simulation was performed using hybrid-EPOCH with the intention of replicating the heating of buried layers observed in recent Orion experiments [4,5] as a means of validating the code against experimental results. A plastic target, containing a thin sample layer of aluminium, was modelled with parameters selected so as to replicate the experimental conditions as closely as possible.

The simulated target consisted of fully-ionised ‘plastic’ ions, with mass number 6.5 and atomic number 3.5 to represent both hydrogen and carbon ions, at a density of 1.0 g/cc. A 150 nm sample of Al$^{12+}$ at 2.7 g/cc was placed 12 µm into the plastic. The target was preceded by an exponential density profile of the form $s e^{x/L_1} + (1 - s) e^{x/L_2}$, where $s$ is the ratio of the critical density to the peak electron density in the front plastic layer, $L_1 = 3$ µm and $L_2 = 0.5$ µm. Furthermore, the target was rotated so as to be angled 10° relative to the incident laser pulse.

The laser pulse was modelled as having a Gaussian radial profile with 90% of the energy contained within a 20 µm diameter spot, a supergaussian temporal profile with full-width-half-maximum (FWHM) of 0.5 ps, total energy of approximately 100 J, and a wavelength of 0.528 µm.

Approximately $2 \times 10^8$ PIC particles (75% electrons, 5% aluminium ions, 20% ‘plastic’ ions) were modelled on a mesh of $2600 \times 2400$ cells covering $65 \times 60 \mu m^2$. The interface between the Maxwell (PIC) and Ohmic (hybrid) field solvers was set between electron densities of $8 \times 10^{28}$ and $9 \times 10^{28} m^{-3}$, with the electric field update at intermediate densities being interpolated between the two solutions.

Radial temperature and density gradients were observed within the aluminium layer (see figure 1). In order to obtain a single value for comparison with the equivalent experimental

![Figure 1. Background electron temperature ($T_e$) and density ($n_e$), and the Poynting flux ($I$) of the laser, at t = 1ps (shortly after the peak laser interaction).](image-url)
Figure 2. Time history of the spatially-averaged electron temperature (blue, solid) and ion mass density (red, dashed) in the aluminium layer.

results, the electron temperature late was allowed to reach a steady state and spatially-averaged. This yielded a predicted electron temperature of 1779 eV, well in excess of the experimentally observed value of 677 eV (see figure 2).

3. Line emission comparison
The results of the previous section indicate that the maximum spatially-averaged temperature of the aluminium layer predicted by hybrid-EPOCH compared poorly with the experimental values. However, these values are usually inferred from the K-α radiation emitted by the target. Thus comparing the average of a distribution of temperatures with a single inferred temperature may not be a valid approach. For this reason the atomic kinetics code FLY [6] was used to calculate the expected emission spectrum, in the range 1.8–2.15 keV, for the hybrid-EPOCH target. This energy range encompasses the aluminium He-β (1.86 keV) and Ly-β (2.05 keV) emission lines, which are generally used as the main temperature and density diagnostics.

The hybrid-EPOCH cells containing aluminium ions were assigned to 100 eV temperature and 0.1 g/cc density bins, covering the ranges 100–6000 eV and 0.5–4.0 g/cc. FLY calculations for each temperature and density bin were performed, and the resultant emission spectra combined to produce a total expected emission spectrum at late time ($t = 3$ ps, $\sim 2$ ps after the peak laser interaction).

Initial comparisons between the emission spectra predicted using temperature and density conditions from the hybrid-EPOCH simulation and those using a single temperature and density indicated that the hybrid-EPOCH-dependent emission could be well characterised by a spectrum corresponding to aluminium at 600 eV and 2.0 g/cc (see figure 3). These values are broadly consistent with the results of similar experiments [4,7].

4. Conclusion
Two dimensional simulations using hybrid-EPOCH (an adapted version of the particle-in-cell (PIC) code EPOCH [3], employing an algorithm for modelling high density plasmas based on that of Cohen et al. [2]) have been performed to attempt to validate the code against experimental results [4,5,7]. The average temperature of an aluminium layer, embedded 12 µm into a plastic target, predicted by hybrid-EPOCH exceeds the experimental values. However, if the distribution
of temperature and density conditions predicted by the code are used by the atomic kinetics code FLY [6] to produce an expected x-ray emission spectrum good agreement is observed with a single spectrum which corresponds to the approximate temperature and density conditions inferred from experiment. Additional simulations with layers buried at differing depths into the plastic targets are currently underway.

Although the observed x-ray emission spectrum from buried layer targets can be characterised by a single temperature and density, the results presented above suggest that there may be radial temperature and density gradients within the layer. Thus the maximum temperature and density within a small portion of the layer may exceed those inferred from the experimental results.

More generally, the above results indicate that hybrid-EPOCH is a useful tool for modelling the initial stages of a short pulse laser experiment. Namely the laser interaction, energetic electron production and transport, return current generation and the associated heating. However, limits to the code’s physics models still prevent this from being sufficient for modelling the full range of phenomena associated with short pulse laser experiments. Additional codes are required to accurately model target ablation and shock generation by long pulse beams, radiative processes, and longer timescale (~ ns) heating and hydrodynamic expansion. Much initial success has been met in linking suitable codes together to encompass these effects [1]. By making use of models such as that detailed in reference [2], and employed by hybrid-EPOCH, PIC codes are able to access the solid density regime, and thus reinforce any linking of PIC and hybrid transport codes.

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