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List of Acronyms

Rad-MHD Radiative-Magnetohydrodynamics

Rad-Hydro Radiative-Hydrodynamics

HEDP High Energy Density Physics

LPIs Laser-Plasma Instabilities

CBET Cross-Beam Energy Transfer

ICF Inertial Confinement Fusion

PiC Particle in Cell

GO Geometric Optics

IB Inverse-Bremsstrahlung

SBS Stimulated Brillouin Scattering

PCGO Paraxial Complex Geometric Optics

IRT Inverse Ray Tracing

FRT Forward Ray Tracing

LLE Laboratory for Laser Energetics

LLNL Lawrence Livermore National Laboratory

CEA Commissariat à l'Énergie Atomique et aux Energies Alternatives

IAW Ion Acoustic Wave

OpenMP Open Multi-Processing

MPI Message Parsing Interface

inv-Brem Inverse-Bremsstrahlung

EI Etalon Integral

FL Field Limiter

CGT Caustic Gain Truncation

1 SOLAS, A 3-D Laser Ray-Trace and Cross-Beam Energy Transfer Model

This chapter will describe the SOLAS code, a 3-D Laser ray-tracing module implemented in the Radiative-Magnetohydrodynamics (Rad-MHD) code CHIMERA. The chapter begins with a discussion of why ray-tracing is frequently used to model ‘long-pulse’ lasers for High Energy Density Physics (HEDP) experiments and why the standard framework is inadequate to model Laser-Plasma Instabilities (LPIs). It will then go on to describe the ray-trajectory solver, electric-field reconstruction and Cross-Beam Energy Transfer (CBET) components of the model in detail. Discussion of the validity of the model components will be included. The numerical methods will also be presented alongside an extensive set validation problems to verify the implementation.

1.1 Ray-tracing for Hydrodynamic Simulations of Fusion Plasmas

Nanosecond length (‘long-pulse’) lasers are often used as an external energy source in the field of HEDP, for example in laboratory-astrophysics experiments [1–3], equation of state studies [4, 5] or Inertial Confinement Fusion (ICF) implosions [6–8]. Experimental design and analysis for these experiments must often be supported with fluid Rad-MHD simulations. The laser must therefore be described in these codes by a theoretical framework that is both valid to the problem and computationally tractable. The physical processes by which lasers interact with plasma is a result of microscopic couplings between the laser field and particles or plasma waves. The detailed microphysics of these interactions are often studied using Particle in Cell (PiC) codes [9] or wave-based solvers [10], typically for scales and durations of tens of micrometres and hundreds of picoseconds. Coupling these tools directly to multidimensional hydrodynamic simulations, which are often used for millimetre and nanosecond scales, would usually be computationally intractable.

The Geometric Optics (GO) assumptions are often applicable for HEDP laser-plasma interactions (validity discussed in detail for ICF plasmas in Sec. 1.5.8) and therefore ray-tracing offers a computationally tractable approach to modelling lasers in these experiments. By assuming static hydrodynamic profiles (which is normally valid for the propagation time of light through the computational domain) a laser beam can be discretized into a bundle of rays and the ray equations can then be integrated along their path to solve for the trajectory of the light, assuming that refraction dominates over diffraction. A discrete amount of power can also be given to each ray. If there is a suitable model for the power-absorption rate, this can also be integrated along the ray to provide an energy source for the plasma. In many

laser-driven HEDP experiments, frequency-doubled or -tripled lasers and long scale-length plasmas mean that Inverse-Bremsstrahlung (IB) is the dominant deposition process [11, 12]. There are well established models for IB that are suitable for implementation in ray-tracing codes, because they only require knowledge of the local plasma conditions, which are easily accessible via interpolation from the hydrodynamic grid to rays [13, 14]. The combination of the ray equations and IB deposition therefore is the basis for the vast majority of laser-modules coupled to hydrodynamic codes.

In laser-driven ICF experiments however, another class of interaction, LPIs are vitally important to the energetics of the implosion. For example CBET leads to a zeroth-order correction to the energy deposited in direct-drive experiments at the OMEGA laser facility, reducing coupled power late in the implosion to $\sim 50\%$ [15]. LPIs cannot be included in the simple framework described above because they are non-linear¹ and reduced theoretical models of the interaction rely on knowledge of the electric field or intensity of the light [16]. Implementation in a tracing code therefore necessitates a method by which the separate light waves can ‘talk’ to each other. For example, the CBET code described in this chapter stores information for separate components of laser beams on a common grid which can then interact via the ‘pump-depletion iterations’, described in Sec. 1.5.7. Additionally, the knowledge of electric field or intensity is problematic because this is not an attribute which standard GO rays possess. Heuristically, rays have an associated power, so an area is required to obtain an intensity. The evolution of a portion of the beam front’s area is governed by a first order expansion of the Helmholtz equation, rather than the zeroth order expansion which is most commonly used in ray-tracing packages for hydrodynamic codes [17]. The first order expansion introduces an equation for the ray amplitude which can be solved in a variety of ways and used to obtain the electric field of the light. Sec. 1.4 describes the approach taken to solving for the amplitude of the rays in SOLAS, which is to track the area of a triangle² of rays around a standard GO ray.

For direct-drive ICF simulations, it is also desirable to have a 3D ray trace, where rays travel and refract in 3 dimensions. In some computational direct-drive studies, particularly in 1D hydrodynamic simulations, simplified laser models are employed in which rays travel radially toward the target [18]. This simplification is can lead to significant deviations from reality, as it neglects any refractive losses, which become increasingly significant late in the implosion as the target converges. Assuming that rays travel radially inward also leads to deposition occurring closer to the critical surface compared to a true 3D ray trace, leading to an overestimation of the drive. The growth of LPIs also depends on vector summations of light and plasma wavevectors, so a 3D ray trace is necessary when modelling these effects. Predictive direct-drive simulations therefore necessitate a fully 3D ray-trace, even when coupled to just 1D hydrodynamics.

¹Non-linear in this context means that the interaction involves the interaction of multiple light and plasma waves.

²For a 2D ray trace, a pair of rays is used rather than a triangle.

1.2 Existing Cross-Beam Energy Transfer Models

There are a variety of existing computational tools used to model CBET for ICF conditions, which are used to study the interaction from first principles, reduced models to investigate the effect of CBET when coupled to hydrodynamics or validation tools to test the implementation of these reduced models. A non-exhaustive list will be presented here of existing codes, provided mainly as context for the work presented in this chapter.

1.2.1 Ray Based Models

The most common tool to study the coupling of CBET effects into hydrodynamics are reduced ray-based models which use the linear gain theory of Stimulated Brillouin Scattering (SBS), outlined in section???. There are a variety of different codes used to simulate this. The main difference between the models is the way that the electric field or intensity of the laser light is obtained.

Inverse Ray Tracing (IRT) This is an approach, implemented within the IFRIIT code, that creates a mapping between points on an initial beam front and arbitrary locations within the plasma [19, 20]. This is in contrast to Forward Ray Tracing (FRT), which is used in the other ray-based approaches listed below, where discrete points on the beam front are integrated forward to discrete points within the plasma. IRT is a very efficient approach for convex, approximately spherically symmetric plasma profiles, it can not deal well with beams that have multiple caustics³, where the FRT approach is better suited. IFRIIT has been coupled to the 3-D Radiative-Hydrodynamics (Rad-Hydro) code, ASTER from Laboratory for Laser Energetics (LLE), and prior to the development of SOLAS, ASTER-IFRIIT was the only code combination capable of conducting 3-D direct-drive simulations with in-line CBET [15].

Ray Statistics Approach The LASNEX [21], TROLL [22] and DRACO codes [23], developed at Lawrence Livermore National Laboratory (LLNL), Commissariat à l’Énergie Atomique et aux Energies Alternatives (CEA) and LLE respectively, implement field-reconstruction methods which depend heavily on having many rays per computational cell. LASNEX and TROLL, used mainly for indirect-drive hohlraum simulations, obtains the intensity of light by first propagating rays through the mesh and obtaining the deposited power in each grid cell. The intensity is then obtained from the power in each cell using electromagnetic energy conservation. Obtaining the intensity from deposition means that the field cannot be reconstructed in vacuum regions where no deposition occurs.

DRACO uses a similar approach, but the intensity is estimated by multiplying the ray power by the path length in a cell divided by the cell volume, which gives a dimensional estimate for the intensity. Both of these approaches require many rays-per cell to accurately obtain the intensity, $\mathcal{O}(100)$ [24]. For direct-drive simulations this is extremely computationally expensive, because backscatter CBET dominates over sidescatter, therefore the reflected field

³Caustics are defined and discussed in detail in Sec. 1.4.1.

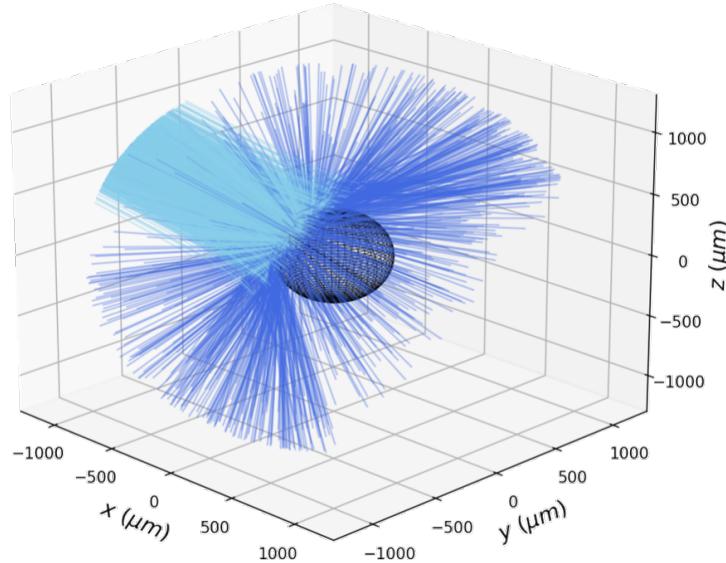


Figure 1.1: 3D ray trajectories through a spherically symmetric, OMEGA direct-drive scale density profile. The incident rays are plotted in cyan and the reflected rays, which spread out over a very large solid angle, are plotted in dark blue. The critical density is represented by the black mesh.

of each beam must be resolved, and each beam spreads out over a large solid angle after reflecting off a convex density profile, as is demonstrated in Fig. 1.1. This means that orders of magnitude more rays are required than for approaches which can accurately obtain the field from a single ray per cell.

Another drawback of both of these approaches is that caustics of beams (regions where the amplitude of rays diverge) are not identifiable, and therefore fields cannot be capped to physically accurate, diffraction-limited values. If a significant amount of CBET occurs at caustics, such as in direct-drive ICF, then erroneous global multipliers to CBET gains must be applied which are effectively free parameters that must be tuned to obtain a pre-known reduction in absorbed energy. This means that it is difficult to trust this approach for predictive direct-drive simulations.

Paraxial Complex Geometric Optics (PCGO) In this approach, each ray has an associated Gaussian intensity profile, the width of which is integrated along the ray trajectory [17, 25]. A single ray can be used per cell as each ray can have an intensity which is interpolated to the mesh, but the reconstructed field at caustics is not accurate and the width evolution is only valid for a short propagation distance. This approach was coupled to the CHIC 2 dimensional hydrodynamics code, but is difficult to extend to 3D as the implementation relied on interacting only rays whose centroids crossed, which does not generically occur in 3D for non-coplanar rays [26].

Neighbouring Rays The BEAMCROSSER code obtains an area for each ray by co-tracing a triangle of neighbouring rays around it that can be converted into a ray amplitude and there-

fore electric field from electromagnetic energy conservation [27]. Integrating the amplitude along the ray trajectory means that the caustics can be identified and therefore fields in those regions capped to diffraction limited values [28]. Each ray also has an individual field value, and it is therefore less dependent on ray-per-cell statistics than geometric models, such as that used in the DRACO code described above [29]. Sec. 1.4 describes the implementation of this approach into the CHIMERA 3D Rad-MHD code, which had not previously been used coupled to hydrodynamics in multidimensional simulations.

1.2.2 Wave Solvers

Solving Maxwell's equations with coupling to a plasma background is a useful tool for the study of LPIs. The main code used in the ICF community that uses this approach is LPSE, which propagates light waves through a prescribed, spatially varying density, temperature and velocity profile in 1D→3D [10, 30]. It then solves the nonlinear coupling of electromagnetic waves by allowing first order plasma perturbations (obtained from the ponderomotive beat pattern between light), which then feed back into the wave propagation. The perturbative approach means that LPSE is limited to linear problems and the temporal and spatial resolution required to resolve the beat frequency mean that coupling to multidimensional Rad-Hydro simulations is not feasible. However, it is an extremely useful tool to validate implementation of CBET models, especially in situations like scattering at laser caustics, such as the test case presented in Sec. 1.5.10.2. It can also be used for many other important studies, such as the mitigation of LPIs via laser bandwidth and the effect of beam smoothing techniques on the growth rate of LPIs [31].

1.2.3 PiC Codes

Both Ray based codes and LPSE are ill-suited to the study of LPIs in the non-linear regime, where the laser intensity becomes sufficiently large that the ponderomotive imprint on the plasma can no longer be treated perturbatively. Understanding this growth and saturation of LPIs in this regime is particularly important for ICF schemes with high peak intensities, such as during the ignitor spike in shock ignition pulses [32]. Often kinetic effects such as ion-trapping become important in non-linear saturation, where ions are trapped and then accelerated in the CBET induced Ion Acoustic Wave (IAW), leading to changes in the IAW phase velocity and therefore a loss of resonance [9]. PiC codes are therefore well suited to model this kinetic saturation, albeit over short timescales and in simulations that are not truly representative of direct-drive conditions, due to computational expense [33]. Kinetic modelling of CBET has demonstrated that the growth of LPIs can be a much more complex, time-dependent problem than is assumed by the linear-models used in ray-based codes, leading to larger net energy transfers [34].

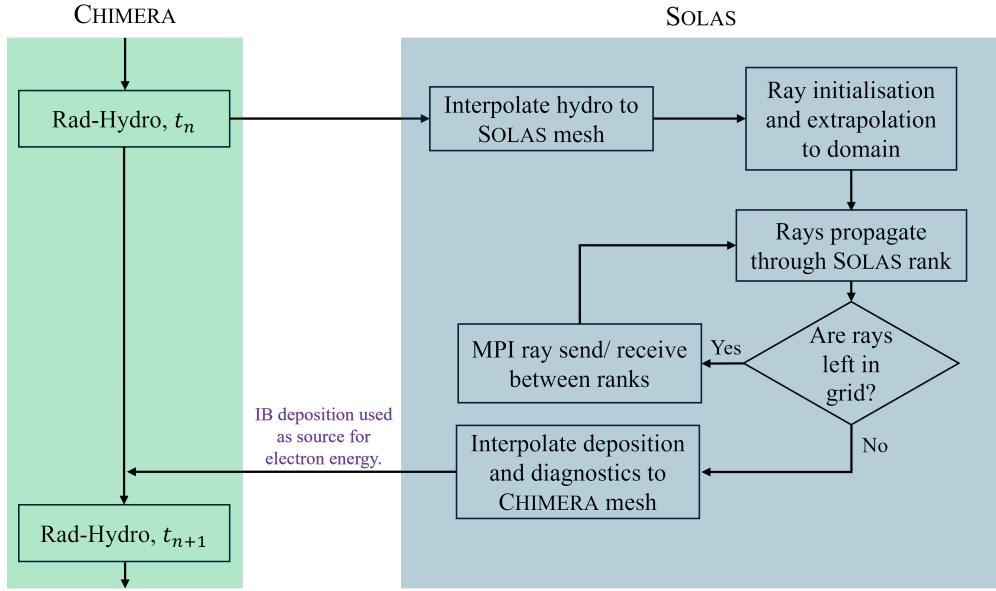


Figure 1.2: A flowchart illustrating the basic interfacing between CHIMERA and SOLAS. The interpolation steps refer simultaneously to the re-domain balancing and cell combination procedures described in Sec. 1.3.2.

1.3 SOLAS 3-D Laser Ray Trace

This section will describe how the ray equations, derived from the Helmholtz equation in Sec. ?? are solved in the SOLAS module for the CHIMERA Rad-MHD code. Details of the mesh used for spherical simulations and load balancing options shall be provided as well as validation problems.

1.3.1 Outline of SOLAS-CHIMERA Interfacing

A simple flowchart for the basic SOLAS operational loop and the interfacing with CHIMERA is shown in Fig. 1.2. At the start of a Rad-Hydro timestep, t_n , the hydrodynamic variables (stored on the Eulerian CHIMERA grid), which are necessary to compute ray trajectories and CBET gains are interpolated to the SOLAS mesh. Rays are then initialised on the beam port locations and extrapolated to the computational domain, before being traced through the grid. SOLAS uses a Message Parsing Interface (MPI) domain balanced approach to parallelization, the reasons for which will be discussed in more detail in Sec. 1.3.2, therefore rays are traced up to the internal borders of the domain subsection used for the MPI rank. Rays are then passed between ranks and moved through their new subdomain until they exit the entire simulation domain. As rays move through the domain, they contribute to total for Inverse-Bremsstrahlung (inv-Brem) deposition in each grid cell and other computational diagnostics. When all rays have exited the domain, the SOLAS quantities such as deposited energy which have been built up from the ray trace are then interpolated onto the CHIMERA grid, where the inv-Brem deposition is used as a source term for the electron energy in the subsequent Rad-Hydro step, t_{n+1} . The interpolation, initialization and propagation steps will be

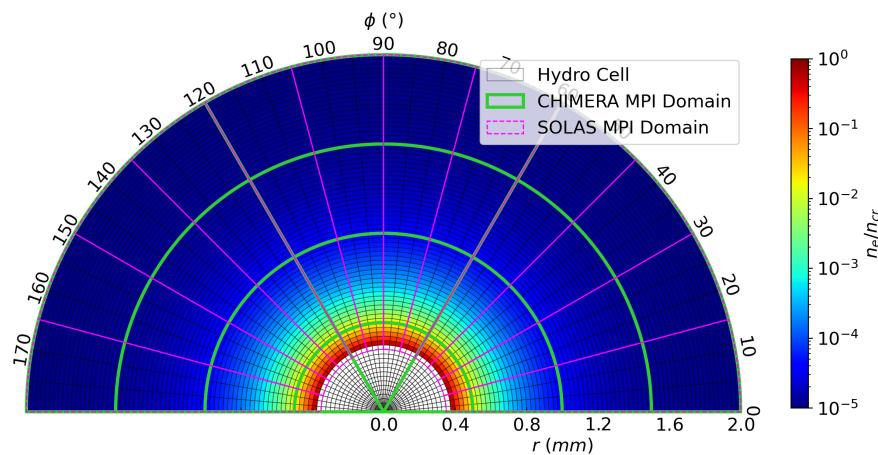


Figure 1.3: An illustrative diagram demonstrating the MPI re-domain balanced grid employed by SOLAS compared to the CHIMERA domain balanced grid for a cylindrical geometry.

outlined in sections 1.3.2, 1.3.3, 1.3.4 respectively.

1.3.2 SOLAS Mesh Structure

For direct-drive ICF simulations which model the laser using ray-tracing, especially those which include CBET, the choice of an appropriate computational mesh on which to conduct the laser ray-trace is crucial to obtaining an accurate and noise-free energy deposition. A well-chosen grid can also significantly reduce the run-time and memory requirements of the calculation. The mesh used for hydrodynamic simulations of these experiments is often not well suited for ray-tracing calculations. For example, hydrodynamic grid resolutions often have excessive resolution in the corona to resolve the gradients in the laser quantities, which greatly increases the expense of tracing rays through the mesh, without significantly enhancing the accuracy of the solution. This section will describe the approach taken in the SOLAS code to create a grid structure which is well suited to direct-drive simulations which we have found to accurately resolve laser energy deposition both with and without CBET in a memory-efficient manner.

1.3.2.1 Re-Domain Balance for Radial Geometries

Rad-MHD codes often employ a domain balanced approach to parallelization⁴, where each computational rank solves a portion of the entire spatial domain each discrete timestep. Additional ‘ghost-cells’ are stored in the subdomains and used to calculate gradients on the boundaries between ranks, which are updated with inter-rank communications each timestep. The hydrodynamic grid for CHIMERA is Eulerian, with options for Cartesian, cylindrical or spherical-polar grids.

⁴This includes the CHIMERA code for which SOLAS has been developed.

The optimal domain balancing minimises communication between ranks, which leads to cubic⁵ subdomains. If computing a laser raytrace through this domain however for a typical direct-drive calculation however, initially rays travel approximately radially and therefore regularly encounter processor boundaries where they must be transferred between ranks. A more optimal domain decomposition for the raytrace minimises radial splitting to avoid excessive passing of rays. When required for spherical and cylindrical simulations, SOLAS therefore takes the hydrodynamic variables on the CHIMERA grid and re-domain balances the grid for the raytrace, such that the splitting does not occur in the radial coordinate. An example of this re-domain balancing is shown in Fig. 1.3 for an illustrative cylindrical mesh. The CHIMERA domain decomposition divides the radial and azimuthal extent into 4 and 3 respectively, whereas SOLAS' division is purely in the azimuthal direction. For spherical and cylindrical direct-drive simulations where there is a defined, global minimum critical radius, SOLAS' mesh excludes the grid cells below this minimum radius beyond which the rays cannot reach in order to reduce the memory burden of the re-gridding.

An alternative approach to domain-decomposition parallelization of the module would be to use the Open Multi-Processing (OpenMP) package, where processors share memory across a computational node. In this approach, the entire laser grid would be stored once on the shared memory of the node and separate ranks would trace rays through the entire domain without the need for transfers. While this is certainly a preferable approach for a standard raytrace to the MPI procedure described above, including a model for CBET is more challenging with this approach. This is because CBET requires communication between beams and therefore large amounts of information must be stored on the grid, which can lead to large memory overheads. Therefore, using multiple computing nodes is often a necessity for 3D CBET calculations and OpenMP-MPI hybrid approaches are required which was deemed too significant an undertaking for the scope of the work presented in this thesis.

1.3.2.2 Semi-Structured Eulerian Grid with Combined Cells

Ideal ICF experiments are spherically symmetric and departures from this symmetry are usually next-order corrections to a spherical implosion. Simulations of these experiments therefore typically employ a computational grid with spherical symmetry. CHIMERA typically simulates direct-drive implosions with a spherical-polar Eulerian mesh, shown in Fig. 1.4.a. This grid has the advantage of simplicity to take gradients across cells and develop new physics modules for the code, however it has the disadvantage that cell edge lengths go to zero as the radial coordinate, $r \rightarrow 0$ and the polar coordinate, $\theta \rightarrow 0, \pi$. This limits the hydrodynamic timestep as stable explicit timesteps are inversely proportional to edge lengths, increasing the cost of 3D spherical simulations. The issue is circumvented at late times in the implosion by remapping onto a Cartesian grid, which does not have vanishing edge length and face areas [35].

Computing CBET however required at least a single ray from each interacting beam to pass through each computational grid cell where the interaction should be important. For

⁵Cubic in cell dimension, not necessarily in physical space for non-Cartesian geometries.

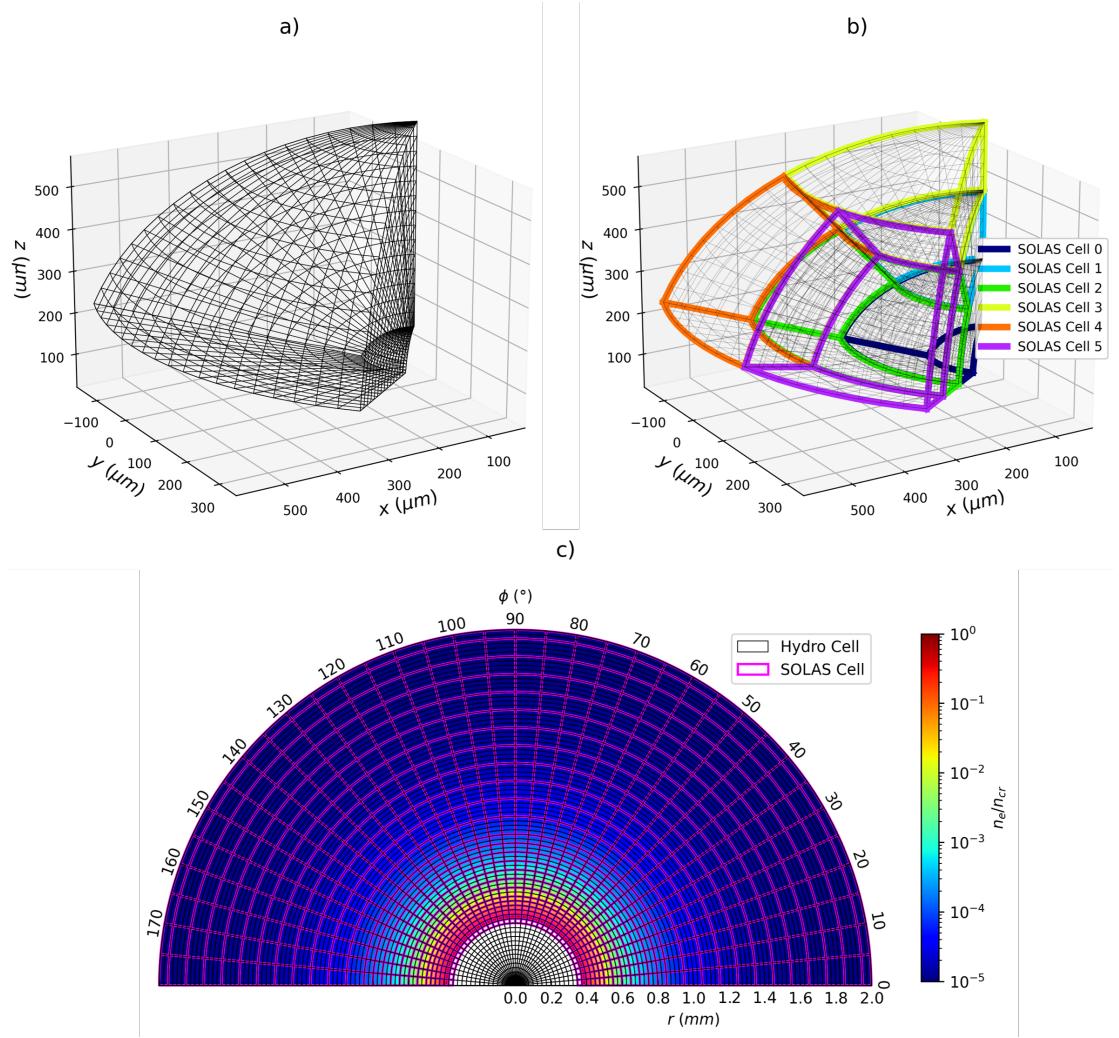


Figure 1.4: Illustrative diagrams demonstrating a) the spherical polar mesh used by CHIMERA for hydrodynamic calculations, b) the cell combination mechanism employed by SOLAS to obtain a roughly equal area grid for spherical simulations and c) the adaptive radial cell combination to reduce resolution in regions where CBET and refraction are unimportant.

spherical-polar meshes the vanishing cell volume therefore sets extreme minimum ray number limits for the calculation to fully resolve all the fields, especially for direct-drive simulations due to the requirement to resolve the reflected fields which spread out over 4π steradians, as is shown in Fig. 1.1. Hydrodynamic resolutions are often also excessive for ray trace calculations to resolve the necessary refraction and energy exchange of the light. Rays must stop at each cell boundary in order to deposit the correct amount of energy into each grid cell and therefore the expense of the ray trace is directly proportional to the number of grid cells that the rays see.

To circumvent this issue cells can be combined around the spherical grid angles in order to make a semi-structured Eulerian grid, as is shown in Fig. 1.4.b. Hydrodynamic grid cells are merged together on the SOLAS mesh in each grid direction until a pre-specified resolution, set by the problem is reached. In Fig. 1.4.b, many cells are combined in each direction to

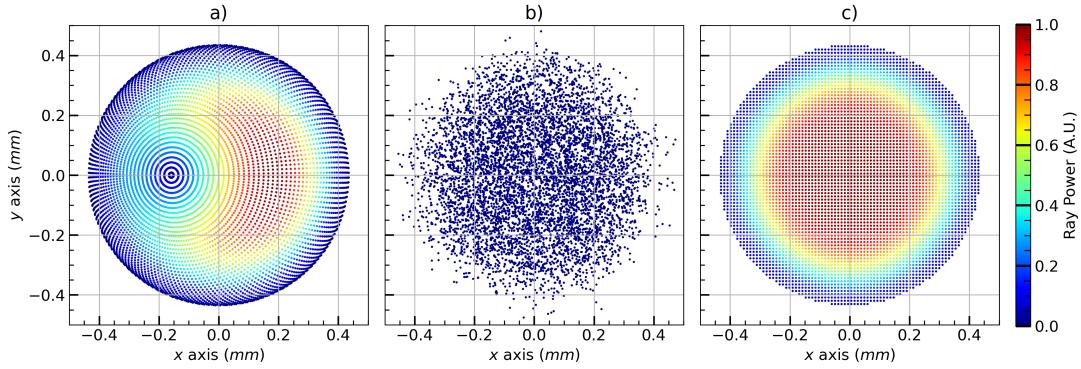


Figure 1.5: Example initial locations for ~ 4000 rays for an OMEGA beam port with super-Gaussian intensity profile, with a shape defined by $n_s = 5.2$ and $\sigma = 352 \mu\text{m}$. The inverse-projection ray locations are shown in sub-figure a) which demonstrate a higher ray density for rays pointed to the pole at $x \sim -0.15\text{mm}$. b) shows the randomly sampled rays where all rays are initialised with the same power, and c) shows uniformly sampled rays.

clearly display the effect. Typically, for spherical simulations however, the cells are not combined in the polar direction, θ and n_φ cells are combined in the azimuthal direction until the azimuthal and polar resolutions match, explicitly $n_\varphi r \Delta\varphi \sin\theta \approx r \Delta\theta$ at a given radius, r .

Fig. 1.4.c demonstrates the capability of the meshing algorithm to adaptively combine cells in the radial direction based upon density gradients. This allows large cells to exist in the coronal plasma where the light refracts minimally and deposits little energy, while the sharp turning point regions close to the critical surface can be well resolved. To find the number of radial cells to combine at a given radius, the cell combination algorithm varies on the number of cells to combine n_r and calculates the maximum gradient length scale from all combined hydrodynamic cells, $L_{n_e} = n_{crit}/|\nabla n_e|_{max}$. The algorithm then finds the optimal number of cells to merge together such that the new cell resolution $n_r \Delta r \approx C_L L_{n_e}$, where C_L is a user parameter⁶ which can be reduced to limit cell combining. A maximum cell size is also set to prevent excessively large cells in regions with minimal density gradients.

Note that many options for equal area computational grids exist which, unlike the semi-structured grid described here, are completely uncorrelated from the hydrodynamic mesh [36, 37]. These have the advantage that the grid can be completely chosen based solely upon the laser ray trace. However, the mesh described in this section has the advantage that interpolation to the hydrodynamic mesh is extremely straightforward as the SOLAS grid cells completely overlap the CHIMERA cells. This also removes minimises artefacts from interpolation between the grids, which have the potential to introduce spurious high order modes to the deposition source term.

1.3.3 Ray Initialisation

To obtain a noise-free energy deposition source term from a ray trace, both the grid and choice of initial rays number and location is crucial. The problems are closely related as a

⁶Default value set to $C_L = 0.05$.

higher resolution grid will require a larger density of rays to get an equivalent ray-per-cell statistics. It is therefore wise to choose the number of rays used in a simulation to be some function of the grid used for the ray-trace. Several methods for ray initialization which have been implemented shall be briefly outlined here, along with a summary of their strengths and weaknesses.

All beams profiles described in this thesis have circularly symmetric super-Gaussian intensity profiles described by the equation,

$$I(r) = I_0 \exp\left(-\left|\frac{r}{\sigma}\right|^{n_s}\right), \quad (1.1)$$

where r is the distance from the centre of the beam port, perpendicular to the beam normal, I_0 is the peak intensity, σ is the beam width⁷ and n_s is the super-Gaussian exponent.

Uniform Sampling In this method of ray initialisation, demonstrated in Fig. 1.5.c, each beam is assigned a number of rays and a maximum ray initialisation width⁸, beyond which rays are not initialised. Rays are then placed in a uniform, square grid on this plane with a power proportional to the intensity value from Eq. 1.1 and removed if their intensity is below $I_0 e^{-3}$, which gives the ray convex hull in 1.5.c the circular shape. For all three procedures described in this subsection, the total summed power of the rays is normalised to the incident beam power after the initialisation of all rays is complete. Typically, for direct-drive, the total number of rays used for spherical simulations is chosen to be,

$$N_{\text{ray}} = C_N \max(N_r N_\varphi, N_r N_\theta, N_\theta N_\varphi), \quad (1.2)$$

where $N_{i=r,\varphi,\theta}$ is the number of SOLAS grid cells in that grid direction and C_N is a user-parameter multiplier which to give better ray statistics for CBET simulations when required. $C_N \sim 2$ is found to give converged deposition when including CBET and so this value is used by default.

When there is sufficiently low ray-per-cell statistics, beat phenomena can occur between the ray spacing and the grid resolution. In this event, especially when using a nearest neighbour interpolation for ray power deposition onto the grid, significant spurious modes can be introduced to the power deposition. To resolve this, ray locations can be ‘dithered’ so that they take a random position within the polygon⁹, defined by neighbouring ray locations. This option is always used for simulations using uniform sampling in this thesis.

Random Sampling Rays can also be randomly sampled according to the intensity profile. Example ray locations from this method are shown in Fig. 1.5.b. Note that the intensity profile purely emerges from the ray locations in this method as all rays have equal power. For no CBET simulations this is a useful method as it minimises coherent build-up of noise from ray-spacing, grid-resolution beating. However, the wings of the intensity profile have

⁷The radius at which $I = I_0 e^{-1}$.

⁸The maximum initialisation width is usually set to be the radius at which $I = I_0 e^{-3}$.

⁹This polygon is a square for uniform sampling, but not for inverse-projection

very poor ray statistics so for direct-drive CBET calculations, resolving the reflected field and therefore the dominant backscatter CBET is excessively expensive.

Inverse-Projection Inverse-projection, is a final method that has been implemented for ray initialisation in SOLAS. The algorithm is described in detail in Appendix A of Ref. [23], but is not used for simulations in this thesis and therefore shall only be cursorily outlined. Briefly, the method works by finding several surfaces, defined by fractions of the critical density and then creating aim points in each cell on the surface. These aim points and their associated area on the surface are back-projected onto each beam port and rays are created if the aim point is not obscured by the surface on which it was created. The power of the ray is then the back-projected area multiplied by the intensity at the beam port location. For a spherical polar grid, this gives a ray distribution which varies in ray density according to which region on the beam port maps to regions on the grid with higher or lower cell-face areas. The rays in the higher ray density at the beam port region which maps to the polar region of the grid, at $x \sim -0.16\text{ mm}$ on Fig. 1.5.a have a correspondingly lower power compared to rays at equal radii to give the same intensity.

While inverse-projection does guarantee good ray statistics at given surfaces for the in-bound component of the field, the algorithm does not extend to beyond ray caustics, or the reflected field component. Therefore, ray statistics are not guaranteed to be good for the reflected field, so the advantages of this method are not evident for direct-drive CBET simulations when backscatter must be resolved. However, for no CBET, direct-drive simulations, this is a useful option for ray initialisation.

For all simulations in this thesis, the uniform sampling method with ray dithering is used. This method is found to give the best ray-per cell statistics across the semi-structured Eulerian grid described in Sec. 1.3.2 while minimising the overall number of rays used required to resolve CBET.

After rays are initialised on each of the beam ports, rays are extrapolated to the edge of the computational domain. Beam focussing is typically neglected, so all rays are assigned velocities parallel to the beam normal. This approximation is widely used for codes that simulate OMEGA-scale direct-drive implosions, where the lasers are approximately collimated on the implosion scale [15, 23]. It is assumed that outside of the simulation domain is vacuum and rays are therefore extrapolated to the edge of the computational domain in straight lines, using a simple root finding to find the intersection of the rays with either a spherical, cylindrical or rectangular domain depending on the simulation geometry.

1.3.4 Equations of Rays and Adaptive Integration

In SOLAS, each ray is defined by a position (\mathbf{x}), wavevector (\mathbf{k}), phase (φ), angular frequency (ω) and power (P). The partial differential equations that are integrated along the trajectory

of each ray for these quantities are,

$$\begin{aligned}\frac{d\mathbf{x}}{d\tau} &= \mathbf{k}, \\ \frac{d\mathbf{k}}{d\tau} &= \frac{1}{2} \nabla \varepsilon(\mathbf{x}), \\ \frac{d\varphi}{d\tau} &= \varepsilon(\mathbf{x}), \\ \frac{d\omega}{d\tau} &= \frac{\omega}{2c} \frac{\partial(n_e/n_{cr})}{\partial t}, \\ \frac{dP}{d\tau} &= -\kappa_{IB},\end{aligned}\tag{1.3}$$

where $\varepsilon = 1 - n_e/n_{cr}$ is the dielectric permittivity of the plasma, n_e & n_{cr} are the electron & critical densities, c is the speed of light, t is time, κ_{IB} is the inv-Brem absorption kernel, given explicitly in Eq. ?? and τ is the ray path length. Note that the phase here is defined such that it has the same dimension as path length and therefore has spatial units. The wavevector is normalised such that $|\mathbf{k}| = \sqrt{\varepsilon}$. The optical path length is related to the arc length, ds by the variable change $ds = d\tau \sqrt{\varepsilon}$. In some formulations of the ray-tracing equations, the differential equations are written in terms of the arc length [23, 38], which is equivalent, but more complicated and without benefit. The frequency shift of the light is only significant for the work presented in this thesis when calculating CBET and is discussed in more detail in Sec. 1.5.3, where the equation used to evaluate the right-hand side is given explicitly. Note that the time, t is not related to the ray path length τ , because an operator split approach is taken to the ray trace, such that the hydrodynamic variables are frozen and the ray trace finds the time independent trajectory of the light through these profiles. The path length τ is therefore best seen as a parameterisation of the ray curve.

Adaptive RK45 Solver The default ray evolution algorithm in SOLAS is to solve Eq. 1.3 using an adaptive RK45 algorithm with stepsize control [39]. Ray steps are either limited by the error from this algorithm, or by distance to the next impact with a cell face. Evaluations of the right-hand side of these equations employ trilinear interpolation for n_e , ∇n_e and T_e to obtain varying values for these quantities at different locations throughout the cell. All other quantities are either defined at the ray location, or use nearest neighbour interpolation. The `bspline-fortran` library has also been implemented to allow tricubic interpolation of n_e , which yields a quadratically varying ∇n_e across the grid [40]. This is slow to evaluate many times per ray step as is required in an RK45 algorithm and therefore limits performance, but is used throughout this chapter as a higher order solution to validate accuracy of the default interpolation.

Linear interpolation of n_e and T_e is required for accurate computation of κ_{IB} , especially for ‘cold-start’ simulations where light impacts upon a solid target and the plasma profiles have steep gradients. Interpolation of ∇n_e was found to be necessary to obtain low-noise ray amplitudes from neighbouring rays for CBET evaluation, which is described in more detail in 1.4. Linear interpolation of both n_e and ∇n_e is technically inconsistent, because ∇n_e should be the gradient of n_e , however the test cases presented in Sec. 1.3.4.1 found that this

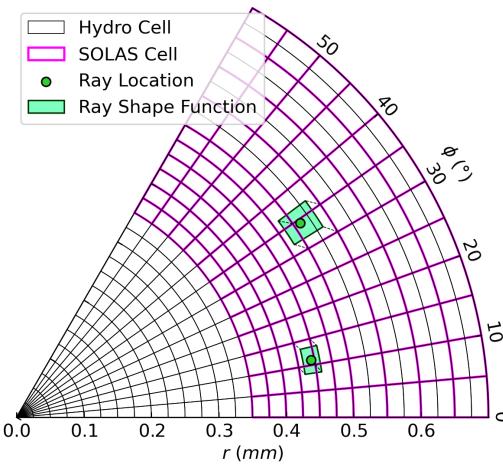


Figure 1.6: Demonstration of the shape function smearing weighting for ray power interpolation to the SOLAS mesh for a cylindrical mesh. The shape function has the same size and geometry as the SOLAS grid cell which the ray is located in. A top-hat shape function is used, so the fraction of the deposited power interpolated to a given cell is proportional to the volume overlap of the shape function with the cell.

did not reduce accuracy compared to the Kaiser algorithm, which employs a self-consistent linear interpolation of n_e and constant ∇n_e within a computational cell.

Kaiser Algorithm The Kaiser algorithm for ray integration has also been implemented [38]. In this algorithm, each cell has a single ∇n_e and an n_e value defined at the cell centre, allowing for linear interpolation of n_e throughout the cell. In a constant ∇n_e region, the trajectory of rays can be analytically shown to follow a parabola. The Kaiser algorithm thus evolves rays over parabolic segments between cells by finding the intersection of the parabola with cell faces, using a root finding algorithm. Assuming constant ∇n_e cells leads to discontinuities in n_e at cell interfaces when the true gradient is not linear and thus Snell's Law is used to refract rays upon cell exit. While this method is often slightly more efficient compared to the adaptive RK45, it was found that when attempting to reconstruct the ray amplitude from the area of neighbouring rays, as outlined in Sec. 1.4, excessive noise was introduced in the amplitude from the discontinuous refraction. Therefore, the adaptive algorithm was used for all work in this thesis, other than where explicitly outlined.

Shape Functions for Ray Deposition Nearest neighbour interpolation of power deposition, which is defined along the ray trajectory, onto the computational grid can result in significant levels of noise in the power deposition profile when ray statistics are not sufficiently high. This is similar to problems experienced in PiC codes when interpolating macro particles to the grid without the use of shape functions [41, 42]. A PiC-inspired shape function approach was taken therefore, where the power deposition from rays is smeared across neighbouring cells. A top hat shape function is used, with a shape function that has the size and

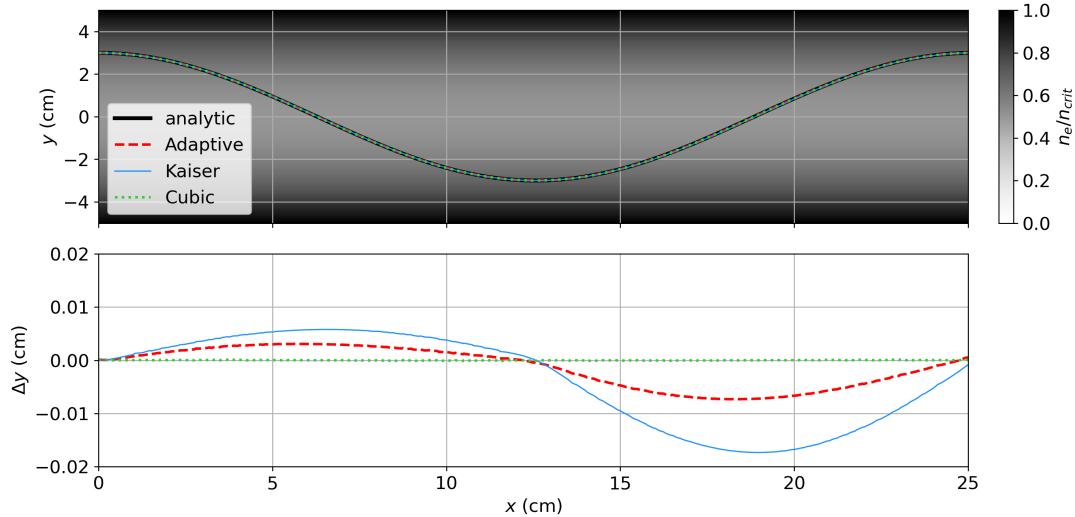


Figure 1.7: This figure demonstrates results of the quadratic trough ray trajectory test problem for the adaptive solver with 3 different cases. These are default settings (linear interpolation of both n_e and ∇n_e), the Kaiser algorithm (linear interpolation of n_e and uniform ∇n_e in a cell) and the adaptive algorithm with tricubic interpolation of n_e). The top plot shows ray trajectories and analytic trajectory and the bottom plot shows absolute errors for the 3 cases.

shape of the cell that the ray is located within, as is shown in Fig. 1.6. The power deposited into each cell that has an overlap with the shape function bounds is therefore proportional to the volume overlap of the shape function with the cell. This approach is more explicitly outlined, particularly for the case of the non- logically rectilinear grids which are present for SOLAS, in Ref. [43]. This smearing is somewhat numerically diffusive and therefore can be optionally disabled. For the work presented in this thesis, the shape function smearing is employed for multidimensional direct-drive simulations, but otherwise disabled.

1.3.4.1 Ray Solver Validation

Several validation problems have been conducted to verify that the ray solver has been implemented correctly. Here we present the quadratic trough and cylindrical helix test problems which compare the path of a single ray in a density profile to an analytic solution to verify that the ray solvers correctly obtain for the trajectory of light. The blast wave problem is also presented which is a test of inv-Brem absorption to an analytic solution in the absence of thermal conduction and hydrodynamic motion.

Quadratic trough The quadratic trough is a test of ray trajectory in a quadratic density trough, which admits an analytic solution of a periodically oscillating ray [38, 44]. The density profile used for the test is defined as,

$$n_e(y) = \frac{n_{e\text{cr}}}{2} \left(1 + \frac{y^2}{y_c^2} \right), \quad (1.4)$$

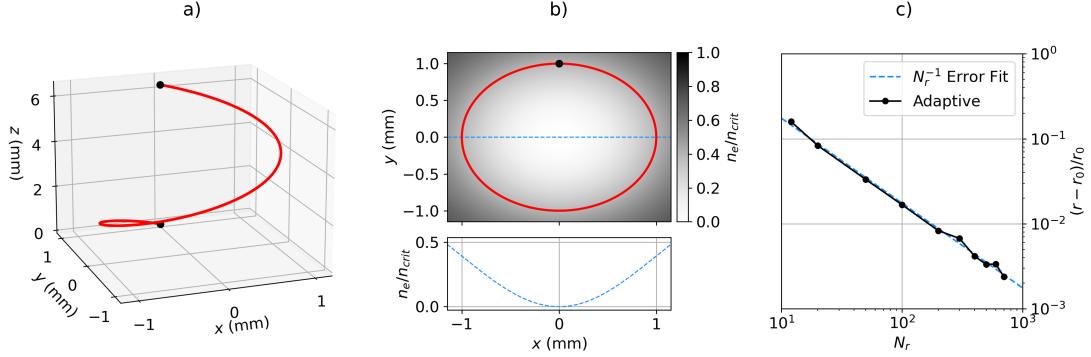


Figure 1.8: This figure illustrates the results from the cylindrical-helix test problem, obtained using the default adaptive RK45 algorithm. a) shows the trajectory of a ray with from a simulation with 100 radial cells in 3-D space. b) shows the trajectory of the ray projected on the $x - y$ plane, along with the n_e profile. c) shows the error of the test, defined as the fractional difference in radius of the ray as it exits the domain from the initial radius, as a function of number of radial cells.

which for light with wavelength $\lambda = 351$ nm, is initialised with $n_{\text{cr}} = 9.049 \times 10^{21} \text{ cm}^{-3}$ and $y_c = 5 \text{ cm}$. The domain has bounds $x \in [0, 25] \text{ cm}$ and $y \in [-5, 5] \text{ cm}$ and a ray enters the domain at $[x_0, y_0] = [0, 3] \text{ cm}$. Analytic integration of the first 2 lines from Eq. 1.3, yields the analytic trajectory as a function of ray path length , τ ,

$$\begin{aligned} x(\tau) &= \tau \sqrt{1 - \frac{n_e(y_0)}{n_{\text{cr}}}}, \\ y(\tau) &= y_0 \cos\left(\frac{\tau}{\sqrt{2}y_c}\right). \end{aligned} \quad (1.5)$$

The analytic trajectory is compared to the solution from the adaptive solver (using both default interpolation and tricubic interpolation of n_e) and the Kaiser algorithm in Fig. 1.7. The associated error, defined as the difference in y at a given x is also plotted. Note that all results were obtained using a grid resolution of 100×100 cells. The top panel demonstrates that all trajectories are identical to the analytic solution by eye. The corresponding errors show that the tricubic interpolation obtains effectively perfectly recreates the analytic solution and the Kaiser error is slightly more significant compared to the default adaptive error. The tricubic error is insignificant because the cubic interpolation perfectly recreates the true density profile, so the errors are purely numeric, not due to the resolution. Errors from the other algorithms would therefore decrease more quickly with increasing resolution as the density profile the ray sees becomes more similar to a quadratic trough. The error from the default adaptive interpolation (linear interpolation of both n_e and ∇n_e) is lower than that of Kaiser (linear n_e and uniform ∇n_e), indicating that the inconsistent interpolation is not a significant issue for resolving ray trajectories.

Cylindrical-Helix The quadratic trough test ensures that the ray evolution algorithm functions correctly in Cartesian geometry. An additional test was desired in non-Cartesian geom-

etry, because CHIMERA also operates with cylindrical and spherical grids. The cylindrical-helix test was therefore devised, where a ray enters an axially symmetric density trough that keeps the ray at a constant, cylindrical radius, r , as is shown in Fig. 1.8.b. As is shown in Fig. 1.8.a, the z extent of the simulation is chosen such that the ray has performed one complete helical spiral when it exits the domain. By requiring that a ray undergo circular motion in the $x - y$ plane and specifying the initial ray direction such that $k_{z0} = \sqrt{k_{x0}^2 + k_{y0}^2}$, it can be derived that a ray entering the domain at r_0 will undergo one complete helical spiral over a z length $\Delta z = 2\pi r_0$, if the density profile has the shape,

$$n_e(r) = n_{cr} \left(1 - \exp \left(\frac{-r^2}{2r_0^2} \right) \right). \quad (1.6)$$

For a ray entering the domain at $[x_0 = 0, y_0 = 1, z_0 = 2\pi]$ mm, with initial wavevector $[k_{x0} = \sqrt{\varepsilon_0/2}, k_{y0} = 0, k_{z0} = -\sqrt{\varepsilon_0/2}]^{10}$, the ray position as a function of path length τ is,

$$\begin{aligned} x(\tau) &= r_0 \sin \left(\sqrt{\frac{\varepsilon_0}{2}} \tau \right), \\ y(\tau) &= r_0 \cos \left(\sqrt{\frac{\varepsilon_0}{2}} \tau \right), \\ z(\tau) &= z_0 - \sqrt{\frac{\varepsilon_0}{2}} \tau. \end{aligned} \quad (1.7)$$

The problem was run in cylindrical geometry for a variety of radial resolutions employing the default adaptive RK45 solver with linear interpolation of both n_e and ∇n_e . The domain bounds for the problem were $r \in [0, 1.5]$ mm, $\varphi \in [0, 2\pi]$ & $z \in [0, 2\pi]$ mm, with a single cell in both the φ & z directions. For all radial resolutions, the ray was observed by eye to exit the domain at the expected location, verifying that the ray trace is functional in non-Cartesian geometries. Plotting the fractional error in ray exit location as a function of number of radial cells, N_r in Fig. 1.8.c, demonstrates that the error in final position of the ray scales as N_r^{-1} . This is because larger N_r more closely recreates the density profile in Eq. 1.6. The error scaling is dictated by the error on the lowest order interpolation used in the algorithm, which is the linear interpolation of n_e for the default adaptive RK45 solver, which yields the N_r^{-1} scaling.

Blast wave The blast wave problem is a validation test of the implementation of inv-Brem absorption [44, 45]. In this problem, a 527 nm, 2 ns laser is incident on a uniform density ($\rho = 1 \text{ mg/cm}^{-3}$), cold gas ($T_{e0} = 1 \text{ eV}$) with fixed ionisation at $Z = 6$, that has an ideal gas equation of state. The $\ln \Lambda$ value used for the κ_{IB} coefficient is fixed at 7. The laser travels in the x direction and has an intensity of $6.4 \times 10^{13} \text{ Wcm}^{-2}$. Hydrodynamic motion and transport is disabled in the simulation. The laser is initially very strongly absorbed in the gas, so energy is not transported beyond the initial layer, perpendicular to the laser propagation direction. As the gas heats up, κ_{IB} decreases and therefore more energy is transported further into the domain by the laser, moving the heatfront forward. The heatfront $x_{\text{analytic}}(t)$, de-

¹⁰ $\varepsilon_0 \equiv \varepsilon(r = r_0)$.

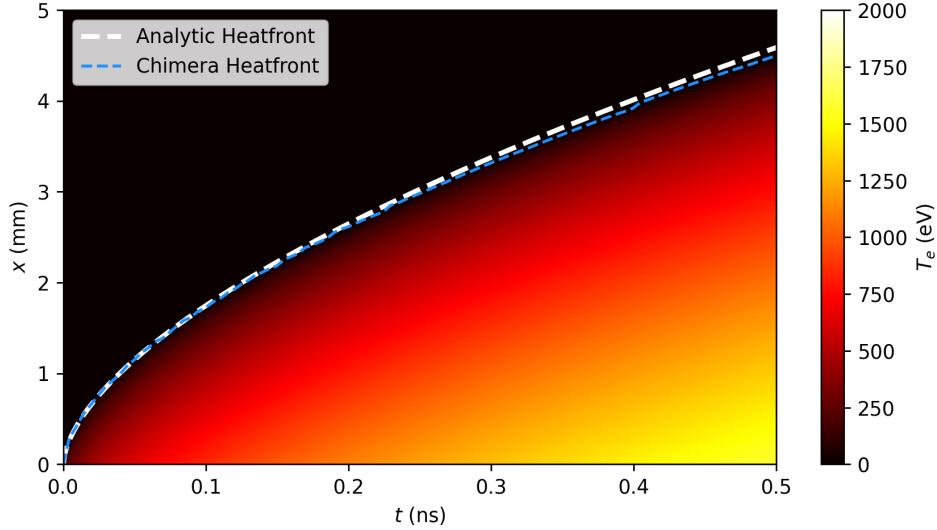


Figure 1.9: This figure shows the results of the blast wave inv-Brem absorption test problem. The colour-plot shows the temperature of the 1-D simulation as a function of time (x -axis) and space (y -axis). The heatfront obtained from CHIMERA, which is the maximum x location where $T_e > T_{e0}$, is in good agreement with the analytic solution.

fined as the largest x coordinate at a time, t where $T_e > T_{e0}$, has an analytic solution under these assumptions, derived by Denavit and Phillion [45],

$$x_{\text{analytic}}(t) = \frac{2}{3\kappa_{\text{IB}}} \left(\frac{5}{3} \frac{\kappa_{\text{IB}} I}{n_e k_B} \right)^{3/5}, \quad (1.8)$$

which can be compared to the result from a ray-tracing simulation.

Fig. 1.9 shows the results for $T_e(x, t)$ and the heatfront location from a CHIMERA-SOLAS simulation of the blast wave problem. The heatfront from the simulation compares well to the analytic heatfront, validating the implementation of the inv-Brem absorption kernel.

1.4 Ray Based Field Reconstruction and Ray Sheets

In order to compute CBET, or other LPIs in a ray-tracing calculation, additional information about the electric field or intensity of the light is required than can be obtained from the ray directly from the routine outlined in Sec. 1.3. In this section the method used in SOLAS to obtain the electric field of the light along the path of each ray shall be outlined. This broadly follows the implementation from Ref. [29].

1.4.1 Ray-Amplitude & Field Estimate from Neighbour Rays

Recalling the formula for the ray-amplitude, A , Eq. ?? from Sec. ??,

$$A(\tau) = A(0) \left| \frac{D(0)}{D(\tau)} \right|^{1/2}, \quad D(\tau) = \begin{bmatrix} \frac{\partial x}{\partial \zeta_1} & \frac{\partial x}{\partial \zeta_2} & \frac{\partial x}{\partial \tau} \\ \frac{\partial y}{\partial \zeta_1} & \frac{\partial y}{\partial \zeta_2} & \frac{\partial y}{\partial \tau} \\ \frac{\partial z}{\partial \zeta_1} & \frac{\partial z}{\partial \zeta_2} & \frac{\partial z}{\partial \tau} \end{bmatrix}, \quad (1.9)$$

where $[x, y, z]$ and $[\zeta_1, \zeta_2, \tau]$ are the ray real-space and phase-space coordinates respectively and D is the Jacobian for the coordinate transform from phase-space to real-space. When refraction forces rays closer together, $|D(\tau)|$ will decrease and equally, when refraction forces rays to separate, $|D(\tau)|$ will increase. The amplitude can therefore be approximated by assuming proportionality between the determinant of the Jacobian and the area, S of an infinitesimally small bundle of rays surrounding the main ray,

$$A(\tau) = \varepsilon^{-1/4} \sqrt{\frac{S(\tau=0)}{S(\tau)}}, \quad (1.10)$$

where the $\varepsilon^{-1/4}$ term accounts for swelling of the field due to the increased optical path through plasma with finite density [29]. Note that the amplitude is a purely geometric quantity, which holds no information about power changes of the light from absorption or LPIs. The electric field outside the caustic region, which shall be discussed in more detail in Sec. 1.4.2, can then be obtained with the formula,

$$\frac{|E(\tau)|}{|E(\tau=0)|} = \sqrt{\frac{P(\tau)}{P(\tau=0)}} A(\tau), \quad (1.11)$$

where P is the power of the ray and the initial (vacuum) electric field $|E(\tau=0)| = \sqrt{2I_0/c\varepsilon_0}$, where I_0 is the intensity of the beam at the ray initialisation point on the beam port.

This method, which has been used successfully to model direct-drive CBET in the BEAM-CROSSER post-process code, is the approach taken to estimate the field in SOLAS. Explicitly, for every ray that initialised for a SOLAS calculation, an additional 3 ‘neighbour-rays’ are initialised in an equilateral triangle around it, perpendicular to the initial direction of propagation at a random angle. Note that when a 2-D ray-trace is used, only 2 neighbour-rays are required as the rays cannot change separation in the out of plane direction. It is important to distinguish the dimension of the ray-trace, which is the number of dimensions in which rays can move in a simulation, to the dimension of the hydrodynamics. For example, a 1-D spherical direct-drive Rad-Hydro simulation still requires a 3-D ray trace where rays can move in $x, y \& z$ for full accuracy.

These neighbour-rays are then co-traced up to the phase of the ‘main-ray’ to evaluate the area of the main ray on its phase front. Practically, the separation distance of the bundle of neighbour-rays (i.e. the side-length of the triangle, Δl) does not need to be infinitesimally small, but small enough that it accurately captures the local change of $|D(\tau)|$. In terms of the hydrodynamic profiles, this means that $\Delta l \ll L_{n_e}$, where L_{n_e} is the density length scale

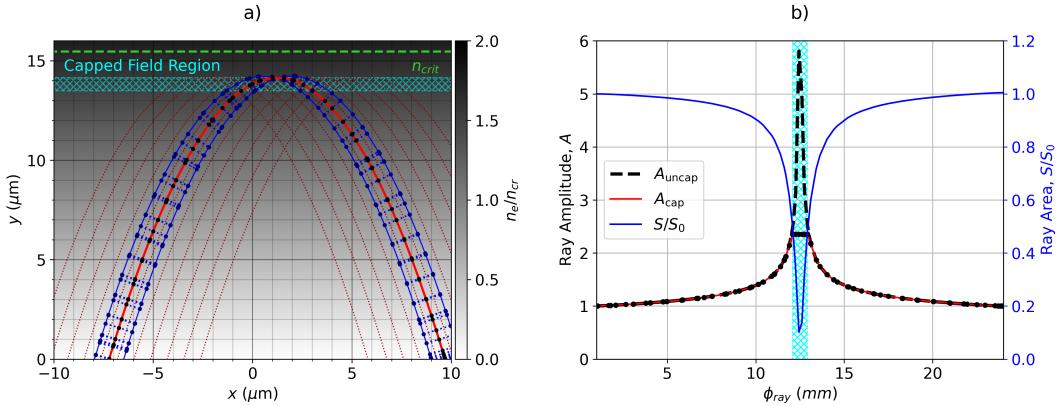


Figure 1.10: This illustrative figure demonstrates how the ray-amplitude is obtained from the area of neighbouring-rays for a beam propagating up a linear density gradient. Fig. a) explicitly shows the trajectory of a main-ray and its neighbour-rays in red and blue respectively, explicitly highlighting the beam's caustic region, where the amplitude of the light is capped. Fig. b) plots the area of the main-ray in blue, which goes through a minimum at the caustic location as a function of the phase of the ray. Also shown are the uncapped and capped amplitudes of the ray.

of the plasma. For OMEGA scale direct-drive simulations, an initial separation of $\Delta l \lesssim 1 \mu\text{m}$ is found to give converged behaviour. If the separation is too small however, floating point arithmetic can lead to noise in the ray-amplitude estimation. For all simulations presented in this thesis, $\Delta l = \lambda_0 / 10 \ll 1 \mu\text{m}$ was used.

As was mentioned in Sec. 1.3.4, it was found that the Kaiser algorithm for ray propagation, which uses a single ∇n_e in each grid cell and discontinuously refracts rays at cell boundaries, led to large levels of noise in the ray-amplitude profiles. In order to obtain smooth profiles for A , linear interpolation of ∇n_e was found to be necessary. The continuously varying ∇n_e , which does not have discontinuities across cell interfaces, allows a smoothly varying area for each ray to be obtained.

Fig. 1.10.a demonstrates this amplitude reconstruction process in a purely illustrative example of a beam travelling up a linear density gradient at an angle, leading to a caustic at its turning point. The trajectory of several main-rays are plotted in dark-dashed red, and a single main-ray is highlighted in a brighter shade of red. The 2 neighbour-rays of this highlighted main-ray are plotted in blue. Note that in this figure, the default initial main-neighbour-ray separation of $\Delta l = \lambda_0 / 10 = 0.035 \mu\text{m}$ was used, but the separation has been magnified on the plot to visualise the amplitude reconstruction from the area more clearly. The locations of the main- and neighbour-rays after a single step of each main-ray are plotted as black and dark-blue spots respectively. The 'area' of the neighbour-rays S , which in this 2-D raytrace example here is simply a distance, is plotted on 1.10.a as a dashed blue line between the neighbour-rays. The neighbour-rays are pushed until they have the same phase as the main-ray, φ_{ray} , at which point the area is evaluated.

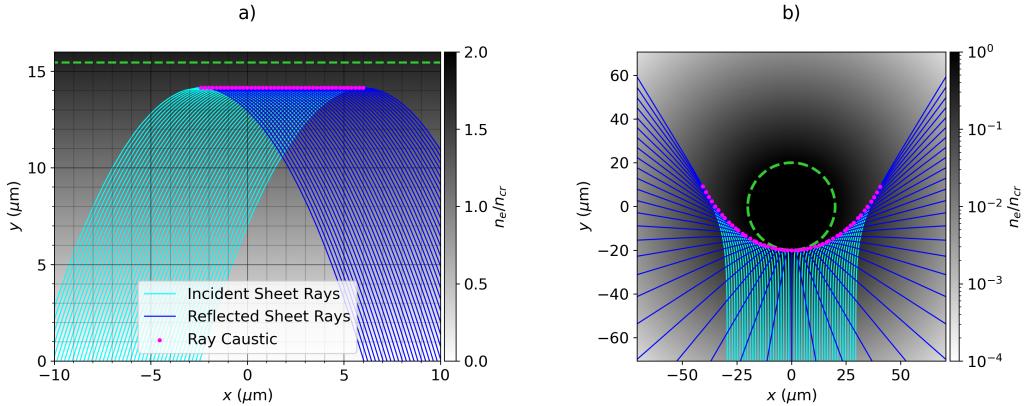


Figure 1.11: This illustrative figure illustrates the concept of caustics and ray sheets. In a), the trajectory of ray traversing up a linear density gradient are plotted. Separate colours are used for the incident and reflected sheets, which are separated by a caustic. In b), rays propagate up a density profile, $n_e = n_{cr} \exp[-(r_{\mu\text{m}} - 20)/100]$. Unlike in a), the ray caustics do not occur at their turning point, *i.e.* the minimum radius.

1.4.1.1 Caustics and Ray-Sheets

Caustics are an important concept in GO, and the reconstructed field in their vicinity must be handled correctly in order to accurately model CBET in ray based codes. Fig. 1.10.b plots the area of the main-ray as a function of main-ray phase in blue. At $\varphi_{ray} \sim 12 \mu\text{m}$, $S \rightarrow 0$, *i.e.* neighbouring-rays cross over each other, which is known as the ray-caustic. In the absence of caustics, rays never cross over each other and therefore the mapping from ray phase-space (beam-port locations, where $\tau = 0$) to real-space is single valued, or in other words each point in space will be reached by (at most) one ray from each beam. In the presence of caustics, this single valued mapping breaks down and a single real-space location is accessible by multiple ray launch locations. A single valued mapping is still possible if each beam is separated into distinct ‘sheets’ after caustics, where each sheet still has a single-valued projection from phase-space to real-space.

This is illustrated in Fig. 1.11.a, where rays from a single beam are plotted propagating up a linear density gradient with $n_e = n_{cr}y_{\mu\text{m}}/15.5$. As the density gradient is purely in the y direction, each ray has translational symmetry in x and therefore each ray-caustic is located at the ray turning point, $y \sim 14 \mu\text{m}$. The portions of the ray trajectories that fall before and after the caustic are separated into the ‘incident’ and ‘reflected’ sheets respectively and plotted in separate shades of blue. Fig. 1.11.b also plots rays from a single beam, but now propagating through a cylindrically symmetric n_e profile. As can be seen from this figure, the caustic is not the same as the ray turning-point¹¹, but the location that the amplitude diverges.

This means that unless the amplitude is tracked along each ray trajectory, the location of the caustic cannot be identified and rays cannot be separated into distinct sheets, both of which have important ramifications for ray-based CBET models. Firstly, because the am-

¹¹Defined here as the location of maximal n_e experienced along the ray trajectory.

plitude diverges, the field values can become very large and therefore must be capped to diffraction limited values, the method for which is discussed in more detail in Sec. 1.4.2. Additionally, if the beam cannot be separated into distinct sheets, then self-CBET, where the reflected component of a beam interacts with the incident component of the same beam, must be neglected. In SOLAS, the neighbour-ray method allows the amplitude to be tracked along each ray, enabling caustic location and sheet-separation. Currently, it is assumed that each sheet has 2 sheet components, *i.e.* an incident and reflected field, but it should be possible to extend this to multiple caustics to accurately model complex CBET interactions such as target-stalk simulations [46–48]. This is an advantage of the forward ray tracing approach to CBET modelling compared to inverse-ray-tracing, where only plasma profiles that result in a single caustic can be modelled [15].

The phase of the light is also evolved along each ray trajectory in equations 1.3, and therefore the coherent sum of all electric fields can be reconstructed which involves interference between sheets. The total electric field is,

$$E = \sum_{j \text{ sheets}} |E_j| \exp(i(k_0 \varphi_j - \pi \alpha_j / 2)), \quad (1.12)$$

where k_0 is the vacuum wavevector of the light and α_j accounts for the $\pi/2$ phase shift that occurs when a ray changes sheet, *i.e.* $\alpha_j = 0$ for the incident sheet and $\alpha_j = 1$ for the reflected sheet [29].

1.4.2 Caustic Field Capping

In the vicinity of beam-caustics, the electric field magnitude of a beam is limited by diffraction which is neglected in GO, so ray based models which do not cap fields near caustics can experience divergent electric fields. For direct-drive simulations, significant amount of CBET occur near caustics and therefore sensibly capping the field value is crucial for accurate simulations [20]. This cannot be achieved without knowledge of the caustic location, which is a severe limitation to the predictive capability of CBET codes that do not track the amplitude. This section shall describe two methods that have been implemented to cap the field values in the vicinity of laser caustics, the Field Limiter (FL) and Etalon Integral (EI) approaches.

Field Limiter This is a straightforward hard cap on the maximum value of the electric field reconstructed during the ray trace. The electric field of light propagating up a linear density gradient has the analytic solution of an Airy function. The field limiter approach is to cap all electric fields to this value,

$$\frac{|E|}{|E(\tau = 0)|} = \sqrt{\frac{P(\tau)}{P(\tau = 0)}} \min \left[A, \sqrt{\zeta} \left(\frac{n_t}{n_{cr}} \right)^{1/4}, \sqrt{\zeta} \sqrt{\frac{S(\tau = 0)}{S(\tau)}} \right], \quad (1.13)$$

$$\zeta = 0.9 (\omega L / c)^{1/3},$$

$$L = n_{cr} / |\nabla n_e|_t,$$

where n_t is the electron density at the caustic, $|\nabla n_e|_t$ is the magnitude of the electron density gradient at the caustic location [28, 49, 50]. The first term in the minimum is the standard field reconstruction from the amplitude away from caustics. The second term is the maximum of the Airy function and the third term is an improvement to the second term for near-normally incident rays [29]. Fig. 1.10.b shows the capped amplitude obtained from the field limiter approach.

Etalon Integral The EI method is an improvement to the FL, which allows for deviations in the density profile away from linearity [19, 51, 52]. Several distinct types of caustic exist for different geometries of problem. For example in direct-drive, the light reflecting from the critical surface forms a ‘fold’-type caustic, whereas focussing light leads to a more complex ‘cusp’-type caustic [53]. If the form of the caustic is assumed, then an approximation of the total field in the vicinity of the caustic is formulated which allows for deviations from the ideal case. In the example of the direct-drive fold caustic, the field is assumed to be the sum of an Airy function and its derivative, which accounts for the deviations from linearity. An expression for the total field can be derived in terms of the ray-amplitude and phase before (A_1, φ_1) and after (A_2, φ_2) the caustic,

$$\begin{aligned} E_T &= \sqrt{\pi} [(-\xi)^{1/4}(A_1 + A_2)\text{Ai}(\xi) - i(-\xi)^{1/4}(A_1 - A_2)\text{Ai}'(\xi)] e^{i(k_0\chi - \pi/4)}, \\ \chi &= \frac{1}{2}(\varphi_1 + \varphi_2), \\ \xi &= -\left[k_0 \frac{3}{4}(\varphi_2 - \varphi_1)\right]^{2/3}, \end{aligned} \quad (1.14)$$

where Ai and Ai' are the Airy function and its derivative. In SOLAS, Ai and Ai' are computed numerically using the `special-functions` library [54]. This total field can then be divided between the incident and reflected sheet by inversion of Eq. 1.12 assuming that $|E_1| = |E_2|$,

$$\frac{|E_j|}{|E_{j,0}|} = \frac{\sqrt{W_j}|E_T|}{\sqrt{2}[1 + \sin(\varphi_2 - \varphi_1)]^{1/2}}. \quad (1.15)$$

The Etalon integral is applied in the ‘caustic-region’, which in Refs. [19, 55, 56], is stated to be equivalent to,

$$|\varphi_1 - \varphi_2| \leq \lambda_0/2, \quad (1.16)$$

where λ_0 is the vacuum wavelength of the light.

Applying the EI method requires evaluation of Eq. 1.16 to determine if a ray is inside its caustic region, which relies on interpolation of the phase of the other sheet from the same beam onto the ray location. If using nearest neighbour interpolation, which is used in SOLAS for interpolation of all field quantities onto rays, this means a resolution of $\Delta \ll \lambda_0$ must be used, which is a much higher resolution than is required for ray-tracing and CBET without the EI. Therefore, the EI method is only used in SOLAS simulations for very high resolution grid test problems, such as those Sec. 1.4.3. The alternative approach would be to implement linear interpolation from the field quantities all beams onto ray locations such as in Ref. [29].

This was not deemed a viable approach however, because the mesh resolution for spherical simulations was found to not be well-enough angularly resolved to interpolate the phase with sufficient accuracy to the rays. The standard procedure for CBET simulations in Solas is to use the FL approach which is found to give satisfactory results compared to the EI method.

1.4.3 Field Reconstruction Validation

In this section several test problems will be presented that compare electric fields obtained using SOLAS field solver in the absence of CBET, to those from the wave based solver LPSE in direct-drive relevant plasma profiles. The LPSE results are presented in Ref. [29], and are available from the repository [57]. In all the following test problems, the laser has a vacuum wavelength, $\lambda_0 = 0.351 \mu\text{m}$ and a Super-Gaussian intensity profile,

$$I(r) = I_0 e^{-(r/\sigma)^{n_s}}, \quad (1.17)$$

where r is the distance from the beam centre, perpendicular to the direction of propagation, σ is the beam width and n_s is the Super-Gaussian exponent. All 1-D and 2-D validation problems assume lasers polarised out of the simulation plane along the z axis. The plasma density profiles are given by,

$$n_e(r) = n_0(d/r)^m, \quad (1.18)$$

where $n_0/n_{text{cr}} = 1.165$, $d = 343 \times S \mu\text{m}$, $m = 3.78$ and S changes the scale of the density profile, where $S = 1$ corresponds to scale lengths from implosions using the full OMEGA laser-energy. These values were obtained from fitting the equation to 1-D Rad-Hydro calculations using the LILAC code.

1.4.3.1 1D Reflected Beam

The first validation problem is for the case of light propagating normally up a density gradient. For this problem, 1-D Cartesian geometry is used, so the density profile is obtained by transforming the spatial coordinate from equation 1.18, $r \rightarrow x - 36.42 \mu\text{m}$, and in this problem, the beam is travelling in the $+\hat{x}$ direction, with $I_0 = 14 \text{ W/cm}^2$. Only a single ray was used because the ray trace is completely 1-D. A scale factor of $S = 1/16$ was used, resulting in a critical surface at $x \sim 14.14 \mu\text{m}$. The simulation has bounds $x \in [-16, 20] \mu\text{m}$ with a resolution of $\Delta x \sim 1 \text{ nm}$. A high resolution is used here in order to resolve the highly oscillatory coherent field sum. Power changes of the rays due to inv-Brem and CBET are also neglected.

The laser in this problem travels up the density gradient, reflecting from the critical surface. For normally incident light up a linear gradient, the critical density is the location of the caustic, because the ray area, $S(\tau)$, is constant and therefore the amplitude diverges when $\varepsilon \rightarrow 0$. The total field is given by the coherent sum between the incident and reflected sheets. Figure 1.12.a shows the LPSE result compared to the field obtained from SOLAS without a cap on the caustic field; using the FL approach; and using the EI approach. The only difference between the SOLAS methods occurs in the caustic region¹², shown more clearly in

¹²i.e. where equation 1.16 is satisfied.

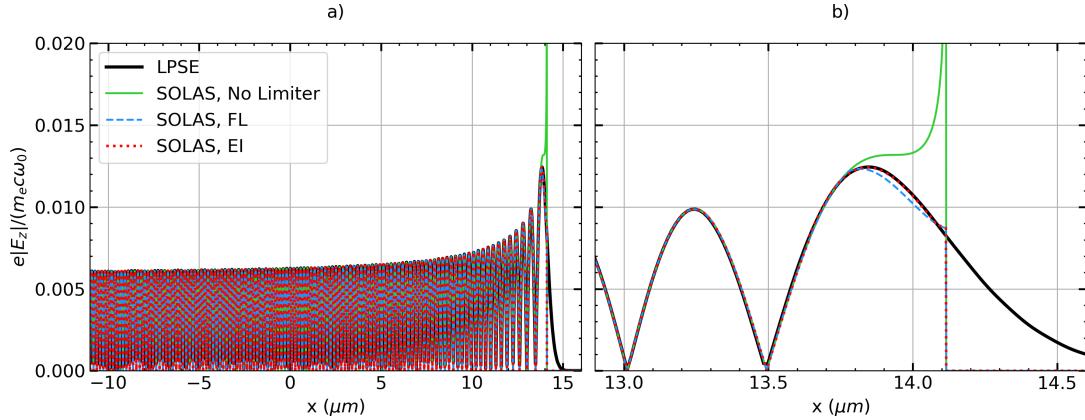


Figure 1.12: This figure shows the results of the 1-D field reconstruction test, comparing SOLAS fields with different caustic field capping methods to the LPSE results. Figure a) shows the oscillatory behaviour of the field solution which arises due to the interference between the incident and reflected sheet. Figure b) plots the same results, but zoomed in on the caustic region to demonstrate the differences in fields obtained from the different methods.

figure 1.12.b, which in this problem is for $x > 13.64 \mu\text{m}$. Failure to cap the caustic field leads to a divergent $|E_z|$ at the critical surface, but both the EI and the FL methods show very good agreement with LPSE. This justifies the default use of the simpler FL method for SOLAS CBET calculations.

Standard GO cannot capture the field beyond the critical surface because rays cannot propagate beyond $\epsilon = 0$. The evanescent field in this region can be reproduced in the complex-GO framework, which integrates rays which have complex-valued properties and can thus be evolved beyond the critical surface [19]. This is not deemed to be necessary for accurate CBET modelling of OMEGA-scale direct-drive implosions, however.

1.4.3.2 2D Reflected Beam

A second field reconstruction test was also implemented in 2-D geometry. Unlike the previous 1-D test, the reconstructed field for this problem also depends on the divergence of neighbouring rays. This is because apart from normally incident rays at the centre of the beam, $\mathbf{k} \nparallel \nabla n_e$, so the area, $S(\tau)$, of the rays vary. Simulations at 1/64 and 1/4 scales are presented here. The $S = 1/64$ simulation had bounds $x, y \in [-20, 20] \mu\text{m}$ and resolution $\Delta \sim 20 \text{ nm}$. The $S = 1/4$ simulation had bounds $x, y \in [-200, 200] \mu\text{m}$ and resolution $\Delta \sim 100 \text{ nm}$. For both scales, a single beam propagated parallel to $+\hat{\mathbf{y}}$ and was centred on $x = 0 \mu\text{m}$. The beam widths were $\sigma = 8 \text{ & } 115 \mu\text{m}$ for the 1/64 and 1/4 scales respectively. The standard uniform sampling procedure described in Sec. 1.3.3 was used with $C_N = 2$. CBET and inv-Brem were again both neglected.

Figure 1.13.a shows the LPSE and SOLAS, FL fields for the $S = 1/64$ setup. Agreement appears to be very good by eye between the LPSE and ray-based field in the sub-critical plasma. The field from the SOLAS FL $S = 1/4$ simulation is plotted in figure 1.13.b, from which it can

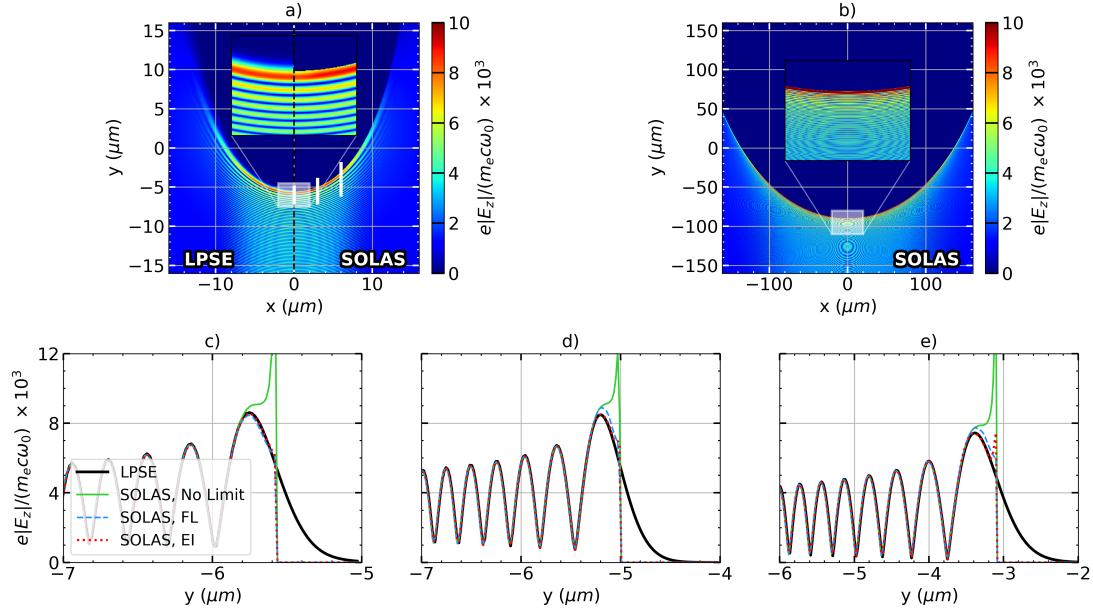


Figure 1.13: This figure shows the results of the 2-D field reconstruction test. Figure a) plots the field from LPSE on the left side and the SOLAS field on the right for the 1/64 OMEGA scale simulation. Figure b) shows the SOLAS field from the 1/4 scale simulation which, when compared to a), demonstrates that as scale increases, the relative size of the caustic region decreases. Figures c), d) & e) are lineouts near the caustic region along y from the 1/64 scale simulations at $x = 0, 3 \& 6 \mu\text{m}$ respectively, the positions of which are indicated by the white lines on a). Note that the circular features in the field in figures a) and b) arise due to aliasing artefacts between the true solution scale, with the resolution of the image and, or simulation grid.

be seen that the caustic region, which has a characteristic width $\sim \lambda_0$, shrinks in relative size as the scale increases. This suggests that at increasing scale, the importance of accurate caustic modelling may decrease in importance. Plotted in figures 1.13.c, 1.13.d & 1.13.e are lineouts from the 1/64 simulations taken at $x = 0, 3 \& 6 \mu\text{m}$ respectively. They all include LPSE and SOLAS results with FL, EI caustic field capping along with no limiting. These plots demonstrate that caustic field limiting is necessary to compare favourably to the LPSE solution and that the FL approach slightly overestimates the caustic field compared to LPSE and the EI method. The discrepancy between the FL and EI results is again deemed sufficiently small to justify the default use of the simpler FL approach. To remind the reader, this choice is because the implementation of the EI method in SOLAS requires grid resolution $\Delta \ll \lambda_0$, the reason for which is described at the end of Sec. 1.4.2.

1.5 Ray Based CBET Model

This section shall describe the implementation of the CBET model in SOLAS. A brief outline of the model works by performing Explain that ray based CBET uses the linear gain discussed in theory section. Say that since this assumes homogeneity, effectively applies to small ray

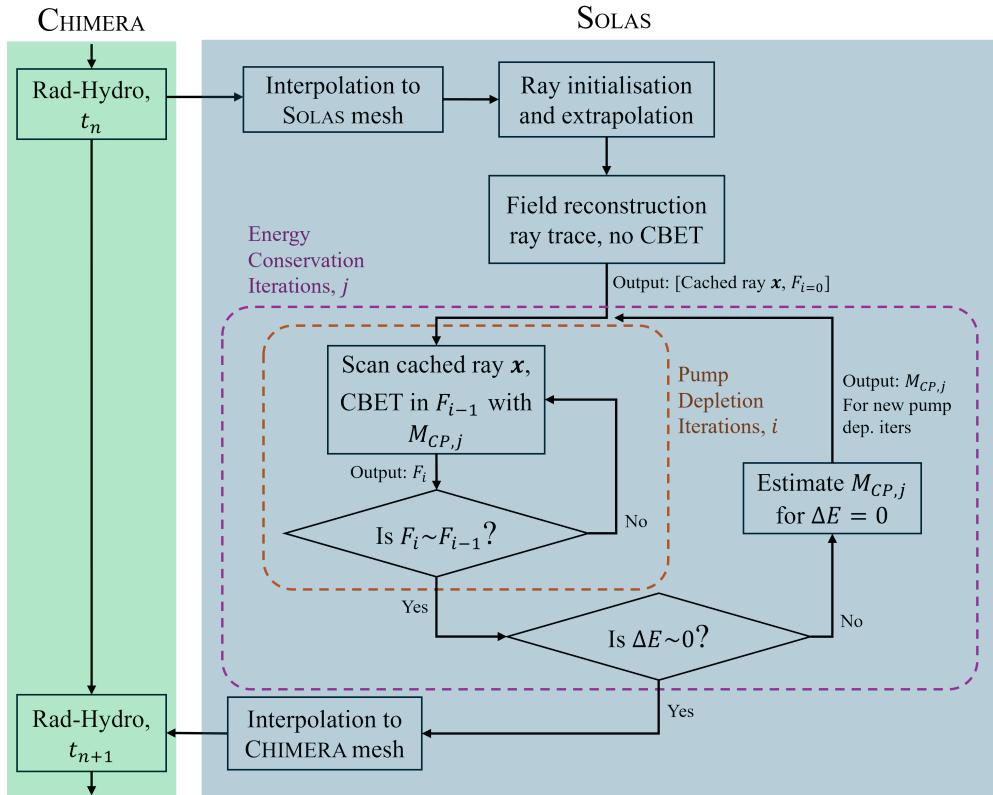


Figure 1.14: A flowchart which illustrates the SOLAS CBET model operation loop.

steps, which is typically well satisfied. Also say that this homogeneity within a computational cell and nearest neighbour interpolation of field means that it is not necessary to adaptively integrate the CBET gain.

1.5.1 Power Change of Rays due to CBET

Describe how ray energy changes due to CBET from linear gain models (either fluid or kinetic). Say how when including with inv brem, the deposited power and CBET change must be got carefully (i.e. Marozas paper).

1.5.1.1 Fluid CBET Gain

Breifly discuss the fluid CBET gain and explain why it is easier to use for code validation.

1.5.1.2 Kinetic CBET Gain

Breifly discuss the kinetic CBET gain and why it is better for predictive simulations.

1.5.2 Dynamic memory structure for storing Fields and CBET Gains

Give the scaling of storing fields and gains for every beam. Say that therefore a dynamic memory structure is used which only stores the fields and gain in cells where they are present. Also state that although the ray trace module must be done in double to numerical errors (for

example, freq differences in resonance and difference between rays), gain is stored as a single which greatly reduces cost. Give an estimate for how much this reduces the overall memory requirements.

1.5.3 Doppler Shift of Frequency

Mention time dependant refractive index results in a frequency shift of light. This is small, however it is significant to include in CBET models as it can shift the resonance.

1.5.4 Caustic Gain Truncation

Say that because nearest neighbour interpolation of the fields is used, there exists unphysical interaction regions where a cell has a field but ray hasn't passed through that portion of the cell. This problem becomes particularly bad at ray turning points, where a significant amount of CBET occurs. Therefore a method called 'CGT' is used to effectively enhance the laser grid resolution in the vicinity of caustics. In cells where a ray from a specific sheet experience a caustic, the field entry for that sheet is divided geometrically, assuming that the caustic is locally a plane. If a ray from another sheet passes through the cell and is on the 'unlit' side of the caustic plane, it will not experience CBET gain. Ray steps are also limited to the caustic plane. Other codes have shown that this approach significantly improves energy conservation.

1.5.5 Coherent Caustic Correction and Caustic Region Identification

Say how the field reconstruction assumption works everywhere apart from at caustics, where it underestimates the field. Follow what Russ says in his paper about CC correction and how it significantly improves energy conservation.

1.5.5.1 Geometric Approach to identifying the caustic region

Other codes find caustic region by phase diff and phase interpolation. We can't interpolate due to resolution issues. Therefore implemented a new, geometric approach to finding the caustic region. Talk about how location of rays is stored for each sheet, partitioned by whether they are over or under the amplitude cap. If a cell has rays from both in a cell, then a plane is found between the two to split the cell into caustic and non-caustic. If a cell has only capped rays then the whole thing is caustic. When a ray from another beam passes through, CC mult is applied if in the caustic region.

1.5.6 Energy Conservation in Ray Based CBET Models

Talk about how energy is conserved away from caustics when converged.

1.5.7 Pump Depletion Iterations

Talk about why it is necessary to iterate the ray trace. Mention that it is possible to store ray locations and avoid performing ray trace all over again, but that approach is not taken due to memory limitations. Talk about convergence parameter. Mention necessity of damping for complicated, many beam simulations.

1.5.8 Model Assumptions, Applicability and Validity to ICF

Discuss the key assumptions of the CBET model and whether it is valid to use for LDD and LID.

1.5.9 Computational Efficiency and Scaling

Talk about how the CBET model is quite expensive. Give the scaling laws from Russ' paper and explain how that means for many beams, CBET is bound to be the dominant cost in the simulation. Also say how it shows that memory is a big consideration for CBET models as the gains and fields must be stored.

1.5.10 CBET Validation

Using Russ' paper with lovely test comparisons to LPSE. Define the electron density profile here.

1.5.10.1 2D CBET Without Caustics

Just a simple test of field capping compared to an analytic problem, without refraction.

1.5.10.2 2D CBET With Caustics

Same as above, but now for non-normally incident rays, accounting for refraction. Show test results in both Cartesian and Cylindrical.

1.6 Coupling to Hydrodynamics and Example Use

Here present an entire explanation for the model working coupled to Hydrodynamics.

1.6.1 Power Deposition

Say that the deposited power is just added as an energy source to the electrons. If running in 1D or 2D, it is integrated over other directions first. Say that when starting from $t = 0$, often use a cold-start routine, which uniformly deposits power at the critical surface of a spherical capsule. This creates an under-dense small region in which the rays can refract and deposit energy. This is unsatisfactory for imprint simulations, where early time imprinting is important, but that is not considered for this thesis.

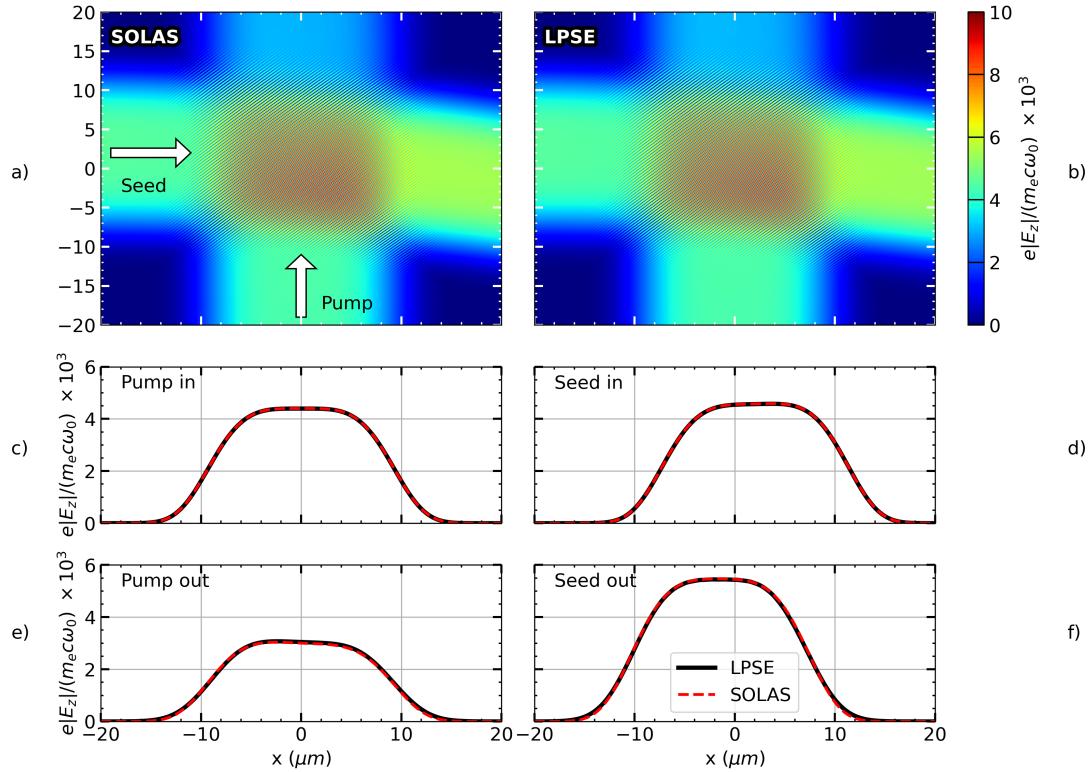


Figure 1.15: This figure shows the results of the 2-D CBET test in the absence of laser caustics.

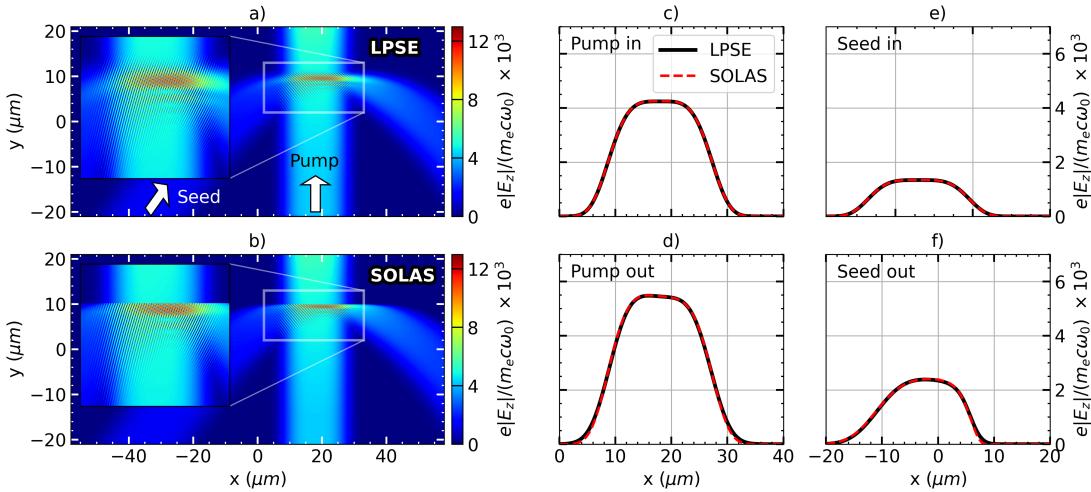


Figure 1.16: This figure shows the results of the 2-D CBET test in the presence of a laser caustic.

1.6.2 Time step limiter

Limit timestep based on the fractional electron energy change. Don't limit timestep in cells far from critical. This is usually the limiting timestep for 'cold start' simulations initially, until deposition begins to occur in hot cells.

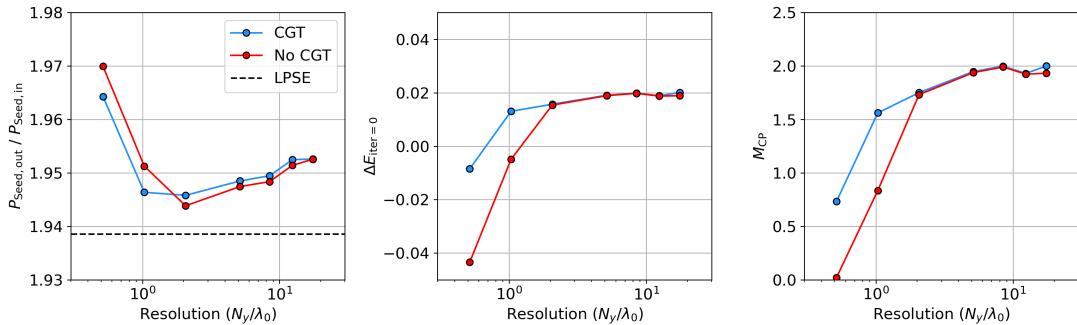


Figure 1.17: This figure shows results from a resolution scan of the 2 beam caustic CBET test both with Caustic Gain Truncation (CGT) and without. Plotted in a), b) & c) are the power amplification of the seed beam, initial energy conservation error before energy conservation iterations & caustic pump multiplier used to obtain energy conservation respectively.

1.6.3 Ray Trace Frequency

For many beam simulations, such as direct-drive simulations, the laser operator (especially with CBET) is typically one of the more expensive parts of the code. In the steady state of an implosion, the coronal plasma conditions don't significantly change on the global hydrodynamic timestep. Therefore the deposition also doesn't change much meaning that previously calculated Pdep can be stored and reapplied on subsequent timesteps. Especially for CBET simulations, this can reduce runtime by order of magnitude. Currently the ray trace is performed every timestep up until a pre-specified ‘warm up’ time has expired. Then the ray trace is performed at a pre-specified frequency by the user. Experimentation has found that for OMEGA scale simulations, increasing frequency of calculations doesn't significantly change the answer above

Because LDD pulses often start with a low intensity and then ramp up, CBET gains are also often minimal until late in the implosion. Therefore field reconstruction and CBET iterations are only performed after a specified start time, normally when the hard-sphere intensity reaches about $1 \times 10^{14} \text{ W cm}^{-2}$. CBET iterations are then performed on the laser frequency.

An improved approach shall soon be implemented where laser iterations occur at $d t_{\text{laser}}$ from Sec. 1.6.2.

1.6.4 Computational Diagnostics

Say that a variety of diagnostics can be output. Qpower with and without CBET. Geometric intensity. Electric field (from single or all beams), optionally split into inbound and reflected components, both with and without CBET.

1.6.5 Example use on OMEGA Shot 89224

First briefly describe the shot, showing pulse shape and target.

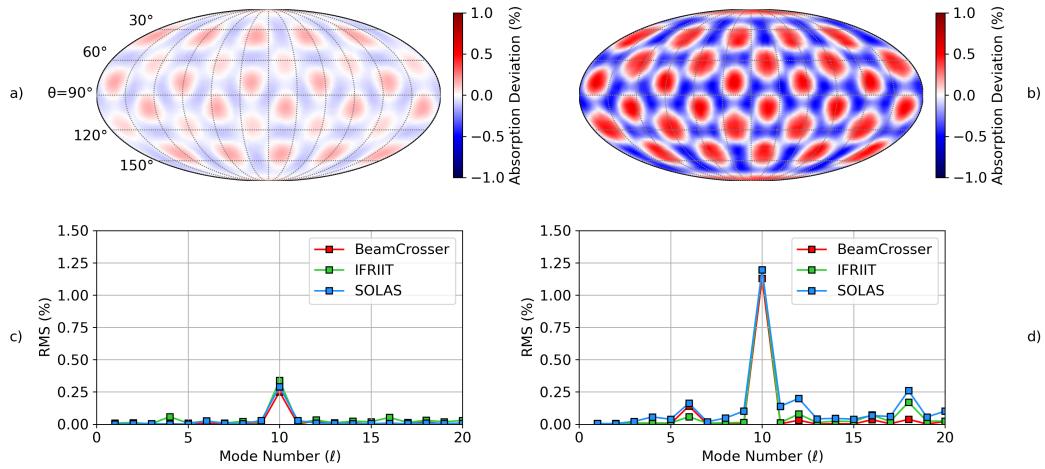


Figure 1.18: This figure shows the results from a 3-D SOLAS post-process of spherically symmetric hydrodynamic data obtained from a LILAC simulation of an OMEGA direct-drive implosion. Figures a) and b) show the deviation in radially integrated deposited power without and with CBET respectively. Figures c) and d) plot the spherical harmonic modal decomposition for these maps alongside results from the IFRIIT and BEAMCROSSER codes without and with CBET respectively.

1.6.5.1 1-D Rad-Hydro, 3-D Ray-Trace with CBET Simulation

Describe the simulation parameters used, e.g. cell resolution, flux limiter etc. Show the absorbed power vs time and effect of CBET. Show instantaneuos radial profiles. Show integrated parameter comparison to LILAC post-shot simulation. Describe the previous method of tuning, involving a 2D scan of flux limiter and power multipliers. Say how it's great that the $f_{lim_e} = 0.06 \rightarrow 0.15$ and CBET combination now gives a predictive capability for OMEGA shots.

1.6.5.2 3-D Post Process of Absorption Non-Uniformity

Mention how the model can also be used as a postprocess. CHIMERA can restart from 1-D data into spherically symmetric 3-D profiles. Ray Trace and CBET can then be performed through these profiles to understand the absorption non-uniformity present due to CBET. Note that comparison of 1-D and 3-D simulations shows that thermal conduction does a good job of smoothing angular deviations in coronal plasma conditions. The assumption of spherically symmetric profiles for the laser is therefore deemed valid, and it is a technique typically used by post-process CBET codes.

MAYBE?? Mention how ray noise means that we can't use direct deposition. Therefore use Pdep from field estimate, which is much cleaner.

Talk about how CBET enhances angular non-uniformity. Show modal decomposition.

1.7 Future Model Extensions

Say that there is even more laser/ CBET physics that is interesting and can be implemented within the ray-tracing framework. Some are straightforward to implement, while others more difficult and computationally expensive.

1.7.1 Langdon Effect on Absorption

Describe Langdon from a kinetic perspective and why it reduces absorption. Describe how you can fit it and include as a modification to ray-tracing absorption if you have the field/intensity. Describe the magnitude of the effect for ICF like conditions. Describe briefly how it would be implemented, say it would not be difficult.

1.7.2 Langdon Effect on CBET

Describe what this is. Say that it is important for high overlapping intensities, eg hohlraum LEH. Say that it is thought to stabilise the CBET interaction in indirect drive configurations and remove the need for artificial clamps. Describe briefly how it would be implemented, say it would not be difficult.

1.7.3 Polarised CBET

Describe how ion acoustic waves are driven by beat between electric fields from light and therefore is polarisation dependent. Say how on OMEGA, RPP smoothing means that each beam is split into 2 sub-beams with linear polarisation. Say that these do not have a symmetry to the configuration about the sphere. Say that this leads to mode-1 on OMEGA. Say that you can track polarisation of rays and trace these sub-beams independently. Would make it more expensive, but definitely feasible.

1.7.4 Bandwidth for CBET Mitigation Studies

Describe how bandwidth should reduce LPI growth rates. Understanding the desired bandwidth to mitigate CBET is a key consideration for design of future laser systems. Fields can be modified to include discrete wavelengths to model bandwidth.

1.7.5 Additional LPIs

Could look at TPD, SBS and SRS. In theory not a difficult problem to do backscatter, but side-SRS is difficult, because additional rays would need to be launched. This could make the model more useful to indirect-drive experiments and design of ignition scale direct-drive facilities, where SRS is thought to be important energetically due to long scale lengths.

1.8 Conclusions

Say that the chapter has described the validity and implementation of SOLAS and validated it. Culminated in demonstrating that the model can reproduce post-shot simulations of an OMEGA shot from the LILAC code which includes a CBET model. This demonstrates that the CHIMERA code now has a predictive capability for OMEGA scale direct drive experiments, as no free parameter tuning was required.

Appendices

A Numerics Appendices

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