Computationally efficient optimization of radiation drives

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For many applications of pulsed radiation, the time-history of the radiation intensity must be optimized to induce a desired time-history of conditions. This optimization is normally performed using multi-physics simulations of the system. The pulse shape is parametrized, and multiple simulations are performed in which the parameters are adjusted until the desired response is induced. These simulations are often computationally intensive, and the optimization by iteration of parameters in forward simulations is then expensive and slow. In many cases, the desired response can be expressed such that an instantaneous difference between the actual and desired response can be calculated. In principle, a computer program used to perform the forward simulation could be modified to adjust the instantaneous radiation drive automatically until the desired instantaneous response is achieved. Unfortunately, such modifications may be impracticable in a complicated multi-physics program. However, the computational time increment in such simulations is generally much shorter than the time scale of changes in the desired response. It is much more practicable to adjust the radiation source so that the response tends toward the desired value at later times. This relaxed in-situ optimization method can give an adequate design for a pulse shape in a single forward simulation, giving a typical gain in computational efficiency of tens to thousands. This approach was demonstrated for the design of laser pulse shapes to induce ramp loading to high pressure in target assemblies incorporating ablators of significantly different mechanical impedance than the sample, requiring complicated pulse shaping.

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I. INTRODUCTION

For many applications of pulsed radiation, the time-history of the radiation intensity must be optimized to induce a desired time-history of conditions. For example, temporal shaping of a laser pulse has been used to induce ablation of a solid target, producing a variety of mechanical loading histories in a solid sample, in particular shock [1] and ramp compression [2]. The optimization of the radiation intensity to produce the desired effect is normally performed using multi-physics simulations of the system. Each simulation solves an initial-value problem: the evolution equations are integrated forward in time, using an estimate of the intensity history of the radiation applied to the system [3]. Repeated simulations are performed, adjusting the pulse shape to be used in each until the desired response is induced. These simulations are often computationally intensive, and the optimization by iteration of parameters in forward simulations is then expensive and slow. The workload to a human designer may be reduced, and the accuracy of the design improved, by wrapping the forward simulation in an automated optimizer employing a numerical search strategy [4], but the computational effort is often greater.

In this paper, we discuss an alternative approach that can be applied when the state at some location within the experimental assembly responds rapidly to changes in the radiation intensity, by modifying the intensity automatically during the simulation.

II. MODIFICATIONS TO RADIATION

HYDROCODE FOR PULSE SHAPE DESIGN

In a range of useful applications, including the design of radiation intensities for the generation of mechanical or thermal loading, the state in the sample responds promptly to changes in the intensity. This is the case for the pressure at the critical surface in laser ablation. For a close coupling between applied intensity and resulting response, the multi-physics forward simulation could in principle be modified to adjust the radiation intensity at each instant of time until the desired response is produced. This modification is relatively invasive, requiring significant changes to the structure of the computer program used to perform the simulation. In contrast, an iterative wrapper can be constructed for a forward simulation without any modifications to the simulation program. However, there is an enormous potential advantage in that the intensity history of the radiation pulse could be calculated in a single simulation.

In other applications, the state in the sample does not respond so promptly to changes in the radiation intensity, but it may be related more simply to states induced in a region which does respond promptly. For instance, if an ablator [4] [5] is used to apply a load to a sample in contact with the ablator, the pressure history in the sample can often be related to the pressure history at the critical surface of the ablator using continuum dynamics without radiation transport [7]. In the absence of radiation transport, hydrocode simulations require much less computational effort, and may be accomplished by different means such as the backward propagation of char-
characteristics [5], allowing a desired loading history in the sample to be transformed to a desired pressure history at the ablation surface. Our procedure can then be used to determine the radiation intensity from this modified state history.

Ideally, a single time increment of the radiation hydrocode would be repeated, adjusting the intensity of the radiation source until the desired response is achieved. In practice, this is a relatively complicated modification to a general-purpose, multi-physics computer program. A simpler approach is to perform a sequence of time increments as usual, adjusting the radiation source such that the response becomes closer to the desired response. Usually, the time increments in the simulation are much shorter than the time scale of the desired response, so some degree of lag in the induced response is acceptable. It is difficult to devise a general algorithm to adjust the source intensity so that the response approaches the instantaneous desired value rapidly and monotonically. In practice, reasonable results can be obtained with forward-time schemes which are not completely stable – the induced response, and thus the radiation intensity, may oscillate about the desired history. Conversely, the radiation intensity may respond too slowly, so the approach to the desired response is over-damped. However, a reasonable radiation intensity history may be found by inspection of the calculated intensity history and response history. Improved results can then be obtained by repeating the simulation a small number of times, using the calculated radiation intensity history from the previous simulation, or a smoothed version.

III. EXAMPLES FOR LOADING HISTORIES INDUCED BY LASER ABLATION

The main application motivating this study was to make the design of laser pulse shapes for dynamic loading experiments more efficient. Laser systems are notable in that the power history can be controlled relatively easily to produce highly-structured shapes, and the pressure response of the ablation plasma is relatively rapid. In contrast, the temperature history of radiation within a hohlraum and the current history in an electrical pulsed power discharge can typically not be controlled with the same degree of flexibility.

Radiation hydrodynamics simulations were performed using the LASNEX[9] and HYDRA[10] computer programs. The current incarnation of LASNEX was written using the interpreted language BASIS[11] in the user interface. Pulse-shaping algorithms were written through the BASIS input without requiring any modification to the LASNEX source code. Similarly, HYDRA includes an interface to a Python interpreter, which was used to implement the pulse-shaping algorithms through input files, without changing the HYDRA source code.

The desired response to be controlled by the laser pulse shape was the ablation pressure $p_a$, to reproduce some desired history $p_d(t)$. As material is ablated, the location of the pressure-generating region changes with respect to both the frame of reference of the undisturbed material and also the original location of the material (i.e. in Eulerian and Lagrangian frames). An automated way is needed to locate the ablation region at any instant of time. There are many possible ways to do this, with applicability to different classes of problem. Laser energy is deposited primarily around the critical surface. We found reasonably general metrics to be the region over which the mass density $\rho$ of ablated material drops by a few tens of percent from its initial value. For high-pressure loading, material about to be ablated may have been compressed to significantly higher density, so this metric does not precisely identify the ablation front, but in many cases it locates the critical surface to an adequate accuracy. A higher reference density, representative of the desired loading pressure, can give better results. The instantaneous ablation pressure was estimated as the average pressure over the ablation region identified in this way.

For applications where the desired pressure history increases monotonically in time, an alternative metric is the maximum pressure in the problem. If the simulation includes other materials, where the impedance mismatch induces a higher pressure, this metric is not appropriate. Also, if the power-adjusting algorithm induces a higher pressure than the desired value, it may take significantly longer for the propagating pressure wave to decay than for the ablation pressure to change, so the power-adjusting algorithm may over-compensate for instantaneous discrepancies in ablation pressure.

Ideally, the power would be adjusted at each instant of time until the desired ablation pressure is obtained. This could involve repeatedly integrating the radiation hydrodynamics equations over the same time increment, which would be complicated in multi-physics codes such as LASNEX and HYDRA. The approach tried here was to adjust the laser power in the right direction to correct $p_a$ toward $p_d$. Adjustments were made with respect to a reference laser pulse shape $I_r(t)$, using a scaling factor $\sigma(t)$. An advantage of this approach is that multiple passes of the pulse-shaping algorithm can be used, by taking the results of a previous simulation as the reference pulse. A wide range of strategies could be used to determine the instantaneous value of $\sigma$ given $p_a$, $p_d$, and $I_r$. The loading induced in matter by ablation is often approximated roughly by an irradiance-pressure relation such as

$$p_a = \alpha I^\beta,$$

(1)

where $\beta \sim 0.6-0.8$[11]. Thus, given the current irradiance $I(t) = \sigma(t)I_r(t)$, a modified irradiance is predicted

$$\tilde{I} = I \left( \frac{p_d}{p_a} \right)^{1/\beta},$$

(2)

allowing a modified scaling $\tilde{\sigma}$ to be calculated. In typical simulations, an unstable oscillatory irradiance was
produced if $\sigma$ was used directly for the next time step. Instead, under-relaxation was used to vary the irradiance over time scales over which laser pulse shapes can typically be controlled,

$$\sigma(t + \delta t) = \sigma(t) + \gamma (\tilde{\sigma}(t) - \sigma(t)) \quad (3)$$

where $\gamma$ is a relaxation parameter $\sim 10^{-3}$.

Variants of this scheme were tried, such as limiting the absolute or fractional rate of change of intensity. This mimics the constraints of real lasers (and other sources of pulsed energy), which typically have a finite response time with which pulse shapes can be defined, limited usually by the bandwidth of the electronic and optical modulator components used to control the gain of the amplifiers. In many cases of interest, including pulse-shaping to produce a constant shock pressure, an increasing ramp, or a shock followed by a second shock or a ramp, experiments and simulations show that the irradiance increases monotonically. It was found that oscillatory behavior was reduced by constraining the irradiance to be monotonic, at the expense of tending to exceed the target pressure slightly. The pulse shape could then be improved by performing a further iteration of the algorithm.

Most of the simulations below were performed in one spatial dimension, appropriate when the diameter of the laser spot is large enough that lateral release in the ablation plume does not affect the center of the spot. This constraint is typically more severe than for loading in the condensed target to remain one dimensional, because the speed of sound in the ablating plasma is typically higher than in the condensed target. However, the approach described can be applied equally well to simulations in more than one space dimension, as long as the critical surface can be identified automatically. The advantage in efficiency is then correspondingly greater, although the slower rate at which time increments occur mean that it takes longer to ensure that a given numerical optimization strategy is behaving acceptably.

The optimized pulse shape did not depend on the initial guess chosen, indicating that the solution was unique. The choice of initial guess did affect the quality of the pulse shape resulting from the first iteration, and the number of iterations needed to give a pulse shape of given maximum deviation from the desired pressure history.

### A. Constant ablation pressure

A very common requirement in dynamic loading experiments is to induce a constant ablation pressure, with as fast a rise as possible. Usually, a constant ablation pressure requires a rising irradiance, as the critical surface accelerates away from the surface and the mass density there decreases. If the duration is long enough with respect to the diameter of the drive spot, lateral flow in the ablation plume must also be compensated by increasing the irradiance. Here we consider the case of a large drive spot, so 1D simulations are adequate. The irradiance history was calculated to induce 100 GPa in Al for 10 ns, following a rise from zero over 200 ps, as is common for high energy laser systems. The Al was 500 $\mu$m thick, so release from the rear surface did not affect the ablation region, which would complicate the pulse-shaping.

The simulations were performed with the LASNEX program, version 1604081910. Al was modeled using LEOS 130 [12] and OPAL opacities [13]. Thomas-Fermi ionization was used. The electron flux was limited to 0.05 of the free stream value, a common choice for such simulations [14]. As is necessary for simulations of laser ablation, the spatial zoning varied exponentially from the free surface of the ablating target, so that the optical skin depth was properly resolved [1].

The optimization parameters chosen were $\beta = 0.8$, $\gamma = 2.5 \times 10^{-3}$. Optimization was made less sensitive while the laser pulse was coming up to power, to allow the ablation plume to establish itself without trying to follow any detailed pressure history. The ablation region was identified as that where $0.5 < \rho/\rho_0 < 0.99$, with $\rho_0 = 2.7$ g/cm$^3$ for Al. The initial guess for the irradiance was a constant 1 TW/cm$^2$.

With the parameters chosen, a single pass of the pulse-shaping algorithm gave a pressure history that reproduced the desired history to around 10%, and to better than 10% toward the end of the pulse. By performing a small number of iterations, the pressure could be brought to within a few percent of the desired history over almost all of the pulse. (Figs 1 and 2)

### B. Ramp loading

Another common requirement is to induce a monotonically-increasing pressure such that a shock does not form as the ramp propagates through some finite

![FIG. 1: Pressure histories for design of constant-pressure shock in Al.](image)
thickness of the target [2, 15]. Approaching the limits of irradiance and pulse length for a given laser, shocks can form for relatively modest imperfections in the pulse shape [18], so it may be crucial to follow the ideal pulse shape [15] as accurately as possible.

Here we simulate the pulse shape needed to give the ideal ramp shape to 1000 GPa over 15 ns in a diamond ablator, followed by a constant ablation pressure for 5 ns. The diamond was modeled using an early version of a multiphase EOS constructed using electronic structure calculations [16], an empirical strength model including electronic structure calculations of shear modulus [17], and OPAL opacities. A single pass of the algorithm gave a pulse shape which reproduced the desired pressure to 200 GPa during the ramp, but induced oscillations during the pressure hold. Again, a small number of passes of the algorithm reproduced the desired pressure history to arbitrary accuracy. The algorithm was very stable during the ramp, but changes in the optimizer parameters were needed for stability during the pressure hold. (Figs 3 and 4.)

On further investigation, including the other pulse shapes described below, oscillations tended to be triggered by the transition from one type of loading to another, here from ramp to constant. Different choices for the numerical optimization parameters were found to make the irradiance and pressure more stable, but we did not find a universal prescription. At any instant of time, the plasma plume reflects the loading history induced up to that point. We hypothesize that the plume must in effect be reconfigured for the change in loading history, and this cannot be achieved instantaneously; attempting to do so induces oscillations. Thus, in order to induce a ramp followed by a constant pressure, near the peak of the ramp, the pulse shape should anticipate the peak pressure by reducing the loading rate gradually, rather than having it fall instantaneously to zero. In practice, it was not necessary to guess a suitable target pressure history in detail to achieve this effect. Either the optimization parameters could be adjusted around the time of the change to be less sensitive to pressure discrepancies and thus avoid ‘hunting’ for the correct solution, introducing oscillations which could grow, or an improved pulse shape could be estimated by eye from the average baseline around any oscillations, and used as a closer estimate for the next iteration.

C. Shock followed by ramp

Another useful loading path is to induce a steady shock, followed some time later by a ramp to a higher pressure, which is then sustained for some finite time.
FIG. 5: Pressure histories for design of shock-ramp-hold in kapton.

This loading history has been used to study solidification from the liquid, where the shock is strong enough to melt the sample, and the ramp is strong enough to pass back through the melt curve and into the solid [19, 20]. Shock-ramp loading can also be used when a laser system does not allow long enough pulses to induce a ramp from zero pressure: if weak enough, the entropy of the shock may be a small perturbation from the isentrope in return for a significantly shorter overall pulse [21].

Here we simulate the pulse shape needed to give a shock to 200 GPa, supported for 10 ns, followed by a ramp to 500 GPa over 10 ns, sustained for 5 ns, in a kapton ablator. The kapton was modeled using LEOS 5040 and OPAL opacities. The first pass of the algorithm gave a pulse shape which reproduced the desired pressure of the first shock, but induced strong oscillations during the ramp drive. Three further iterations with different optimization parameters were needed to define the pulse shape for the ramp and sustained peak pressure. A few additional calculations were performed to select the parameters. (Figs. 5 and 6.)

We observed that, if the ramp was sufficiently steep, the simulations predicted that a second critical surface could form downstream of the original one, and initially decoupled from the first. The ramp in the sample was then delayed significantly until the critical surfaces merged, significantly perturbing the desired pressure history. The irradiance, adjusted automatically to try to induce the desired pressure history, could then become incompatible with the conditions in the plasma plume, inducing oscillations much as were observed at the constant pressure peak following a ramp. There seems therefore to be a maximum rate at which the nature of the pulse shape should be changed, depending on the instantaneous plasma conditions: a constraint to consider when designing pulse shapes.

FIG. 6: Irradiance histories for design of shock-ramp-hold in kapton.

IV. CONCLUSIONS

An alternative approach to iterative forward optimization was investigated for the design of radiation pulses to produce a desired response in a target, by modifying the simulation program to adjust the irradiance automatically during a simulation such that the response approached the desired history. This approach was investigated in the design of laser pulses to induce a variety of loading histories for experiments on the response of condensed matter to dynamic loading. Existing multiphysics simulation programs were used, and the irradiance was adjusted such that the load induced at the critical surface tended toward the instantaneously-desired value, rather than inducing the desired value at all times, which would have required significant modification to these complicated programs.

Several optimization strategies were investigated, i.e. algorithms for adjusting the irradiance given the instantaneous discrepancy between calculated and desired ablation pressure. In some cases, an acceptable pulse shape was found in a single such simulation. More commonly, the induced pressure history exhibited significant discrepancies and oscillations, and a small number of irradiance-adjusting simulations were needed, each using the output of the previous simulation as an initial guess, with smoothing through oscillations if of large amplitude.

It was found possible to induce oscillatory modes in the plasma that seemed to be more than simply naive optimization strategies that overshot the desired conditions, though the choice of optimization parameters could certainly make the oscillations stronger and unstable. We hypothesize an effective ‘memory’ in the ablation plume, making it necessary to change gradually between loading conditions of different nature. In the case of ramp loading following a previously induced constant (elevated) pres-
sure, the initial ramp loading rate must be slow enough to avoid the development of a second critical surface down-stream of the original one.

Overall, the use of this approach seemed to significantly reduce the human and computational effort required to design pulse shapes for laser loading experiments.

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