LA-UR-18-29211

Machine Learning to Estimate Dante Response for Hohlraum Design

Ryan G. McClarren[1,2], PhD, Grace Cummings[2], & I. L. Tregillis[3], PhD
[1]CCS-2; [2]University of Notre Dame; XCP-6

NECDC 2018

Hohlraum Simulation Model

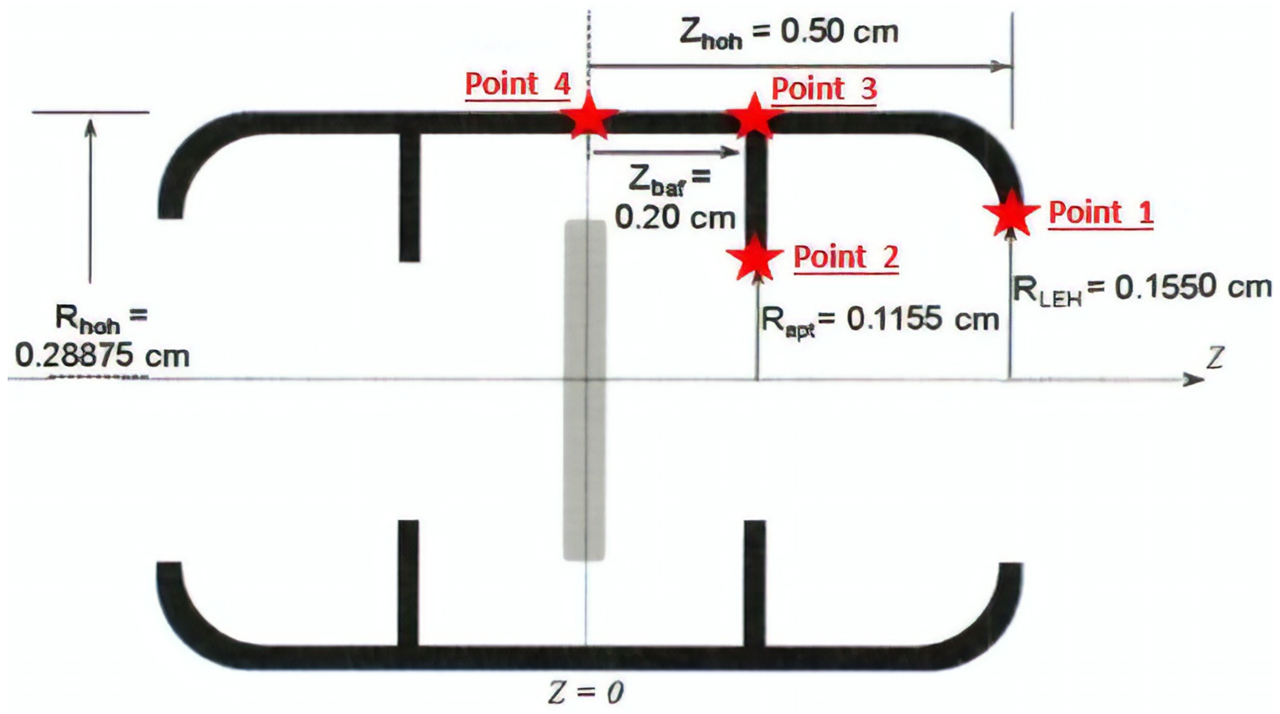

Figure 1: The nominal hohlraum design used in this study [1]. In the terminology of this report this hohlraum has scale = sc length = Rapt = 1. The (r, z) values of the 4 indicated points are used as inputs to the machine learning model.

This work considers the design of hohlraums to obtain a desired temperature profiles. Our objective is to train machine learning models using simulations to predict the simulated Dante response. The machine learning method will then be used to optimize the design.

The hohlraum design and parameter variation simulations were undertaken by I.L. Tregillis as described in LA-UR 17-22657. For completeness, we repeat some of the discussion in that report.

We consider a nominal hohlraum design as shown in Figure 1. In the parlance of opacity experiments, the region in the center of the hohlraum is called the sample chamber and it is bounded by two radial baffles a distance of Z_{baf} from the center of hohlraum. The radial distance from the edge of a baffle to the centerline of the hohlraum is the radius of the aperture.

In our study we considered variations to this nominal hohlraum defined by four different parameters:

- A `scale` parameter where every dimension (R_{hoh}, R_{apt}, R_{LEH}, Z_{hoh}, and Z_{baf}) is scaled by a factor. When scaling the hohlraum in this way, the wall thickness is not changed. As an example, if $\texttt{scale} = 0.5$, then every dimension would be halved.
- The `sc_length` perturbation scales Z_{baf} by a factor *while keeping the ratio* $R_{\mathrm{apt}}/Z_{\mathrm{baf}}$ a constant.
- An R_{apt} perturbation where the dimension of the aperture to the sample chamber is scaled *independently* of Z_{baf}.
- `pulse_length` is the length of the laser pulse drive, scaled to deliver the same amount of energy, 250 kJ.

The parameter variations can be mapped to eight input variables: the (r, z) values of four points that determine the hohlraum shape as shown in Fig. 1.

Simulated DANTE Response

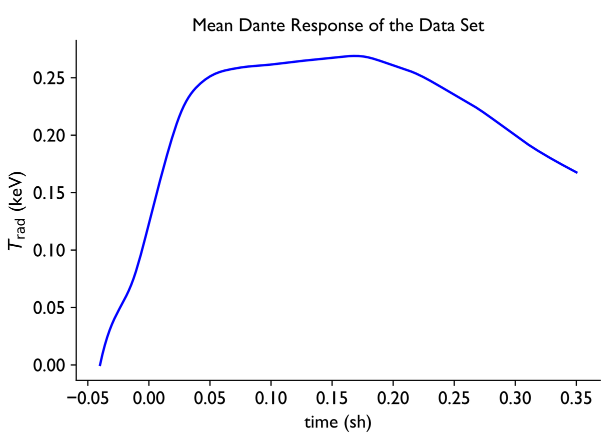

Figure 2: Mean Dante response as a function of time for the 61 simulations

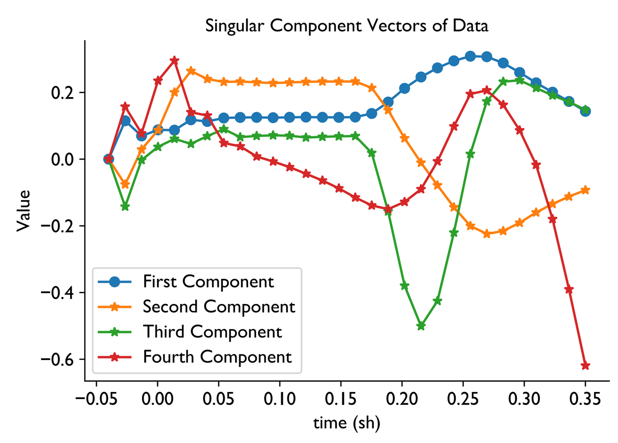

Figure 3: Four most important basis vectors in the simulation data

From the completed simulations, we extracted the response for the Dante-1 temperature estimate at 30 times equally spaced between the minimum and maximum times reported in the set of simulations, and 30 points was determined to be enough time points to reconstruct the Dante-1 results using cubic splines. When the reported data does not correspond to one of time points of interest, we use a cubic spline to interpolate the data to that time. We use the same splines in our plots of Dante output.

As a result of the time sample, for each simulation we have a list of 30 temperatures, corresponding to the 30 time points. We assemble the vectors from the 15 simulations into a rectangular matrix $\mathbf{A}$, where each row of this matrix is a Dante-1 temperature profile at the 30 time points.

This matrix is called the data matrix. From the data matrix we can compute the mean of each column (i.e., the mean temperature at each time point). This mean temperature profile is shown in Figure 2. We then subtract this mean vector from each row of $\mathbf{A}$ to get a mean zero data matrix $\hat{\mathbf{A}}$.

The singular value decomposition is then taken of the matrix $\hat{\mathbf{A}}$. This procedure takes the 30 correlated values of the temperature as a function of time as a projection onto a set of 30 uncorrelated basis vectors. In particular, the SVD of $\hat{\mathbf{A}}$ is $\hat{\mathbf{A}} = \mathbf{USV}^{\mathrm{T}}$ The matrix $\mathbf{V}$ has orthonormal columns that are the coefficients of the linear combinations of the original temperatures to create the uncorrelated variables. $\mathbf{U}$ contains orthonormal columns that are the projection of the data onto the uncorrelated values. The matrix $\mathbf{S} = \mathrm{diag}(\sigma_1, \ldots \sigma_{15})$ is ordered so that $\sigma_1 > \sigma_2 > \ldots$. The σ_i are known as singular values. From the partial sums, the first four singular values explain about 92% of the variance in the data.

Data-Driven Modeling

We will use the 61 simulations that ran to completion to build machine learning models to predict the four coefficients for the bases found from the SVD. That is, for a given set of points defining the hohlraum, plus the laser pulse length, we seek to find a model of the form

$$[u_1, u_2, u_3, u_4] = f(\texttt{scale}, \texttt{sc\_length}, \mathrm{R}_{apt}, \texttt{pulse}).$$

From these u_i we can reconstruct the Dante response as a function of time. We used several different techniques for modeling the relationship between inputs and outputs, and results from a Gaussian process model are shown here.

The figure below shows the behavior of the output as the laser pulse length is changed. The legend denotes the values for $[\texttt{scale}, \texttt{sc\_length}, \mathrm{R}_{apt}, \texttt{pulse}]$. These results are a leave-one-out cross validation where all of the simulations except the one being predicted is used to build the model to predict the Dante response.

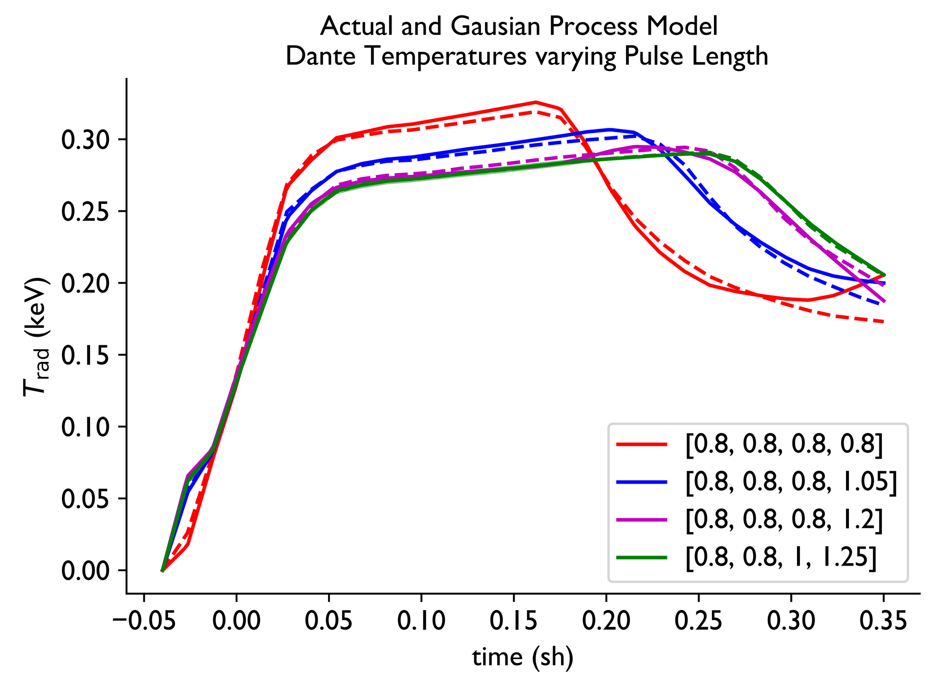

Figure 4: Changing the duration of the laser pulse adjusts both the height and duration of the temperature plateau. The solid lines are the GP model results and the dashed lines are the simulation results.

It is possible to use the GP model to predict the response of simulations that crashed before running to completion. We did not use these to train the model, however, in Figure 5 we can see that the GP follows the simulations for the data that we do have.

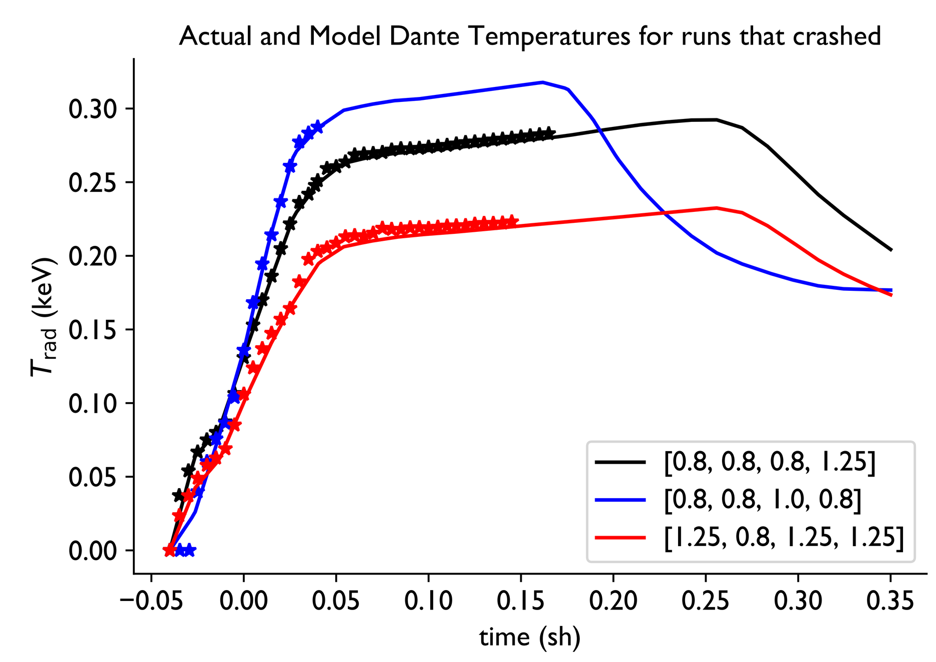

Figure 5: These are predictions from the GP model for HEDP simulations that crashed during the simulation. Those simulations where not used to train the model.

Different Hohlraum Shapes

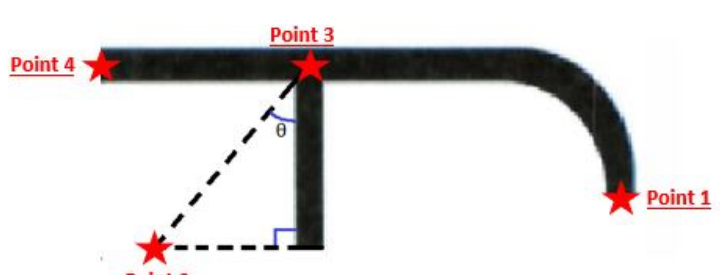

Figure 6: Illustration of how the baffle angle may change and affect point 2 in the hohlraum description.

We are interested in how changing the geometry of the sample chamber/aperture affects the evolution of the radiation temperature. To this end we have used the GP model to predict the behavior when point 2 moves to cause the inner baffle of the hohlraum to open up. These are blind predictions because we only have simulation data for perpendicular baffles. We cannot trust the GP model or its confidence intervals in such an extrapolation.

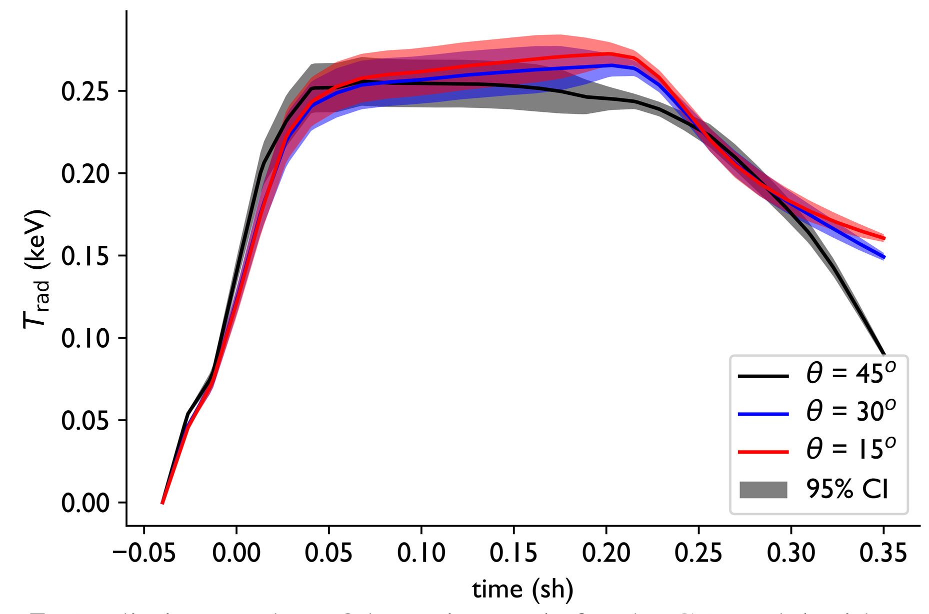

Figure 7: Predictions and confidence intervals for the GP model with varying angle of the baffle.

Radiation Transport Simulations

Given the cost of acquiring more simulation data for the full experiment, we have developed a radiation-only model of the hohlraum that uses gray, flux-limited diffusion to model the propagation of energy in the hohlraum. A simple, inverse bremsstrahlung model is used for the opacity in the metal of $20T^{-3.5}$ cm^{-1} for T in keV. The interior has the same opacity but multiplied by 10^{-3}. The heat capacity is constant at 0.25 GJ/keV/cm^3 in the metal and 0.001 times that in the interior. In the simulation the laser is on for 2.5 nanoseconds and deposits 250 KJ at a constant rate into a volume of 0.002 cm^3 inside the hohlraum wall.

We can generate data from this model much more rapidly and will be using this data to develop models for a variety of hohlraum shapes. To date we have data for the "lampshade" hohlraum that is shown below. We will be generating data on this and other holhraum shapes and applying our modeling techniques to them.

In these simulations we can see that the late time behavior of the radiation temperature is not affected much by the angle of the baffle, but the early and intermediate times have a strong effect. Though we should not read too much into the idiosyncrasies of a flux-limited diffusion calculation, we can see that the larger angle of the baffle exposes it to more radiation from the laser spot. Furthermore, the temperature of the baffle is much hotter when $\theta > 0$.

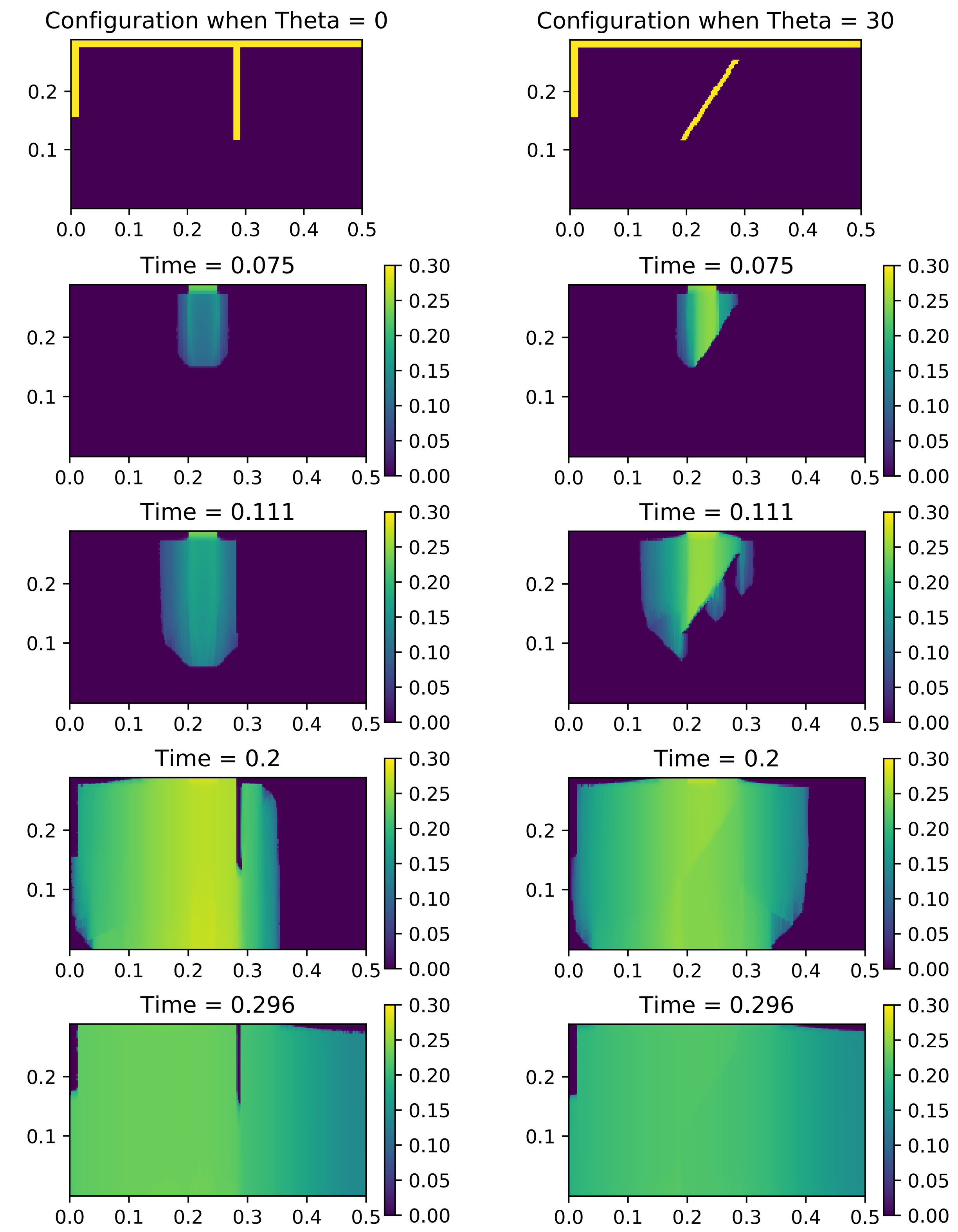

Figure 8: Time evolution of the radiation temperature (keV) for the radiation-only, gray, flux-limited diffusion model of a hohlraum with two different baffle angles. Only the left half of the hohlraum is shown. Notice that the baffle angle is the opposite of that in Figure 6 (the baffle bends toward the hohlraum opening).

If we average the radiation temperature in the middle of the sample chamber near the axis, we can obtain temperature profiles for the experiment. These profiles indicate that the angle of the baffle will affect both the peak temperature and the shape of the profile as a function of time.

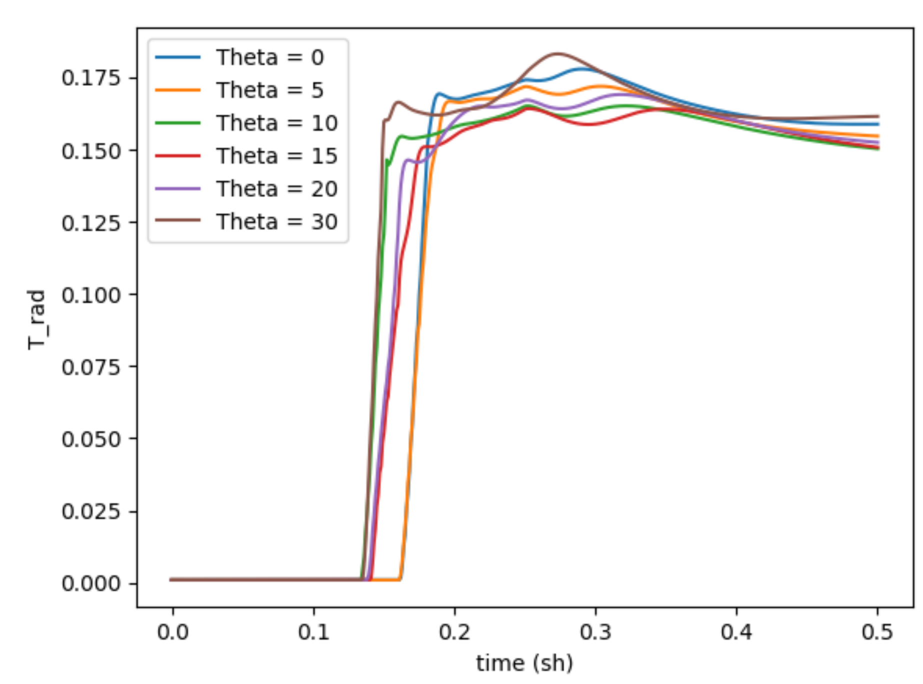

Figure 9: Time profiles of the temperature in the middle of the sample chamber near the axis (r=0).

[1] I. L. Tregillis. Synthetic Dante-1 temperatures from parameter variations of NIF hohlraums (phase 01). Technical Report LA-UR-17-22657, Los Alamos National Laboratory, March 2017.

[2] Dodd, E. S., DeVolder, B. G., Martin, M. E., Krasheninnikova, N. S., Tregillis, I. L., Perry, T. S., et al. (2018). Hohlraum modeling for opacity experiments on the National Ignition Facility. *Physics of Plasmas*, *25*(6), 063301–11. http://doi.org/10.1063/1.5026285

Los Alamos National Laboratory EST. 1943 · AWE · Lawrence Livermore National Laboratory · Sandia National Laboratories · NNSA National Nuclear Security Administration · Department of Energy