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Report from the Integrated Modeling Panel at the Workshop on the Science of Ignition on NIF

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1.0 PANEL SUMMARY SECTION 6 — INTEGRATED MODELING

1.1 Introduction (1 Paragraph)

– This section deals with multiphysics radiation hydrodynamics codes used to design and simulate targets in the ignition campaign. These topics encompass all the physical processes they model, and include consideration of any approximations necessary due to finite computer resources. The section focuses on what developments would have the highest impact on reducing uncertainties in modeling most relevant to experimental observations. It considers how the ICF codes should be employed in the ignition campaign. This includes a consideration of how the experiments can be best structured to test the physical models the codes employ.

1.2 Status of the Physics (1 page)

1.2.1 **Underlying processes and properties** – Physical processes modeled in the codes include radiation transport, electron and ion thermal transport, thermonuclear burn and transport of burn products. Production of radiochemical isotopes is modeled. These codes include models for transport of laser light and the various processes that affect it. They also include a treatment of magnetohydrodyanmics and the effects of magnetic fields on transport processes. Ingredients in the integrated models include atomic physics, in particular models for opacities and equations of state, both LTE and NLTE. These codes employ single fluid, two temperature hydrodynamics which resolves hydrodynamic instabilities directly.

1.2.2 Status of theory and modeling – Simulations used to model experiments in the ICF program fall into two broad categories: 1) integrated hohlraum simulations and 2) capsule only simulations. The former type models the hohlraum and capsule and may include patches and reentrant cones in the targets. These can calculate both intrinsic and extrinsic drive asymmetry (due to pointing and power balance errors). Recently this technique has been extended in HYDRA to include the roughnesses on the capsule surfaces. The latter capsule only simulations are often run with high resolution and include roughnesses on all surfaces, a representative ice groove, the effect of the fill tube and tent and drive asymmetries. The capability to perform these simulations has been developed and validated in the ICF program over many years. The ICF program relies heavily upon simulations carried out in 2D using Lasnex and 2D/3D using HYDRA. Modeling techniques employed in these codes have been tested extensively against experimental data obtained on the Shiva, Nova and Omega lasers for a wide variety of experiments. The RAGE code has also undergone experimental validation against ICF experiments, to a less extensive degree. Historically hohlraum simulations performed using the XSN NLTE opacities and flux-limited conduction have been able to calculate radiation drive temperatures in a wide variety of hohlraums to within 10%. These account for measured energy scattered out of the hohlraum due to laser plasma instabilities (LPI) through adjustments to the input laser powers. Simulations of experiments on Nova and Omega demonstrated their ability to model pole-to-waist (P_2) asymmetry as the power was varied from the inner to outer cones. The ability of these codes to model the ablative Rayleigh-Taylor instability itself has been validated experimentally in the linear and nonlinear saturated regime, with single mode, two mode, and multimode perturbations, including shape effects in both 2D and 3D. Capsule only simulations have demonstrated an ability to calculate the variation in yield as the amplitudes of controlled surface perturbations were varied.

1.2.3 **Impact of experimental results** – Early vacuum hohlraum experiments on NIF in 2009 showed higher radiation drive temperatures than were predicted with hohlraum temperatures using the historical models. Simulations using new more detailed models of NLTE opacities/EOS obtained from the detailed configuration accounting (DCA) model and a detailed model for nonlocal thermal transport produced a higher radiation drive which was a better match to experimental measurements. With this "high flux model" the plasma temperatures and densities calculated for *gas filled* hohlraums were closer to values inferred indirectly from LPI measurements, using a linear theory for backscattered power. In contrast to the vacuum hohlraums, the most recent analysis of drive measurements for gas filled ignition hohlraums indicate this high flux model predicts a flux which is systematically too high, by about ~13% during the peak. We note that in these gas filled hohlraums the evolution of the gold bubbles is restricted by the gas fill, and quite different from the bubble dynamics in vacuum hohlraums.

To account for errors in the energy flow in hohlraum simulations a time varying multiplier is applied to the laser power, constrained to match shock timing data from keyhole experiments and the bang time. With this adjustment to the "push" delivered the capsule simulations can match many observables from implosions experiments, such as mass averaged velocity and radius vs. time, shell thickness and peak shell density vs. time. The implosion velocity versus remaining mass fraction agrees within experimental error bars. The shell areal density deduced from the neutron downscatter fraction can also match well the experimental values, and is ~85% the value specified for the point design. And the ion temperature deduced from neutronic measurements is usually close to the simulated value. The experimental neutron yields are low by a factor of several to 10 times compared to 2D calculations using the renormalized drive. The hot spot pressure and density inferred from the experiments performed with cryogenic ignition capsules are also low. The calculations show a significant amount of bootstrapping from alpha particle deposition, not observed in the experiments due to depressed yields. When bootstrapping due to alpha deposition is disabled in the simulations the experimental yields are lower than calculated values by a factor of 2 – 5 times.

Since energy transfer between crossed laser beams is important on NIF, as was anticipated, a semi-empirical model for the energy transfer is now routinely used in modeling. It is employed by post-processing results of a hohlraum simulation, accounting for the color separation specified between individual beam cones. The model for cross beam transfer contains a single adjustable saturation parameter, which is tuned to match the implosion symmetry. Making use of this model, the simulations match the variation in pole-to-waist asymmetry as the color separation between beam cones is varied across a similar set of experiments. Benefitting from guidance provided by simulations, the hot spot symmetry which meets ignition specifications has been achieved by adjusting hohlraum geometry, and power balance and wavelength shifts between inner and outer cones.

1.3 Opportunities for progress (1-2 pages)

What are the most important uncertainties and why -

In the discussion of specific Priority Research Directions, we show in detail how simulations and experiments in each area can advance our ability to perform predictive simulations of NIF experiments and our understanding of the physics involved. Here we first provide a brief overview of the opportunities for progress in these areas and a few others.

Integrated modeling and simulation has a vital role to play in the design, execution, and analysis of NIF experiments. Given the vital role of integrated modeling and simulation in achieving ignition, it is exceedingly important to track down sources of error in the simulations, so the codes can be more effective in guiding the experiments and helping to identify possible missing physics. Simulating the results of experiments has many sources of error. As well as the codes themselves which combine many approximations, there are also the databases containing tables of Equations of State, Atomic and Nuclear Physics, and input files that describe the initial "as shot" target geometry, zonal and frequency resolution, laser pulse specifications and instructions to the code describing which models should be used and how. We need to make progress in each of these areas to better understand and resolve the discrepancies between simulation and experiment. Integrated experiments with incomplete diagnostics are particularly difficult to use as a means to discover which particular models, databases or input errors are responsible for a discrepancy. It is likely that there is more than one thing wrong and we should expect that fixing some errors will move the simulated results farther from experiment. Only by doing less integrated experiments will we be able to validate our models and simulations of the individual processes involved.

For these reasons, execution of a rigorous, science-based validation campaign provides the greatest opportunity for progress in integrated modeling. This campaign has several components including a hierarchical directed validation experiment strategy that breaks down the fully integrated experiments into separate parts that can better validate the simulation ingredients, and a hierarchical simulation strategy in which capstone simulations having the highest possible fidelity are done, as well as many modest fidelity simulations. Another component is enhancing the techniques for sensitivity analysis developed within NIC by combining them with quantifications of uncertainties in both inputs and measurements. This can be used to discriminate which inputs and model ingredients are most for responsible uncertainties in modeling, and to help guide efforts to improve model ingredients. Unraveling the sources of the discrepancies between the predictions of the simulations and the experimental data in non-linear, tightly coupled, fully integrated experiments conducted in the NIC is nearly impossible. Several hypotheses can be put forward for each discrepancy. Directed validation experiments that single out one key physical process in the physical regime encountered in the NIF experiments are therefore crucially needed to cut this Gordian knot. The campaign also includes continued code-to-code comparisons for verification and validation.

Successfully modeling hohlraum energetics is crucially important. Presently the location of some 170 kJ of energy (~10%) in the NIF ignition hohlraum is not well understood. This involves accurately modeling a plethora of challenging physics models and processes, including equations of state, non-LTE opacities, laser-plasma interactions, non-local electron thermal transport, fluid instabilities, and spontaneously generated magnetic fields.

Recently, several physical processes have been identified that could affect thermonuclear reaction rates in the hot spot. It is important to investigate these processes through both simulations and experiments because the neutron yield in the NIF experiments is a factor ~ 5 lower than simulations predict, in spite of the expected areal densities and reasonable ion temperatures being obtained. Physical processes that should be investigated include the separation of deuterium and tritium nuclei by electric fields and barodiffusion, depletion of the tail of the velocity distribution by the DT reaction itself, and non-local electron thermal transport that may play a role in the early formation of the hot spot and the flow of energy into the dense fuel.

In addition to these three Priority Research Directions, the Panel believes our ability to model non-local electron energy transport, a fundamental physical process that plays a key role in hohlraum energetics and may play an important role in the creation and evolution of the hot spot, should be improved. The Panel also strongly encourages exploration using both simulations and experiments of the variety of effects spontaneously generated magnetic fields could have on energy transport, fluid velocities, and instabilities, as well as the possible dynamical importance of magnetic fields at and behind the shock fronts that compress the capsule.

1.4 Priority Research Direction 1 (2 pages)

A Science-Based Validation Campaign

Introduction – Integrated modeling and simulation has a vital role to play in the design, execution, and analysis of NIF experiments, including those directed toward achieving ignition. For modeling and simulation to play this role, the simulation codes must faithfully predict complex, multi-scale, multi-physics experiments to within the accuracy of diagnostic measurements.

The pathway to predictive capability is a science-based validation campaign in which comparisons of simulation results to experimental data uncover limitations or weaknesses in the integrated model, which is followed by new experiments designed to illuminate further the origins of the discrepancies [1,2]. Improvement of models through validation is a continuous process leading to predictive capability.

Decades of validation experiments and predictive science model improvements for non-ignition targets lead to a demonstrated ability to model well the wide variety of physical effects related to radiation drive and asymmetry in hohlraums, and implosion physics, including hydrodynamic instabilities. The capability was developed by testing the models against a wide range of experiments, many of which focused upon specific, individual effects. For NIF ignition experiments these models must be extended to systems with 100 times as much energy as Nova, much larger spatial and temperature scales, higher convergence ratios and rather different plasma conditions. As these models are extended to these new regimes, comparison with integrated experiments places the greatest stresses on their predictive capability; those simulations require a wide variety of model ingredients, with each having significant bearing on the ability to model the whole system. Isolating specific the ingredient(s) responsible for disagreements in modeling the integrated experiments alone is exceedingly difficult.

Near-term improvements and approaches to theory and modeling - The Integrated Modeling Panel consequently believes execution of a rigorous, science-based validation campaign provides the greatest opportunity for rapid progress in integrated modeling. Such a campaign should have several components.

The Science-Based Validation Campaign includes continued code-to-code comparisons and appropriate studies of numerical convergence. Such comparisons are an important, though incomplete, way of checking that (i) the codes have implemented the physics models correctly, (ii) the algorithms used in the codes are as accurate and efficient as possible, and (iii) the infrastructure of the codes is operating correctly. In the ICF program code-to-code comparisons are generally done on simplified problems to reduce to a manageable level the effort required to locate sources of differences. Also some codes lack the full set of physics to do the actual problem. As an example simulations of simplified problem containing a fill tube run with dissimilar hydrodynamics methods can test if they converge to a similar result. Excessive dependence upon code-to-code comparisons should be avoided. For one it would tend to result in different codes implementing the very same models. Also code-to-code comparisons produce information regarding similarity of results obtained, but they do not test which methods and models are best at modeling the actual experiments.

The Science-Based Validation Campaign includes a hierarchical directed validation experiment strategy that focuses on crucial aspects of the fully integrated experiments. This is essential because the fully integrated experiments are too complicated to be able to easily identify the reasons for the discrepancies between the predicted and the experimentally measured values, and because the ability to obtain data on the quantities of greatest interest is usually very limited and may times impossible. Close and continuing cooperation between simulators and experimentalists will be essential to the success of such validation experiments, as will be the willingness of project leaders to direct resources to the execution of such experiments.

The Science-Based Validation Campaign also includes a hierarchical simulation strategy that includes a number of simulations performed at the highest possible fidelity. High fidelity includes high spatial resolution, or a high level of detail of physics models employed, as well as detailed 3D simulations. The high fidelity simulations provide valuable information about the importance of the various physics models, enabling informed choices to be made about how to reduce the models to make it possible to do many simulations, while retaining the ability to accurately predict the experimental quantities of greatest interest. Many modest fidelity simulations will be needed to do parameter sensitivity studies and to understand the uncertainties in the predictions made by the simulations. The willingness of project leaders to provide the resources necessary to improve existing physics models, develop new physics models, enable the simulation codes to run at scale on existing and future platforms, and carry out a hierarchical simulation strategy will be essential to its success.

Some of the effort within the Science-Based Validation Campaign should be devoted to performing a sensitivity analysis for the most relevant performance metrics to specific model inputs. The NIC has developed a capability to perform sensitivity analysis by executing thousands of 1D and 2D capsule only simulations with HYDRA [POP **19** 056316 (2012)] in which many parameters are varied to map out a multi-dimensional response function of the "quantities of interest." [1] As has been noted [1] generating response function surfaces for every input parameter variation is not practical. It would result in an underfit response function that would not be useful. Rather one must choose a limited number of free parameters, based upon physical intuition, so that the number of simulations required to generate the response functions becomes tractable. Such a sensitivity analysis yields important insights on which inputs of the reduced model have the most important impacts on the quantities of interest. We recommend that the program enhance the usefulness of capsule sensitivity studies, by combining them with knowledge of the uncertainties in the individual model inputs, to assess systematically the impacts of those uncertainties. This will help to identify the specific inputs for which the uncertainties have the greatest impact on quantities of interest. This analysis, combined with quantitative knowledge of the uncertainties in measured quantities of interest could help the program determine which model inputs and ingredients are most strongly associated with errors in modeling of capsule performance. Such an analysis could help the program to determine which focused experiments should receive the highest priority. Examples of approaches for performing this analysis have been reviewed [1, 2]. As part of simulated ignition campaigns carried out previously within NIC, estimates for uncertainties in the ingredients of many models have been assembled.

With respect to 2D hohlraum simulations, running many thousands of these is not practical at present. Nevertheless we believe that a systematic assessment of the sensitivities to uncertainties in each of the physics models is feasible and should be performed. This could be accomplished by varying the appropriate settings for each, one at a time, within a set of hohlraum simulations. This version of a systematic sensitivity analysis, combined with knowledge of the uncertainties in inputs, could help to discriminate which model ingredients are most responsible for overall uncertainties in the calculated hohlraum drive. As the model ingredients are improved, this process can be employed iteratively to help speed convergence. [3]

High impact experiments on HED facilities to address uncertainties in critical physics models - The ICF program has a long history of validating the ability of its modeling tools to simulate successfully essentially every physical process regarded as important in an ignition target design. During the Nova technical contract and for subsequent experiments at Omega laser facility, simulations of the performance of various ablators was validated against the results of experiments that measured hydrodynamic performance, and a range of hydrodynamic instability effects in planar [PRL **80** 4426 (1998), POP **2** 241 (1995), POP **1** 3652 (1994), Phys. Fluids B **4** 967 (1992)] and converging geometry [POP **3** 2070 (1996), PRL **89** 165001 (2002), POP **7** 2033 (2000)]. The ability to model hohlraum drive [PRL **80** 2845 (1998)] and implosion symmetry [POP **10** 2429 (2003), UCRL-JC-135811] were also validated for a variety of targets, as was the ability to control laser plasma instabilities [POP **14** 055705 (2007), PRL **101** 115002 (2008), PRL **103** 045006 (2008), POP **17** 056302 (2010), POP **15** 056313 (2010)].

Ignition experiments at the NIF probe plasma densities, temperatures, and pressures that are well beyond the ranges that could be achieved and explored on Nova and at the Omega laser facility. Thus the physics models used in the simulation codes for opacities, equations of state, conductivities, etc. have of necessity been applied well outside the regimes for which they were validated in previous experiments. For example at radiation drive temperatures of NIF the carbon K shell experiences significant ionization, not present in previous experiments with lower drives. Due to the exigencies of the NIC, the experiments that have been carried out are complex and highly integrated. As a result, each of the experimental results can be related to multiple hypotheses, making it difficult to identify the reasons for the discrepancies between the predicted values and the experimentally measured values.

The Panel therefore recommends a series of directed validation experiments that will gather data on individual physical processes for the physical regimes encountered at NIF. This data can be then be used to validate the models used in the simulation codes in the appropriate regimes. The following are examples of the kinds of experiments the Panel recommends be done:

- Planar foil experiments could measure the performance of various ablators for 300 eV drives using side-on radiography. These could include position vs. time and the rate of foil burn-through. They could also include experiments with planar foils having pre-imposed perturbations, diagnosed through face-on radiography with a backlighter. By employing foils of the same composition as the capsule ablators, the experiments could be used to validate directly the ability of the simulations to model ablation front growth for relevant drive conditions.

- Experiments measuring the growth of individual features imposed on a backlit capsule implosion diagnosed with radiography could be used to validate simulations of ablation front hydrodynamic instability growth for spherical geometry in the NIF regime.

- Of all the materials employed in the ignition capsules, the program has the least experience with cryogenic DT fuel. Measuring the release of DT in both the keyhole and planar geometry could help constrain the equation of state of DT in this cold, dense regime.
    - In planar geometry, a CH/D2 composite target could release through a vacuum onto a witness plate. Measurement of the pressure at the witness plate vs. time using VISAR would help constrain the physics related to early stages of hot spot formation.
    - The strength and timing of the stagnation shock could also be measured using the keyhole geometry. Uncertainties in shock timing measurements could be reduced by performing keyhole experiments using DT ice, rather than liquid D2.
- Experiments that measure the growth of fill tube perturbations using high-resolution radiography could further constrain modeling uncertainties.

An alternative path for validation recommended by the Panel is to identify an integrated experiment matched by the current model. Then, starting from there, march along various paths towards the point design and see where the model breaks down. The HEP4 experiments performed on Nova are a candidate for this approach, since the neutron yield was modeled well by simulations for a set of experiments in which various controlled perturbations were imposed on the capsule surface.[POP **3,** 2070 (1996)] The capsules consisted of a single germanium-doped polystyrene ablator layer of uniform dopant concentration, with a thin interior mandrel. They were filled with deuterium gas at room temperature. The specific changes that would be required to march to the point design are the following: (i) going from a two shock to a four shock drive, extending out to 20 ns, (ii) replacing GDP with silicon dopant, (iii) replacing D2 gas with cryogenic DT fuel, (iv) replacing a single dopant ablator layer with a graded dopant layer, (v) raising the peak drive to 300 eV, and (vi) obtaining a low fuel adiabat to increase the convergence ratio from ~15 to ~37.

Long-term goals and outlook - Executing a rigorous, science-based validation campaign will enable the ICF program to identify the specific physical effects responsible for the low neutron yields measured experimentally. It will produce a better understanding of where the discrepancy between simulation and experiment becomes significant as one marches away from points in the experimental parameter space where the simulation codes were successfully validated. This will provide a better way to discrimination of competing hypotheses. The end result will be increased ability to do predictive science, and greater community and customer confidence in the simulation tools**.**

[1] M. L. Adams and D. L. Higdon. *Assessing the Reliability of Complex Models: Mathematical and Statistical Foundations of Verification, Validation, and Uncertainty Quantification*. The National Academies Press, 2012. ISBN 978052111301.

[2] W. L. Oberkampf and C. J. Roy. *Verification and Validation in Scientific Computing*. Cambridge University Press, 2010. ISBN 9780521113601.

[3] C. Graziani, T. J. Loredo, and M. Anitescu. Adaptive design of computer experiments and simulation fidelity hierarchies. Technical report, University of Chicago Flash Center for Computaitonal Science, 210. http://flash.uchicago.edu/car/adaptive_design.pdf

1.5 Priority Research Direction 2

Improved Modeling of Hohlraum energetics

1.5.1 **Introduction** – Integrated simulations of hohlraums model a wide variety physical processes, including laser energy deposition, thermal transport and transport of radiation energy. The ablation of various surfaces and the implosion hydrodynamics, including hydrodynamic instabilities, must be resolved. Several factors add to the challenge of hohlraum modeling. The necessity of including detailed inline models for non-local thermodynamic equilibrium (NLTE) kinetics to generate opacities and equations of state is one. In addition the collisional mean-free-path λ_c of electrons is long enough to violate the condition for local transport $\lambda_c \ll L$, there are MegaGauss level spontaneously generated B-fields [Li et al., PRL 102, (2009)] which are of sufficient strength to influence electron transport in the gas-fill, and the B-field topology is complicated. Laser plasma instabilities (LPI), principally Stimulated Brillouin (SBS) and Raman (SRS) Scattering, redirect significant amounts of energy through backscatter. The SRS electron plasma wave can produce hot electrons which could preheat the capsule. Cross beam energy transfer can shift substantial amounts of energy between laser beams. Distorted electron distribution functions due to non-local transport and from intense inverse bremsstrahlung heating can influence plasma profiles. They could also potentially directly affect the production of x-rays from the hohlraum wall, through interplay with NLTE atomic physics. Distorted electron distribution functions might affect the LPI by changing Landau damping rates.

With respect to spontaneously generated magnetic fields simulations of gas filled ignition hohlraums carried out using the Lasnex code have shown a Hall parameter $\omega\tau_c$ having a peak value of ~5 in the hohlraum [R. Town, Bull. Am. Phys. Society, DPP, **49**, 2004, pp. 25], indicating the plasma is not strongly magnetized. And the magnetic field effects on x-ray drive and associated drive asymmetry are indicated to be rather weak in simulations. So these simulations indicate the principal effect of these magnetic fields on hohlraum performance is a modest change in plasma densities and temperatures in low density regions interior to the hohlraum, which might influence LPI, and some reduction in mobility of hot electrons.

During the experimental campaigns on Nova and Omega hohlraums were routinely modeled, with a high degree of success, using XSN average atom opacities and flux limited electron conduction, with a flux limiter of 0.05. With this long time model the calculated radiation flux was regularly within 10% of the experimentally determined value. By comparison Dante, the principal diagnostic to measure the hohlraum x-ray flux, typically has an uncertainty of 12% on the flux. As computer power available has increased rapidly the modeling tools HYDRA and Lasnex have been able to incorporate more detailed and complex models for NLTE kinetics in the form of the Detailed Configuration Accounting model (DCA). Also a multigroup model for non-local electron transport had been installed in HYDRA, and later in Lasnex [G. P. Schurtz, P. D. Nicolai, and M. Busquet, Phys. Plasmas 7, 4238 (2000)], which in principal enables a more accurate treatment of the thermal electron heat flow in the hohlraum. Early experiments on the NIF in 2009 using *vacuum* hohlraums showed higher electron temperatures than were predicted with the historic model. Simulations run using the DCA model along with the nonlocal electron transport model, elements of the "high flux model", agreed better with the vacuum hohlraum drive measured on NIF. Plasma temperatures indirectly inferred from LPI backscatter measurements in *gas filled* hohlraums on NIF, using linear models for LPI backscatter, were also closer to the lower values calculated with the high flux model. In more recent NIF experiments performed with *gas filled* hohlraums the high flux model predicts a drive on the capsule which is systematically too high, by about 13% during the peak of the pulse.

Recent analysis of time integrated images of the laser entrance hole aperture imply the numerical simulations are predicting it closes somewhat faster than the experiment. This results in an area that is inferred to be ~20% smaller than the experiment at late time. When this difference in aperture area is accounted for, the drive deduced from Dante is within 4% of the drive required to match the shock timing data. This is within the experimental error bars on Dante.

To match the shock timing data obtained from keyhole experiments, and the bang time, a time varying multiplier on the laser power is applied to hohlraum simulations performed with the high flux model. We note that a series of very recent simulations of shock timing data from keyhole experiments, which use different physics models, is matching well the data for a range of ignition hohlraum experiments without any multipliers on the laser power at all. This module employs the older XSN NLTE opacities and EOS, new LTE tabular opacities and a higher flux limiter, representative of results obtained with the non-local electron transport model. The shots matched include both gold and uranium hohlraums and different rates of rise for the laser pulse [Harry Robey, private communication]. Clearly uncertainties in modeling of NLTE kinetics and the equations of state can account for significant variations in the simulation results, and should be the subject of further research. Other significant uncertainties include nonlocal electron transport, LPI and cross beam transfer and effects of self-generated magnetic fields.

1.5.2 **Near-term improvements and approaches to theory and modeling** – First principles modeling of the SRS and SBS backscatter is a grand challenge problem carried out at resolution comparable to the wavelength of light and over the light transit time. Because of the very short spatial and temporal scales involved, it is far too expensive to include inline in a radiation hydrodynamics simulation of a hohlraum. In practice the effect of laser plasma instabilities has generally been accounted for in hohlraum simulations by subtracting off the backscattered light energy from the laser source. And the effect of cross beam energy transfer has been calculated by postprocessing results of a hohlraum simulation. The energy at the laser lens is then modified to model the resulting effect of cross beam transfer. Recently a model for energy transfer between cross laser beams [P. Michel…] has been implemented inline in HYDRA. Also semi-empirical models for energy backscatter due to SRS and SBS were implemented in HYDRA and Lasnex. A simulation run using these new models would improve modeling by producing a much more self-consistent treatment of energy flow due to LPI effects. For example the changes in laser momentum deposition due to the cross beam transfer are included, as well as the absorption of redirected energy flow. The resulting plasma conditions can thus be calculated self-consistently. These models should be employed and tested on simulations of experiments, including ignition targets.

Improving modeling of NLTE kinetics is one of the highest leverage items for improving simulations on hohlraum energetics. There are several areas in the DCA NLTE kinetics model which should be pursued. One such area lies in the transition from tabulated LTE data to NLTE calculations. This should occur as soon as NLTE effects begin to become significant. However, DCA results do not match the LTE data well for the relevant conditions in the hohlraum wall, so the transition region is not well modeled by either LTE or NLTE methods and simulation results end up being sensitive to this transition. Also, detection of when the transition should occur is not currently informed by kinetics, although this is under development. The limitations of DCA in this area are primarily due to the use of very simple atomic models which do not adequately model the complexities of ions with 40-50 electrons. A second area requiring improvement is modeling M-band radiation. Here, DCA does a surprisingly good job, as measured by comparisons with benchmark calculations by detailed codes. However, that still allows uncertainties in the range of 20-40%. The limitation here is likely due to an overly simplistic description of excited states of M-shell ions. These are approximated as having a single energy based upon the principal quantum number. Resolving the energy distributions of the levels would improve the overall model accuracy. Lastly an examination of the accuracy of the model for continuum lowering in DCA is warranted.

Atomic models with better fidelity are available from detailed NLTE codes, but with a level of description which makes their usage several orders of magnitude too expensive for integrated simulations. The improvements necessary for using high-fidelity data inline lie in producing atomic models which reproduce these features with only moderately increased computational requirements over the models currently used with DCA. This is a challenging area for research.

Hohlraum simulations which employ the Schurtz non-local electron transport model [G. P. Schurtz, P. D. Nicolai, and M. Busquet, Phys. Plasmas 7, 4238 (2000)] are believed to have the most accurate treatment of thermal transport. Alternatively the simulations done with the high flux model may use flux limited thermal conduction to model thermal transport, with the flux limiter is calibrated to produce results similar to those obtained from the non-local model. Kinetic codes for electron transport exist which are well suited for modeling non-local transport and which include self-consistent B-fields. IMPACT and IMPACTA are implicit 2D (Eulerian x-y grid), parallelized Vlasov-Fokker-Planck codes using the "diffusive approximation" $f=f_o+f_1$ and including anisotropic pressure $f=f_o+f_1+f_2$, respectively. They include B_z and full B, respectively. The Schurtz model should be tested more thoroughly against a Vlasov-Fokker-Planck calculation of a simplified system, perhaps using IMPACT / IMPACTA, with plasma conditions relevant to a NIF hohlraum. Besides improving our understanding of the accuracy of the non-local model under the conditions specific to NIF experiments, this effort could result in a better reduced model, having an improved value of a flux limiter.

1.5.3 **High impact experiments on HED facilities to address uncertainties in critical physics models** – Opacities of the gold and uranium used in hohlraums are critically important in determining the amount of energy absorbed by the hohlraum wall and retained by coronal plasma ablated off the wall. Measurements of opacities for these materials can help constrain opacity models used in the simulations. Experiments of the type performed by Foord [PRL **85** (2000)] and Heeter [PRL **99** (2007)] produce detailed opacity data for plasma conditions of interest in hohlraum, including the relevant ionization states. We recommend that more measurements be made of the opacities of these materials, for NIF relevant plasma parameters, to constrain better the opacities models used. Many of these experiments can be performed on the Omega laser and other facilities.

A time-resolved measurement of the closure of the LEH is important for resolving outstanding questions regarding energy balance. Making this measurement for a set of relevant x-ray energies would be desirable.

Hohlraum experiments using different fill gases and pressures to study laser plasma instabilities would be helpful. Varying the laser power would also allow a study of the variation of LPI with plasma conditions.

Dedicated experiments can help tests the accuracy of the non-local electron transport models in a long scale length plasma. One approach would be to scale up the Gregori [PRL **92** (2004)] and Froula [PRL **98** (2007)] type JANUS (gas-jet) experiments to conditions more indicative of the NIF hohlraum. These involve higher electron density, higher power, 2 parallel beams (to mock up beam bundles in cones), and 2 crossed beams (to mock up LEH area). The experiment would use square aperture beams as are used in NIF.

Another approach would be a direct experimental measurement of the heat flow and electron distribution function. This would be a follow on of the experiment of Hawreliak et al. [J. Phys B **37** (2004)]. The experiment would produce more detailed and direct validation data for non-local and kinetic transport models. In particular the distortion of the electron distribution function by the non-local transport and intense inverse bremsstrahlung heating and the resultant affect upon the heat flow would be of primary interest. This would be done for a laser spot intensity and size like those of a NIF hohlraum, creating similar plasma conditions. Though it would not necessarily need to be done on the NIF laser.

1.5.4 **New capabilities (diagnostics, models) needed** – One feature of the high flux model is sharply lower predicted electron temperatures in the hohlraum. There are presently no diagnostics on NIF which can measure electron densities and temperatures in hohlraum experiments. Electron densities and temperatures in hohlraums have been *inferred* indirectly, based upon backscatter measurements, using linear models for LPI backscatter. A direct measurement of the plasma electron density and electron temperature is needed to constrain models used in hohlraum simulations. A Thomson scattering diagnostic with a 4ω probe laser has been proposed for this purpose. In addition a simultaneous measurement of the magnetic fields in the hohlraum would help the program to understand its role in modifying the plasma temperature profiles. This could be accomplished using proton radiography, measuring along the lines of the sight, similar to the approach taken on the Omega laser. With direct simultaneous measurements of the aforementioned plasma quantities the program would be able to discriminate between the models.

Measurements indicate that laser plasma instabilities such as SRS and SBS scatter about ~17% of the laser energy back out of the hohlraum. This is of the order of the modification in energy input required to match capsule implosion dynamics with the high flux model. Presently the backscatter is measured on only a handful of NIF beams. Given the importance of backscattered energy on the drive, and uncertainties surrounding its, a more comprehensive set of measurements of LPI-induced energy redirection is warranted. LPI-induced energy redirection includes the generation of suprathermal electrons which could be detected by any resulting x-ray emission. To this effect, effort should be directed at improving the spatial and temporal resolution of the FABS (Full Aperture Back Scatter) diagnostic to enhance understanding of SRS and SBS processes, and implementing simultaneous measurements on more beams. In addition, we recommend that the temporal resolution of the DANTE and filter fluorescer (FFLEX) diagnostics be improved.

With respect to modeling, improving the Vlasov-Fokker-Planck codes to model r-z and r-theta geometries would allow better applicability to hohlraum and greater overall flexibility. Improving the overall physics capabilities of those codes would make them more useful for assessing the importance of kinetic effects is actual hohlraum experiments.

An improved, more comprehensive and robust treatment of magnetized transport effects particularly, Righi-Leduc heat flow ($\kappa_\wedge$) and Nernst advection ($\beta_\wedge$) – into hohlraum simulation codes is also important. This would enable a better assessment of the significance of magnetic field effects upon transport and resulting modifications to plasma temperature and density profiles. This work is underway in HYDRA and Lasnex, at different stages of development in 2D and 3D, and extends over a several year time frame.

1.5.5 Long-term goals and outlook – By validating individual elements of the models used in hohlraum simulations the program will also improve validation of the integrated model itself. The ultimate result of these efforts will be an improved predictive capability for modeling capsule drive and preheat. An improved understanding can ultimately lead to achievement of a higher radiation drive. The figure of merit of an ignition capsule implosion has a very strong dependence upon implosion velocity and thus the peak drive. Thus achieving a higher radiation will strongly benefit the campaign to achieve ignition.

1.6 Priority Research Direction 3

Investigate Kinetic Effects on Thermonuclear Yield

1.6.1 **Introduction** – Recently several processes have been identified that could modify thermonuclear reactions rates due to the fuel plasma being a non-ideal fluid. These process include the separation of deuterium and tritium nuclei by electric fields and barodiffusion [P. Amendt, S. C. Wilks, C. Bellei, C. K. Li & R. D. Petrasso, Phys. Plasmas 18, 56308 (2011)], the loss of reactive ions in the high energy tail of the distribution function due to their long mean free paths [K. Molvig, N. M. Hoffman, B. J. Albright & R. B. Webster, LA-UR 12-0150 (2012)] as well as various infinite medium processes such as tail enhancement by large angle alpha particle collisions, tail depletion due to the DT reaction itself and lack of time to fill out the tail. Non-local transport can also play a role in the early formation of the hot spot and the heat flow from the hot spot into the dense fuel. These kinetic and non-local effects are more significant when the first shock reaches the center of the capsule. In a cryogenic NIF capsule the hot spot mass increases many times during the implosion due to conductive ablation of fuel from the dense capsule shell. The compression of the hot spot, coupled with the increase in its mass, cause the collisionality to increase. For example, when the capsule has converged to minimum radius and the hot spot is approaching ignition, for a central density of 100 g/cm^3 and the ion temperature of 5 keV, the hot spot is over 1000 deuteron mean free paths in radius. As a result most of these effects will be small as the fuel is beginning to ignite and become more important during vigorous thermonuclear burn. Analysis done to date suggests these effects would not be expected to account for the yields being low by a factor of several in current NIC experiments with ignition capsules. Given that experiments show low yields in spite of the expected areal densities and reasonable ion temperatures being obtained, the Integrated Modeling Panel recommends that the aforementioned effects be assessed systematically using the best available models.

1.6.2 **Near-term improvements and approaches to theory and modeling** - In the near term we should apply the best existing models and codes to ignition conditions to learn more about when these various processes are important and to estimate their impact. This effort should include using PIC codes such as LSP [D. R. Welch, D. V. Rose, B. V. Oliver & R. E. Clark, Nucl. Instrum. Methods Phys. Res. A **464**, 134 (2001)] to investigate simplified localized geometries and to validate the models used in larger scale codes like Vlasov-Fokker-Planck [A. G. R. Thomas, M. Tzoufras, A. P. L. Robinson, R. J. Kingham, C. P. Ridgers, M. Sherlock & A. R. Bell, J. Comp. Phys. **231**, 1051 (2012)]. Among PIC codes LSP is well suited because it can run in 1D spherically converging geometry and contains and expanded set of physical models. These tools enable the program to study all of the aforementioned processes. Specific effects can be studied using idealized problems that resemble the hot spot and capsule shell geometry of the ignition capsule. In addition plasma profiles from a 1-D simulation of an ignition capsule can be linked near peak implosion velocity for example to LSP and the simulation carried through. By comparing the evolution of the profiles between the radiation hydrodynamic code and the LSP PIC code the significance of effects such as species separation can be assessed for a specific target design. If any specific effects above appear to be significant then reduced models of these processes should be developed in the short term and tested against PIC and VFP codes. Once validated they would be implemented in multi-dimensional hydrodynamic and transport codes. This would enable these effects to be evaluated self-consistently in a full physics code. Efforts have begun to assess these effects using the LSP code. [S.C. Wilks, private communincation]

1.6.3 High impact experiments on HED facilities to address uncertainties in critical physics models – Shock timing experiments performed in the keyhole geometry to date have used DD as a surrogate main fuel layer. In the actual DT cryogenic capsule effects of rarefactions launched as individual shocks break out is accounted for by scaling data from DD equation of state measurements. This is a source of uncertainty in the shock timing obtained. Plans exist to conduct VISAR experiments of shock propagation in a DT fuel layer to test the surrogacy of the DD fuels. Such tests would provide required data on species separation effects. It would also allow for an assessment of whether the adiabat of the fuel is anomalously high compared with predictions of the radiation hydrodynamics codes.

1.6.4 **New capabilities (diagnostics, models) needed** - Assuming that further analysis reinforces the need for better non-ideal fluid models in the hydro codes we should develop models that can capture the important physics without overburdening our computational resources. Adding electric fields and barodiffusion to multi-dimensional hydrocodes should be reasonably straightforward and inexpensive to run if limited to a single velocity "diffusion drag" model. Developing a non-local or multi-group model to capture the non-Maxwellian ion tail distribution and using it consistently should also be possible if limited to a nearly isotropic approximation. In the interests of speed and robustness we should probably first develop these models in the absence of magnetic fields, but it will be necessary to include magnetic fields in true multi-dimensional simulations.

An experimental measurement of electric fields in the hot spot is possible using proton radiography. This technique has been carried out in direct drive implosion experiments fielded on the Omega laser [C. K. Li, et al., Phys. Rev. Lett. 100, 225001 (2008)], where strong electric fields were reported to be measured inside the imploding capsule. We recommend proton radiography measurements of electric fields in the hot spot of capsule implosions be made on NIF. These would yield valuable information to compare with kinetic models of the aforementioned effects.

1.6.5 Long-term goals and outlook – In the long term we would like to have any kinetic model for the hot spot validated by experimental measurements**.** This seems difficult to do given the integrated nature of ignition experiments. We may have to be satisfied with models in hydro codes that can reproduce the effects seen in Fokker-Planck and PIC codes for relevant plasma conditions. By assessing the several aforementioned kinetic effects with the best existing models and codes we can resolve whether any are significant contributors to the yield discrepancy. Eliminating specific effects allows the program to focus on other hypotheses. To the extent the investigations warrant, this research direction will result in the development of non-ideal fluid models for more accurate modeling of hot spot physics and associated yields.

1.7 **Conclusions (1 page)** - The integrated modeling panel advocates the following high priority research directions:

1) Science-Based Validation Campaign

Employ hierarchical directed validation experiments which focus on crucial aspects of the fully integrated experiments. These include planar foil experiments to test ablator performance and growth of imposed perturbations. Experiments in both planar and the keyhole geometry to examine physics of stagnation for cryogenic DT or DD are also valuable.

Employ a hierarchical simulation strategy which includes a number of simulations performed at the highest possible fidelity, including high spatial resolution, high detail in the physics models employed and detailed 3D simulations.

Enhance usefulness of sensitivity analysis studies by combining with quantification of uncertainties in both inputs and measurements. Use this to discriminate which inputs and model ingredients are most for responsible uncertainties in modeling, and to help guide efforts to improve model ingredients.

Continue code-to-code comparisons, focusing on simplified problems.

2) Improved Modeling of Hohlraum Energetics

Simulate experiments using the new inline models in the hydrocodes for cross beam energy transfer and SRS and SBS backscatter.

Improve DCA NLTE kinetics, including accuracy in transition region between LTE and NLTE. Improve energy resolution of excited states. Assess more accurately the model for continuum lowering.

Test the non-local electron model against Vlasov-Fokker-Planck code on simplified geometry for plasma conditions relevant to NIF hohlraum.

Make more extensive measurements of opacities of hohlraum wall materials under NIF relevant plasma conditions.

Perform gas jet experiments to test non-local electron transport model in long scale length plasmas for NIF relevant conditions.

Experimentally measure of heat flow and electron distribution function for NIF relevant plasma conditions.

Measure plasma electron temperature and density via Thomson scattering. Simultaneously measure magnetic fields via proton radiography.

Deploy a more comprehensive set of measurements of LPI-induced energy redirection. This includes improving the spatial and temporal resolution of the FABS, and measuring backscatter on more beams.

Implement a more comprehensive and robust treatment of magnetic fields effects, including Righi-Leduc heat flow and Nernst advection.

3) Investigate Kinetic Effects on Thermonuclear Yield

Apply PIC and Vlasov-Fokker-Planck codes to study several kinetic effects and quantify their effect upon the yield. These processes include the separation of deuterium and tritium nuclei by electric fields and barodiffusion, the loss of reactive ions in the high energy tail due to several effects. Non-local transport in the hot spot and surrounding dense fuel is also of interest.

If results of kinetic simulations indicate a need, develop a reduced model for the physical effect and implement into hydrocodes for self-consistent treatment.

Conduct VISAR experiments of shock propagation in a DT fuel layer in keyhole geometry to test the surrogacy of the DD fuels. This would also provide required data on species separation effects.

Deploy proton radiography to measure electric fields in the hot spot on NIF. This will yield valuable data for comparison with kinetic models of the aforementioned effects.

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Roger Vesey
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Robert Kingham
Paula Rosen
Andy Schmitt
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Two Side-bars (with figures)

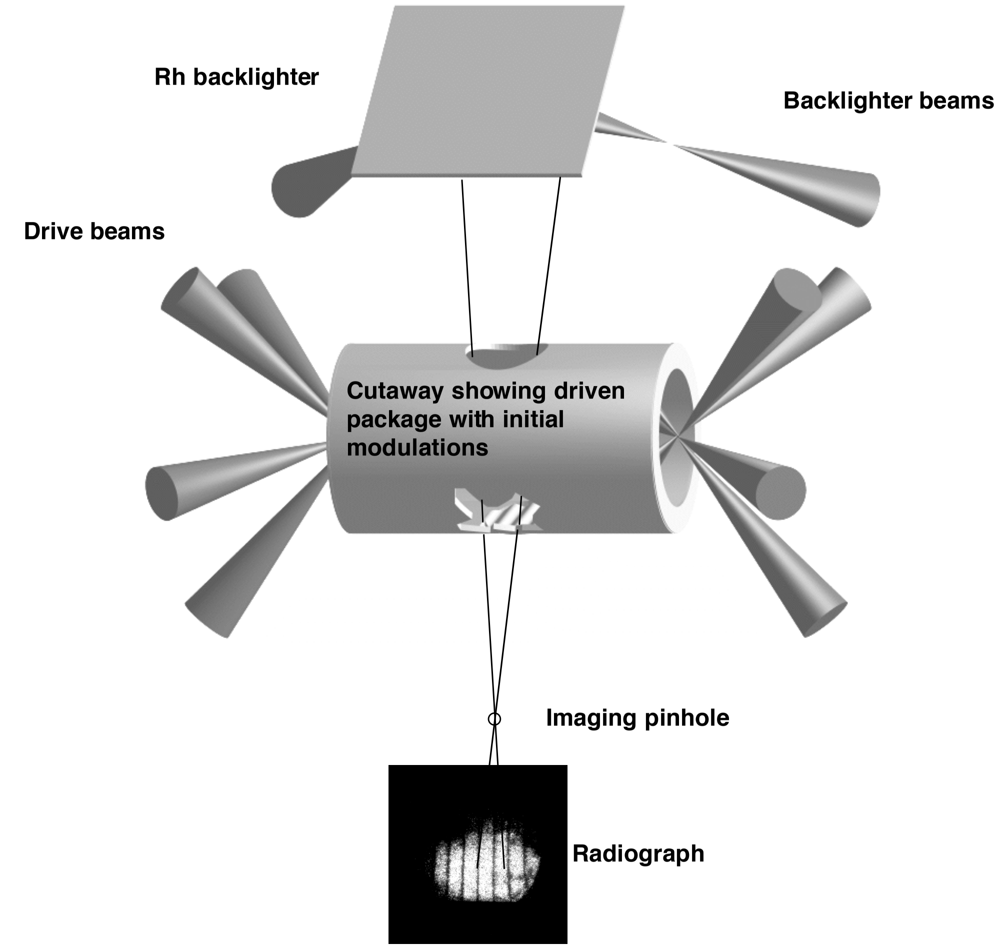
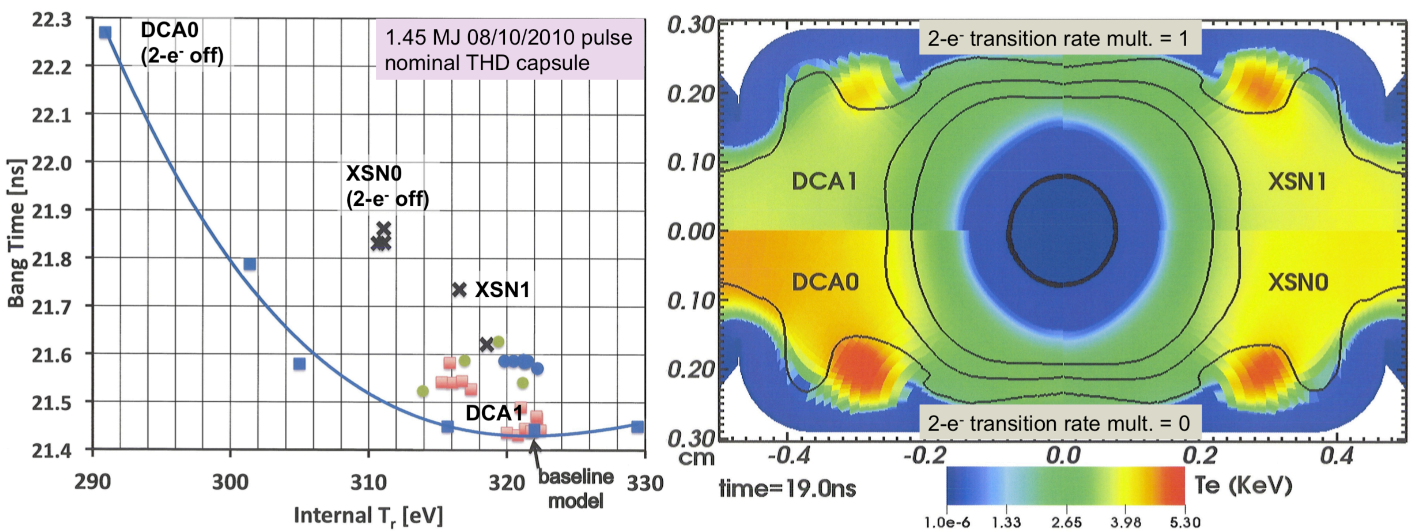
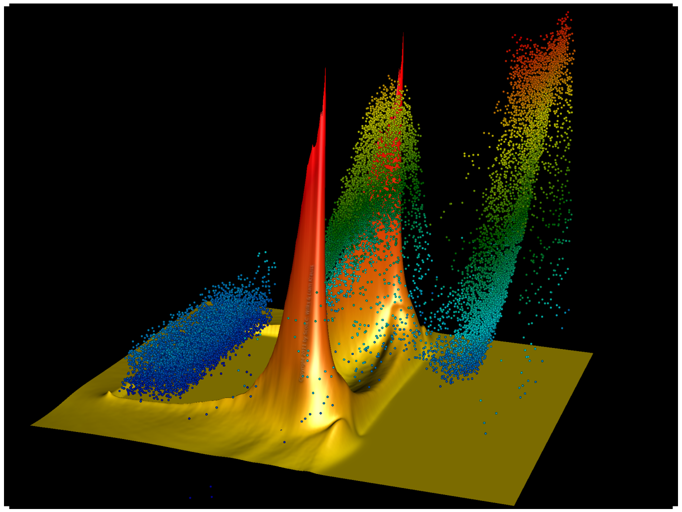


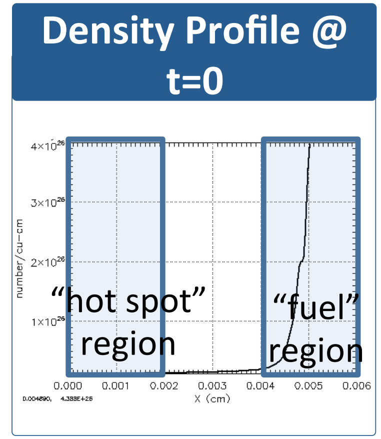
Figure 1. Schematic of the geometry for experiments with face on radiography

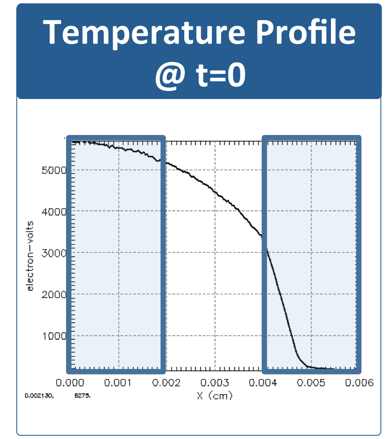
Experimental diagnostics that could help constrain NLTE modeling choices would be particularly useful given that NLTE modeling uncertainties account for at least 200 ps of the approximately 300 – 800 ps discrepancy between observed bang times and predictions.

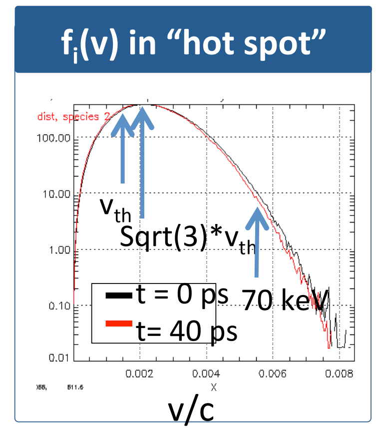


***Left**:* Figure illustrating the sensitivity of the radiation drive and predicted bang times to NLTE modeling parameter variations. Each point represents the result of a 2D integrated HYDRA hohlraum simulation of a nominal NIF target. Justifiable variations (e.g. dielectronic recombination (DR) rate multiplier of 0.1-2.0) can result in ~200 ps delays in bang times, bringing them closer to the measurements which typically come in over 400 ps later than predicted. The solid line fits through points in which the DR rate multiplier varies from 0.0 to 2.0. ***Right**:* Electron temperature maps taken from simulations corresponding to the 4 labeled points in the figure on the left. The solid lines indicate material boundaries. The top left (DCA1) corresponds to the current baseline model, while the map below (DCA0) shows the effect of turning off DR. The same variations for XSN are shown on the right, with XSN0 representing the old Point Design XSN model. The plasma conditions from the integrated simulations are used to obtain spectra of the backscattered light that can be compared with measurements. (Source: LLNL/M.V. Patel)









Left: Electric field (surface plot) driven by laser light accelerating bunches of particles as they move through and exit a target in a simulation performed with the LSP PIC code. Particle height indicates particle energy. The PIC simulation resolves particles both in physical and velocity space with self-consistent electric and magnetic fields. **Right:** Top plots show radial electron density and temperature profiles respectively representing conditions in the hot spot of an ignition capsule. Bottom plot shows evolution of deuterium ion velocity distribution function in hot spot at 0 and 40 psec from LSP simulation. Slight depletion of the tail ions results from energetic ions escaping the hot spot. LSP simulation can assess the affect upon fusion reactivity.