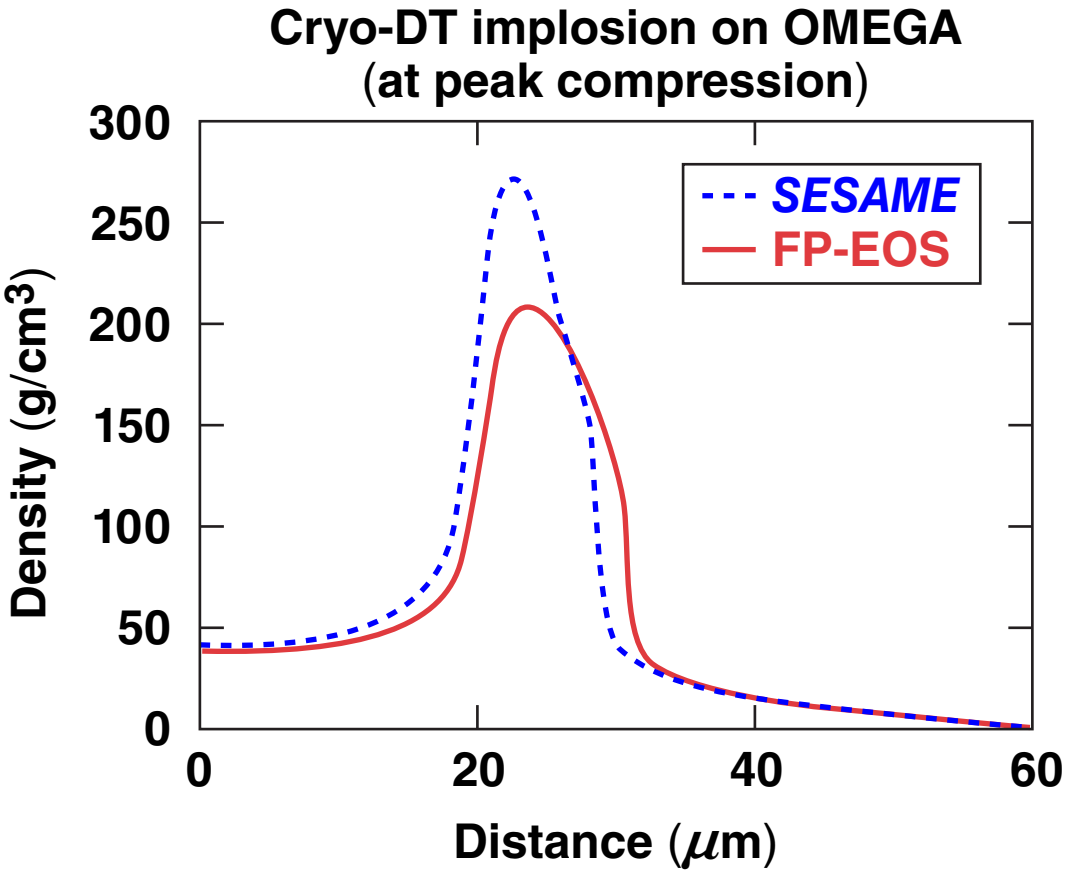
Theoretical Investigation of Strong Coupling and Degeneracy Effects in ICF Implosions



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Summary

An equation-of-state table of deuterium from first-principles calculations has been established and has indicated significance in ICF implosions

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- We have established a first-principles equation-of-state (FP-EOS) table for deuterium, using the restricted path-integral Monte Carlo (PIMC) method, which covers typical ICF fuel conditions of $\rho \approx 0.002 \sim 673$ g/cm^3 and $T \approx 1.35$ eV ~ 5.5 keV
- The FP-EOS table shows discrepancies in pressures and energies in the moderate coupling ($\Gamma \geq 1$) and degenerate ($\theta \leq 1$) regimes when compared to the *SESAME* table
- Hydrodynamics simulations of cryogenic ICF implosions using the FP-EOS table have indicated significant differences in peak density, ρR, and neutron yield relative to *SESAME*-EOS simulations

Collaborators

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Low-adiabat ICF implosion designs routinely access to strongly coupled and degenerate plasma conditions!

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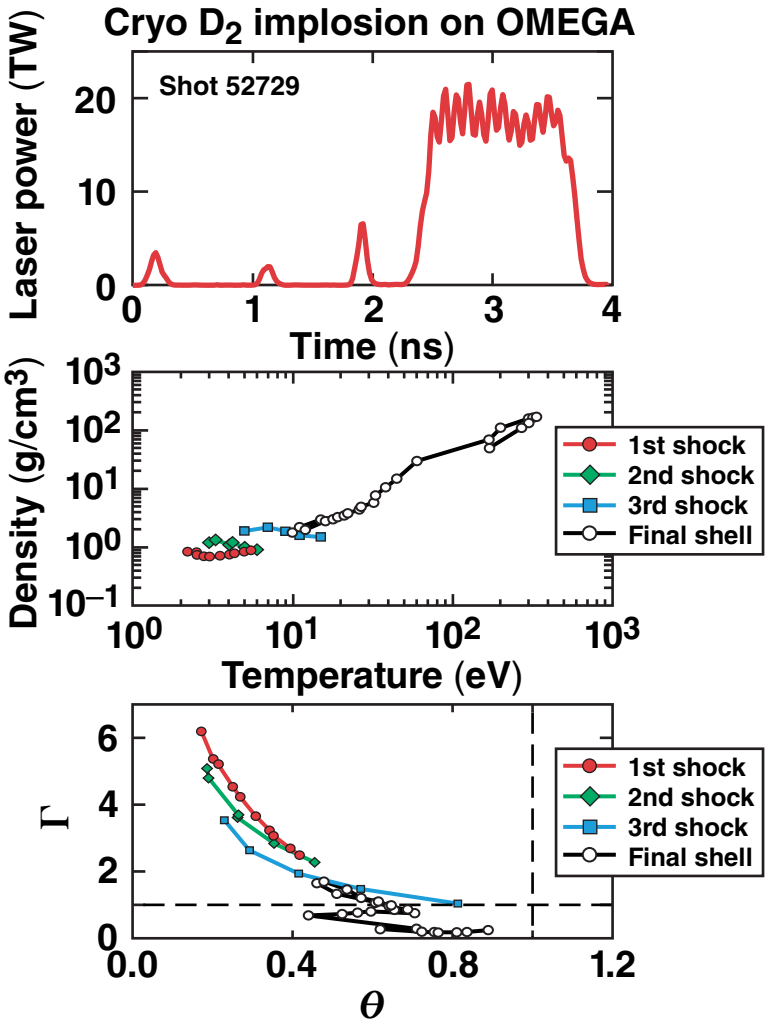

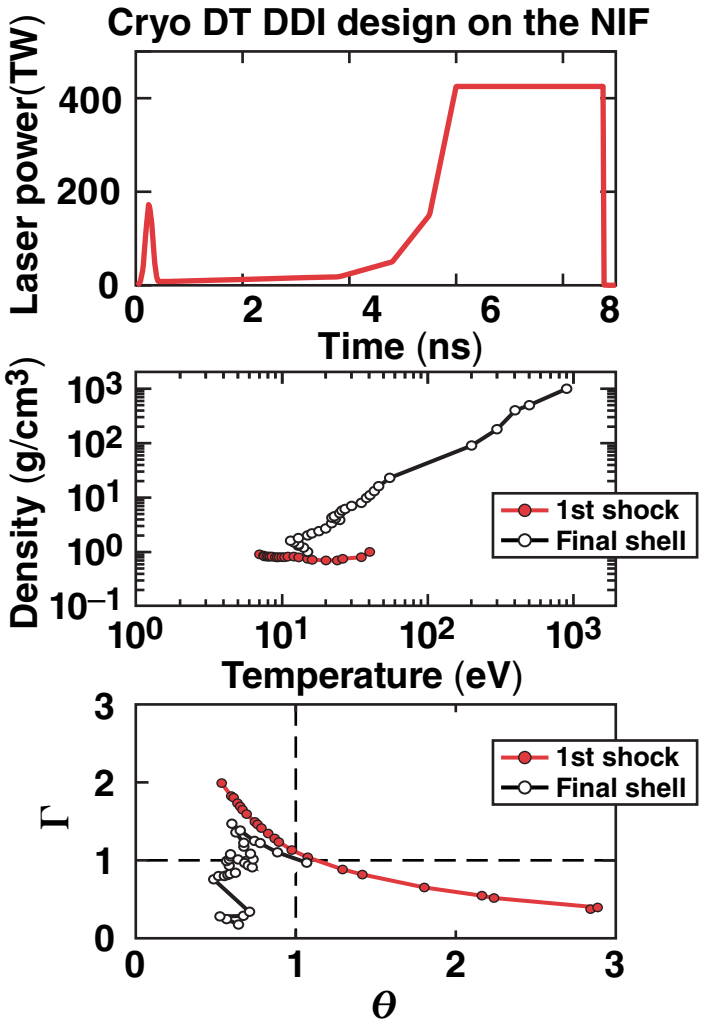

$\Gamma = 1/a\ kT$, a – the Wigner–Seitz radius
$\theta = T/T_F$, T_F – the Fermi temperature

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The *SESAME*-EOS table is based upon the "chemical model" of matter*, which does not fully account for strong-coupling and degeneracy effects

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The essential physical models in the *SESAME*-EOS table:

- The molecular solid phase: is valid only in low-T and not-too-high density ($\rho \leq 4$ g/cm^3) regimes where molecular identity still exists.
- The atomic solid phase: The zero-Kelvin cold curve used in the atomic-solid model is still uncertain*.
- The molecular/atomic fluid phase: The first-order expansion was used in the liquid perturbation theory to only account for the nearest neighbor interactions.

→ Strong-coupling and many-body degeneracy effects are not fully accounted.

*G. I. Kerley, SAND2003-3613 Report.

The first-principles method of path-integral Monte Carlo (PIMC) was used to calculate the FP-EOS of deuterium

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- For a many-body system in thermal equilibrium at temperature T, the density matrix $\rho(R,R';T)$ uniquely contains all thermodynamic information of the system; $\rho(R,R';T)$ is defined as (in configuration representation)

$$\rho(R,R';T)=\left\langle R\left|e^{-\vec{H}/kT}\right|R'\right\rangle=\sum_n \varphi_n(R)\,\varphi_n(R')\,e^{-E_n/kT} \qquad \left(\vec{H}\varphi_n=E_n\varphi_n;\vec{H}=\vec{K}+\vec{V}\right)$$

- Using the convolution property of $\rho(R,R';\beta)$, one can compute the density matrix from high-T ρ_0

$$\rho(R,R';\beta)=\int dR_1 dR_2 \ldots dR_{M-1}\,\rho_0(R,R_1;\Delta\beta) \times\rho_0(R_1,R_2;\Delta\beta)\ldots\rho_0(R_{M-1},R';\Delta\beta)$$

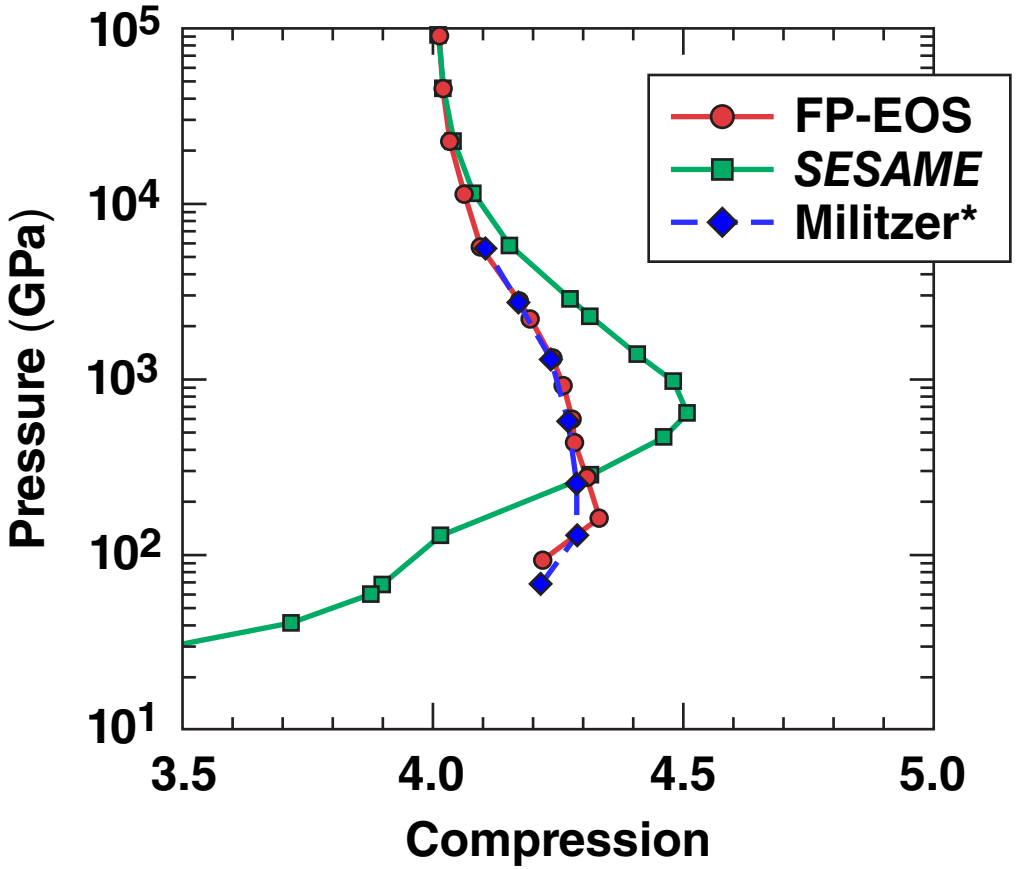
with $\rho_0(R_i,R_{i+1};\Delta\beta)=\exp\left[\frac{-\pi}{\lambda_\Delta^2}(R_i-R_{i+1})^2+\Delta\beta\times V(R_i)\right]$, $\beta=1/kT$, $\Delta\beta=\beta/M$,

and $\lambda_D=\sqrt{2\pi\hbar^2\Delta\beta/m}$ is the DeBroglie wavelength

- Once we know $\rho(R,R';\beta)$, we can calculate the thermodynamic properties of the system with the corresponding operators $\hat{O}$:

$$\langle\hat{O}\rangle=\frac{\int dR dR'\left\langle R\left|\hat{O}\right|R'\right\rangle\left\langle R'\left|\rho(\beta)\right|R\right\rangle}{\int dR\left\langle R\left|\rho(\beta)\right|R\right\rangle}$$

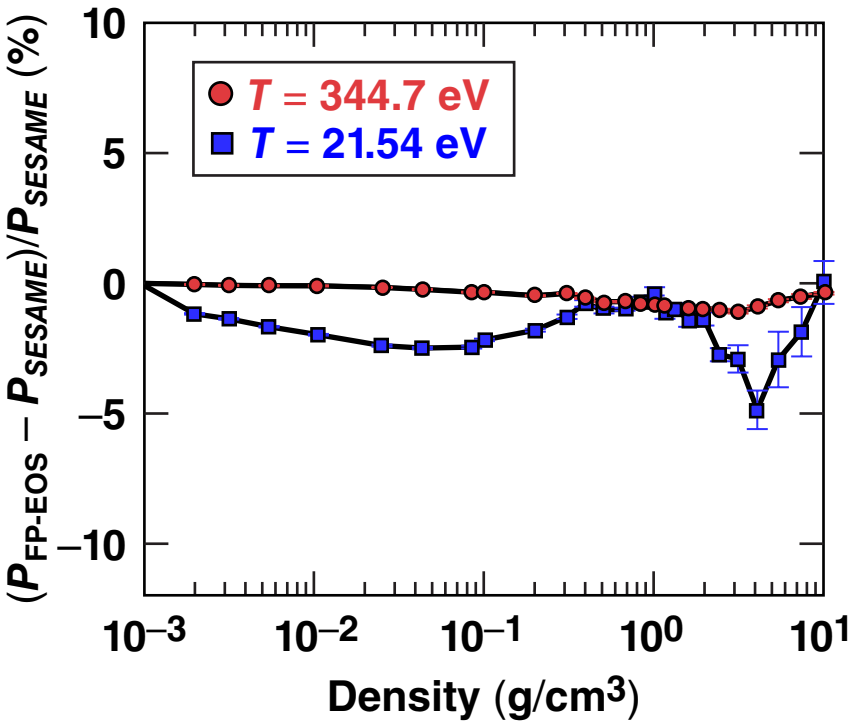
The principal Hugoniot comparison shows that deuterium is slightly softer under ~2 Mbar, but stiffer in FP-EOS than *SESAME* for ~2 Mbar < *P* < ~100 Mbar

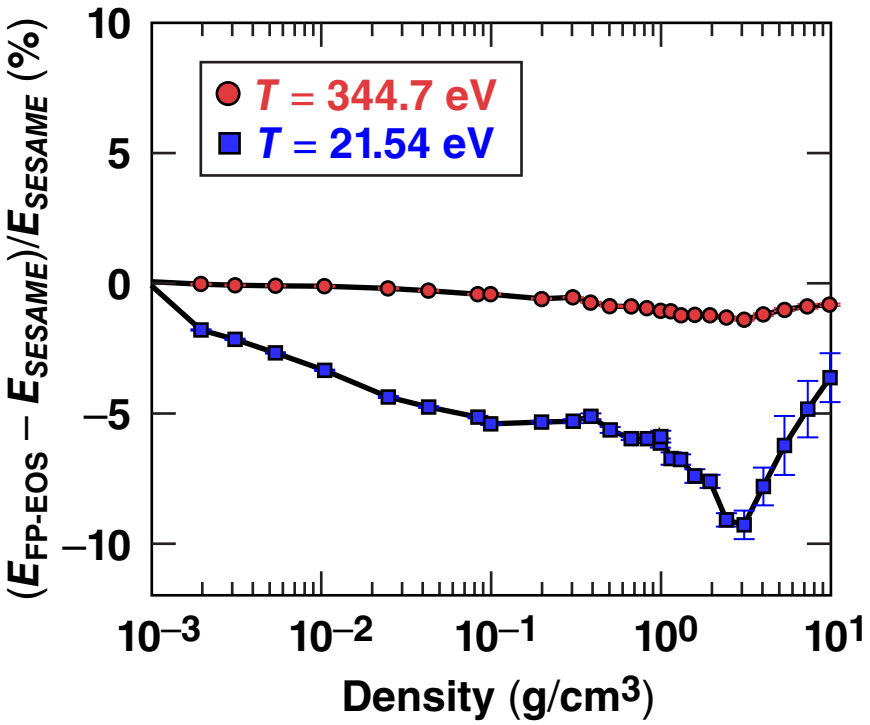


The Hugonoit: $E_f - E_i + 0.5 \times (P_f + P_i) \times (V_f - V_i) = 0$

*B. Militzer and D. M. Ceperley, Phys. Rev. Lett. 85, 1890 (2000).

In comparison to the *SESAME* table, the FP-EOS table has shown large differences, especially in internal energy





The FP-EOS table covers typical fuel conditions of $\rho \approx$ 0.002 ~ 673 g/cm^3 and $T \approx$ 1.35 eV ~ 5.5 keV.

Hydro-simulations of low-adiabat implosions using the FP-EOS has indicated significant differences in ρ_{peak}, ρR, and neutron-yield compared to *SESAME* simulations

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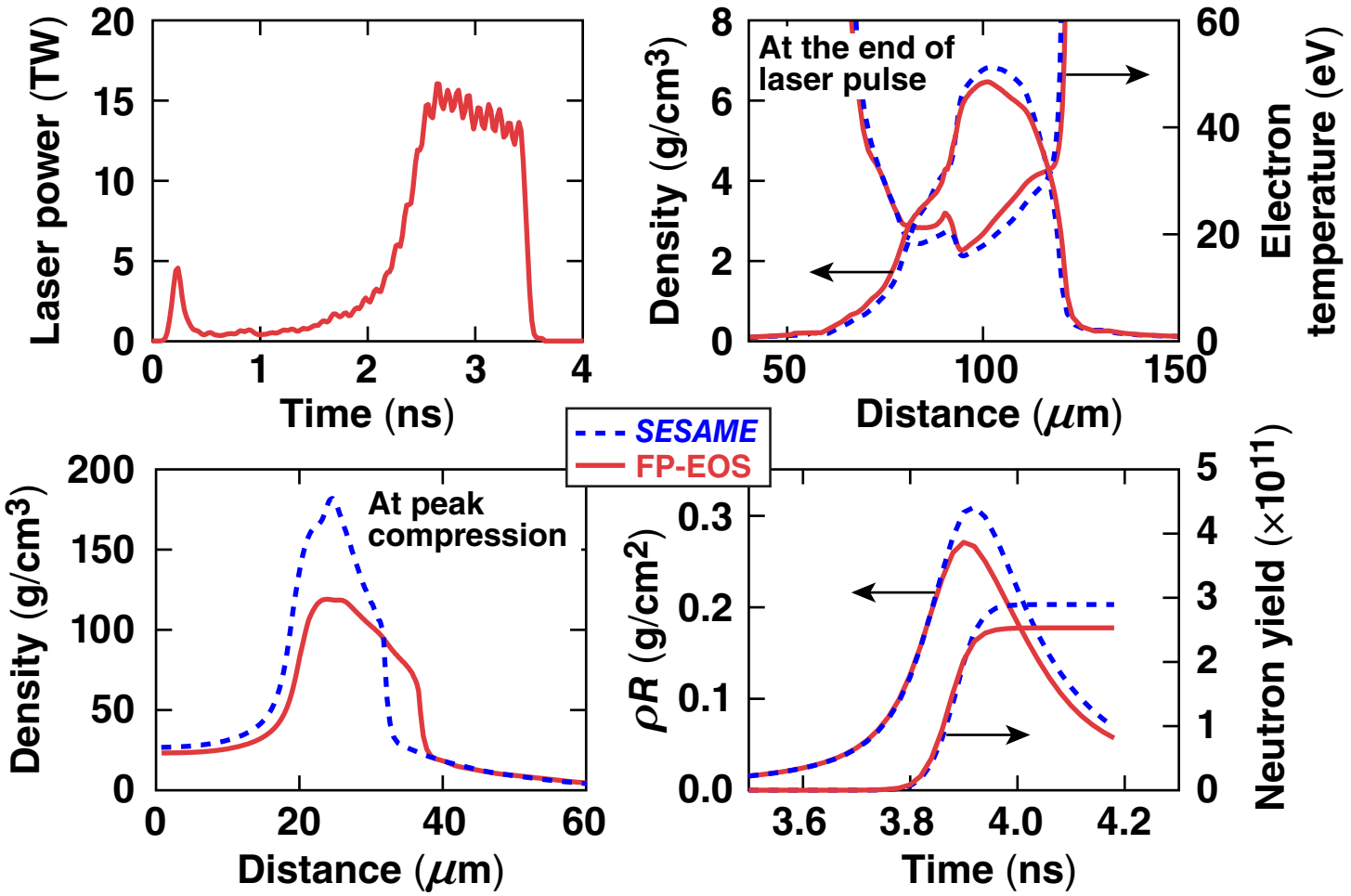
Target: 10-μm CD shell
78-μm D_2 ice
341-μm D_2 gas



SESAME: ρ_{peak} = 182 g/cm^3, ρR = 307 mg/cm^2, Yield = 2.9 × 10^{11}
FP-EOS: ρ_{peak} = 119 g/cm^3, ρR = 268 mg/cm^2, Yield = 2.5 × 10^{11}

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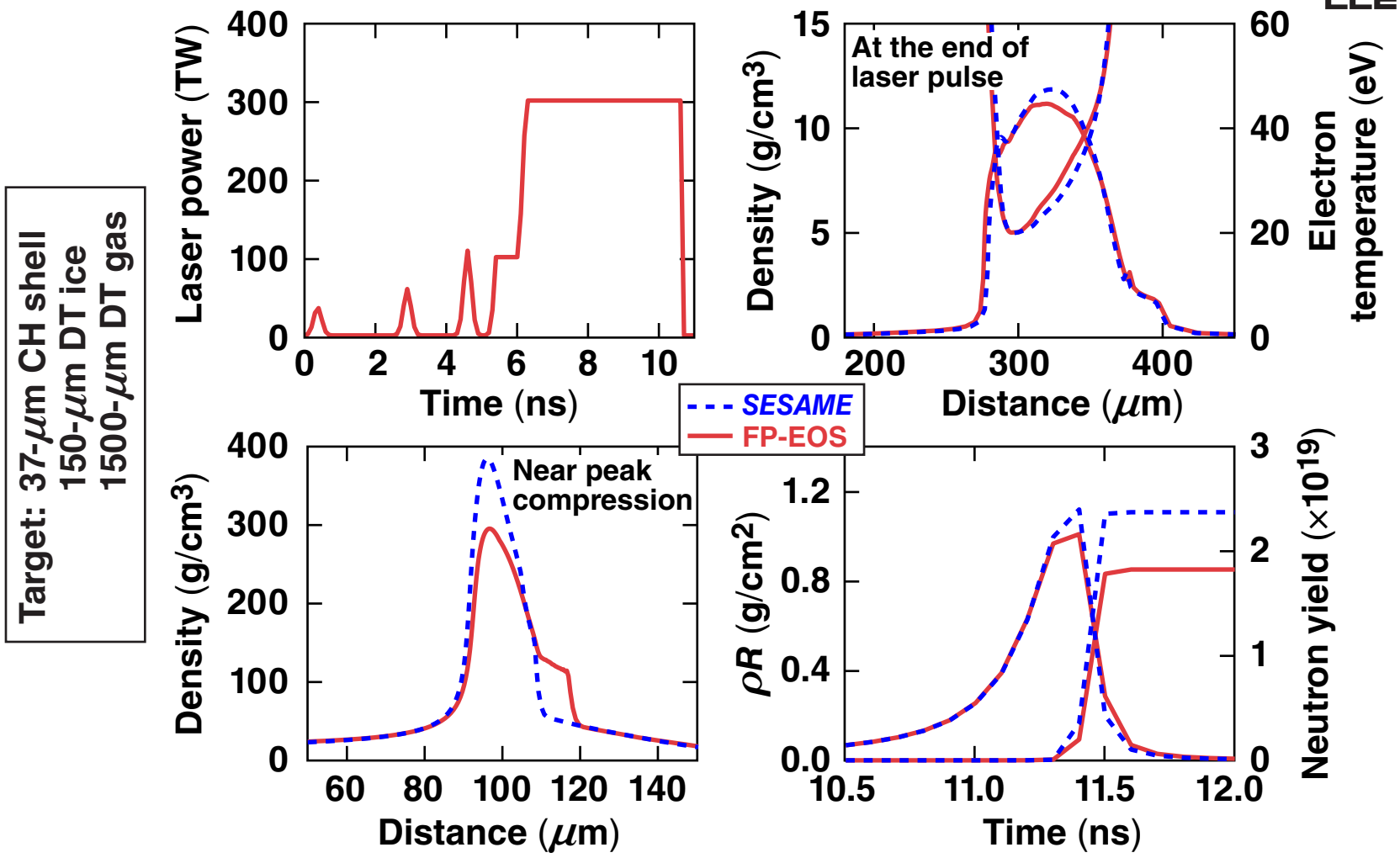
Simulations for NIF direct-drive designs also show significant differences in peak density, yield, and gain



SESAME: ρ_{peak} = 383 g/cm^3, ρR = 1.1 g/cm^2, Yield = 2.4 × 10^{19}, Gain = 45
FP-EOS: ρ_{peak} = 294 g/cm^3, ρR = 1.0 g/cm^2, Yield = 1.8 × 10^{19}, Gain = 34

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Summary/Conclusions

An equation-of-state table of deuterium from first-principles calculations has been established and has indicated significance in ICF implosions

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