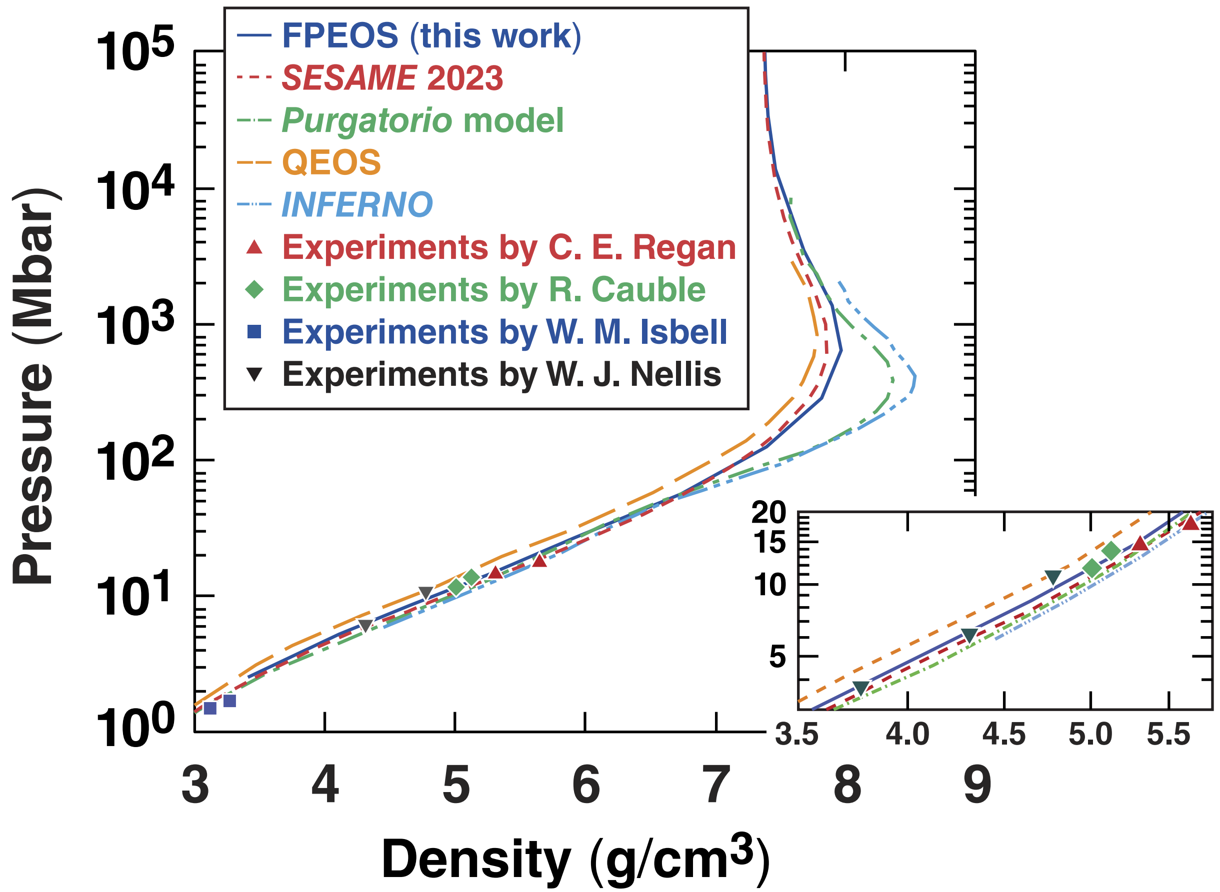
Density-Functional-Theory–Based Equation-of-State Table of Beryllium for Inertial Confinement Fusion Applications



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Summary

An accurate equation-of-state (EOS) table of beryllium has been built from first-principles calculations

- Based on density-functional-theory (DFT) calculations, we have established a wide-range beryllium EOS table of density $\rho = 0.001$ to $\rho = 500$ g/cm^3 and temperature $T = 2000$ to 10^8 K
- The first-principles equation-of-state (FPEOS) table is in good agreement with the widely used *SESAME* EOS table (*SESAME* 2023), but shows a 10% difference in maximum compressibility from *Purgatorio*
- By implementing the FPEOS table into our hydrocodes, we show that the FPEOS simulation predicts a higher neutron yield (~15%) compared to the simulation using the *SESAME* 2023 simulations

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Combining orbital-based DFT and orbital-free molecular dynamics (OFMD), we have investigated wide-ranged EOS tables of beryllium

- Previous FPEOS studies on D_2, CH, and Si show a significant difference from *SESAME* 2023

- As an inertial confinement fusion (ICF) ablator, accurate properties of beryllium under such extreme conditions are essential for designs

- Theoretical EOS models may not provide an accurate EOS in the warm-dense-matter (WDM) regime, where both strongly coupled ($\Gamma > 1$) and degeneracy effects ($\theta < 1$) are important*

- Quantum molecular dynamics (QMD),* based on DFT, has proven to work well for EOS calculations**

*L. Collins *et al.*, Phys. Rev. E 52, 6202 (1995).
**L. X. Benedict *et al.*, Phys. Rev. B 89, 224109 (2014).

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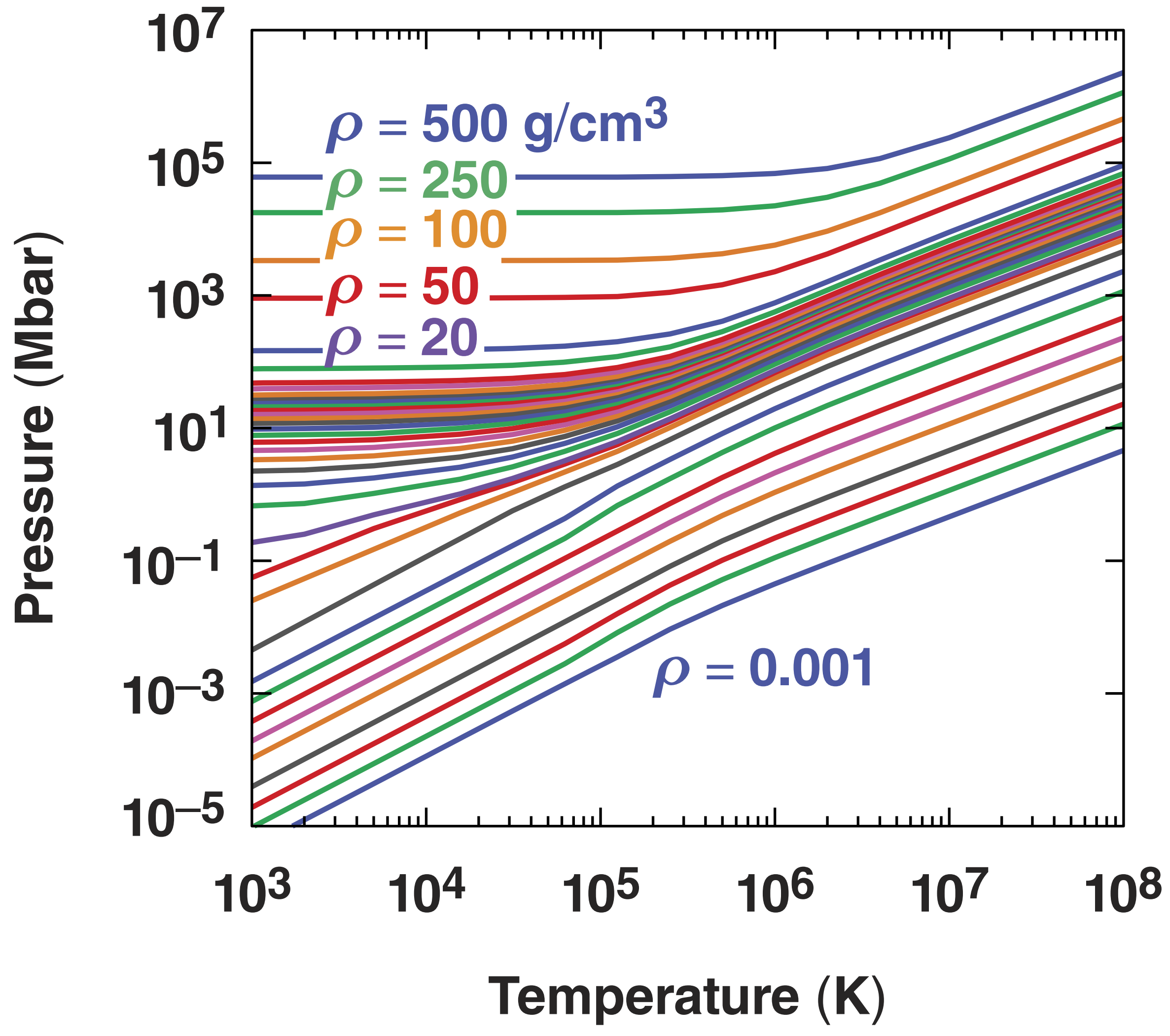
The FPEOS of beryllium has been calculated for densities and temperatures from ρ = 0.001 g/cm^3 to ρ = 500 g/cm^3 and T = 2000 K to 10^8 K



Y. H. Ding and S. X. Hu, Phys. Plasmas 24, 062702 (2017).

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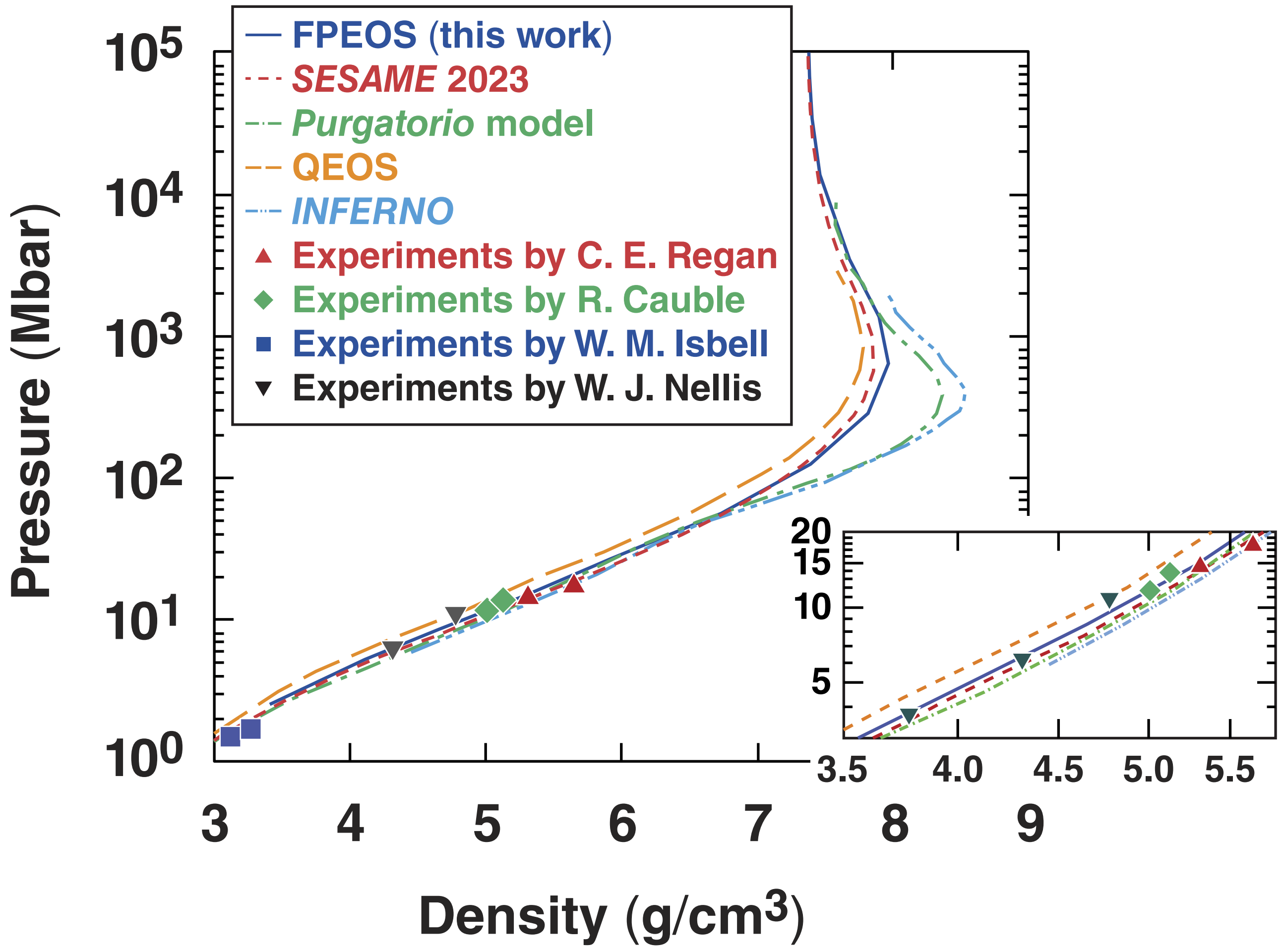
The calculated principal shock Hugoniot of beryllium from FPEOS has been compared with other theoretical models and experiments



The FPEOS Hugoniot pressure of beryllium is in good agreement (within 10%) with the widely used *SESAME* model (*SESAME* 2023) in the low-compression-ratio region; the pressure differences can be up to 30% in the high-compression region.

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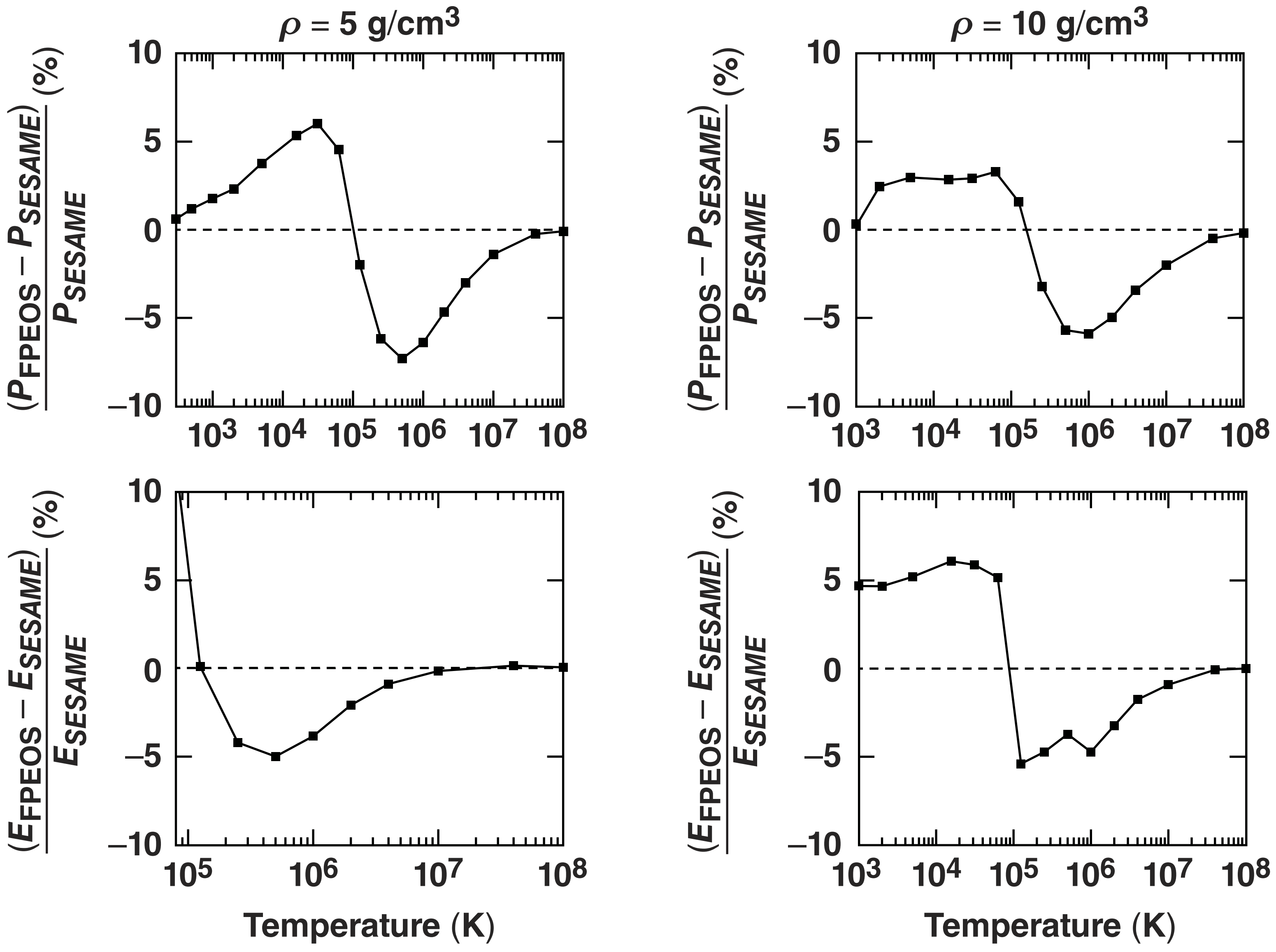
The off-Hugoniot equation of state is compared between FPEOS and *SESAME* at certain densities



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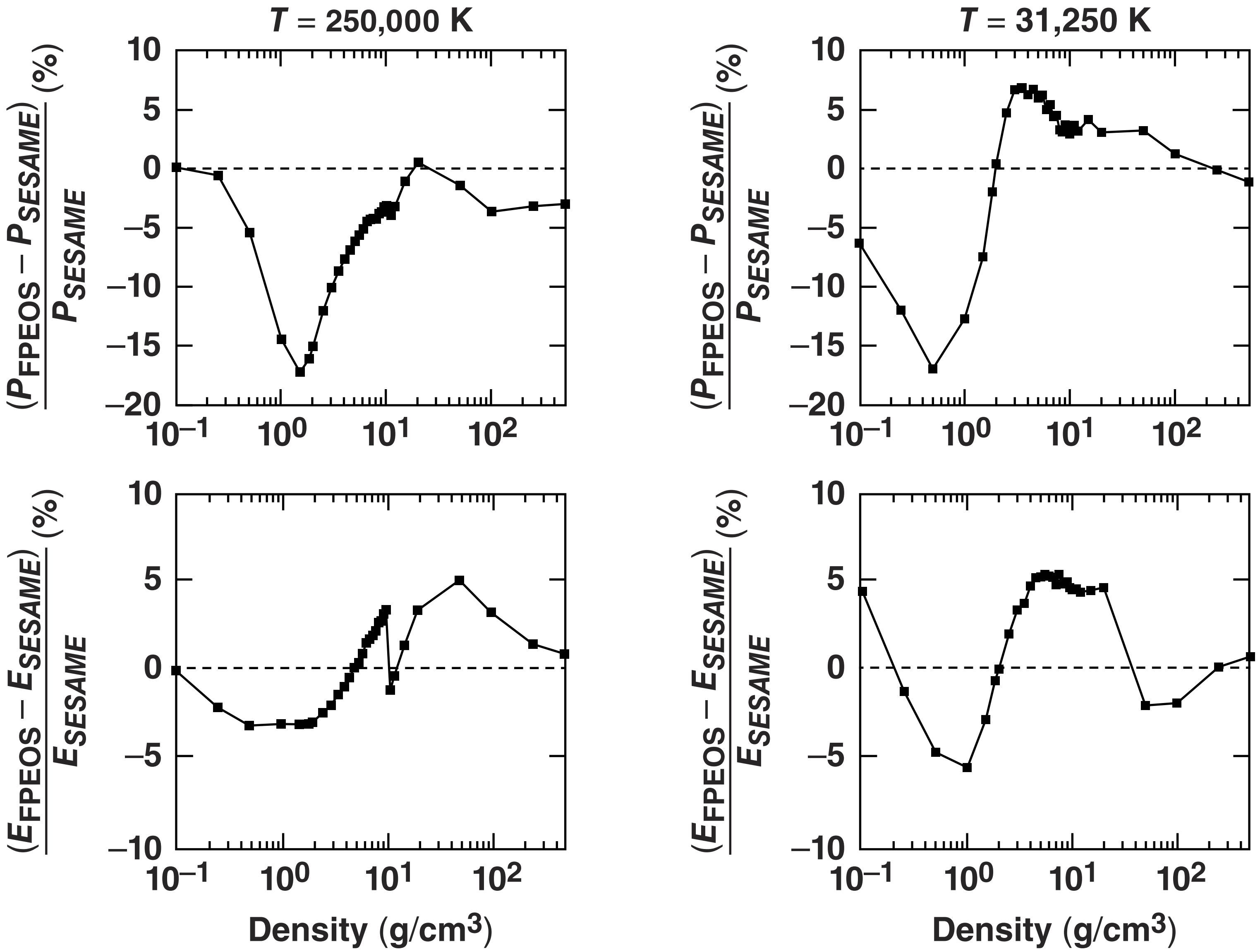
In the WDM regime the difference between FPEOS and *SESAME* 2023 can reach a maximum of 20%



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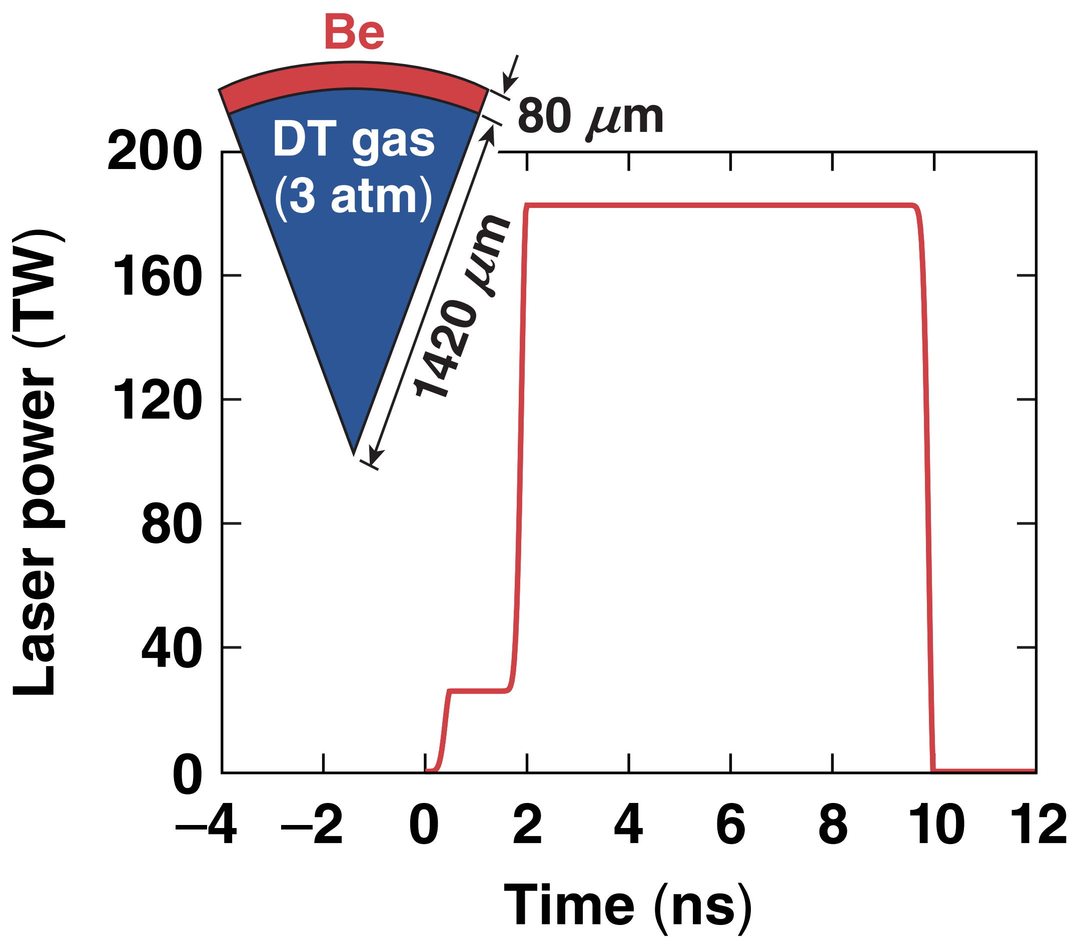
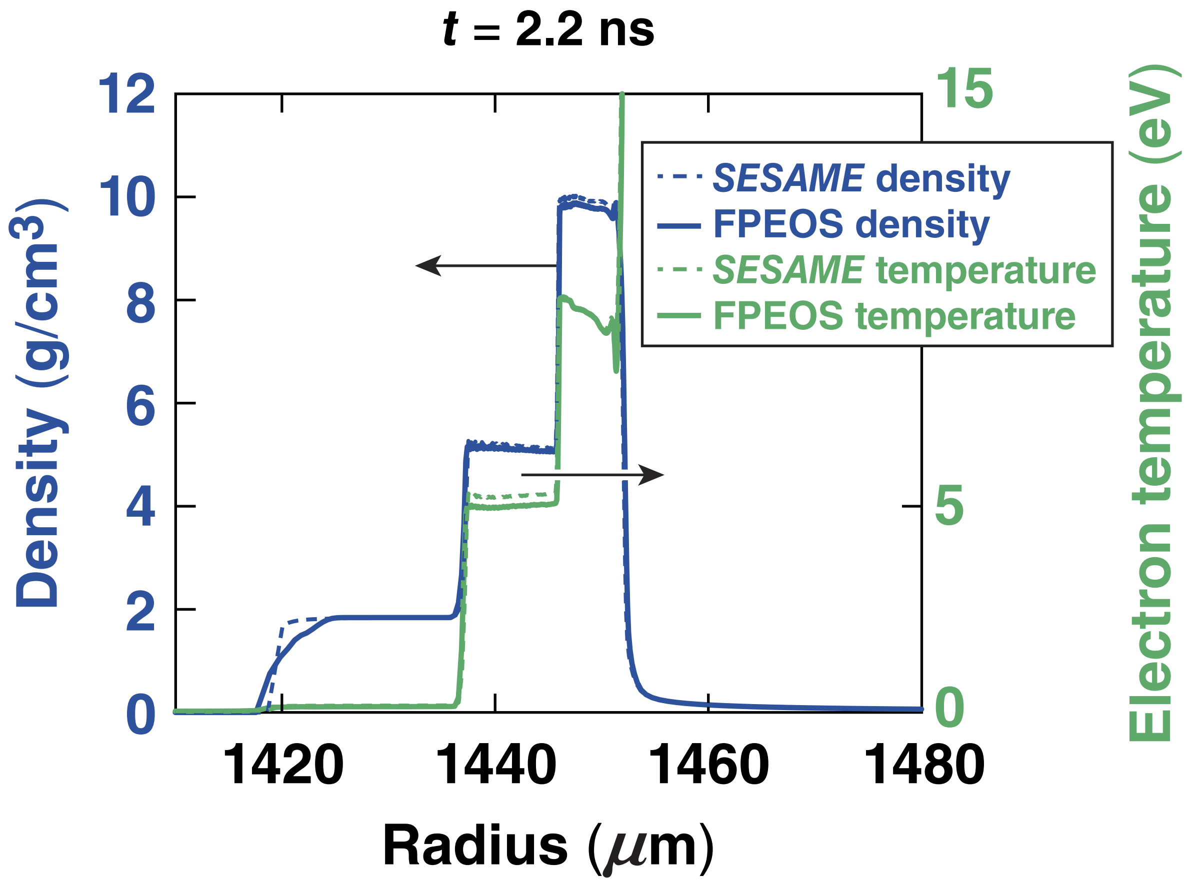
The implication of Be FPEOS for ICF designs has been examined





For DT, two gas simulations used the same FPEOS table and the first-principles opacity table.

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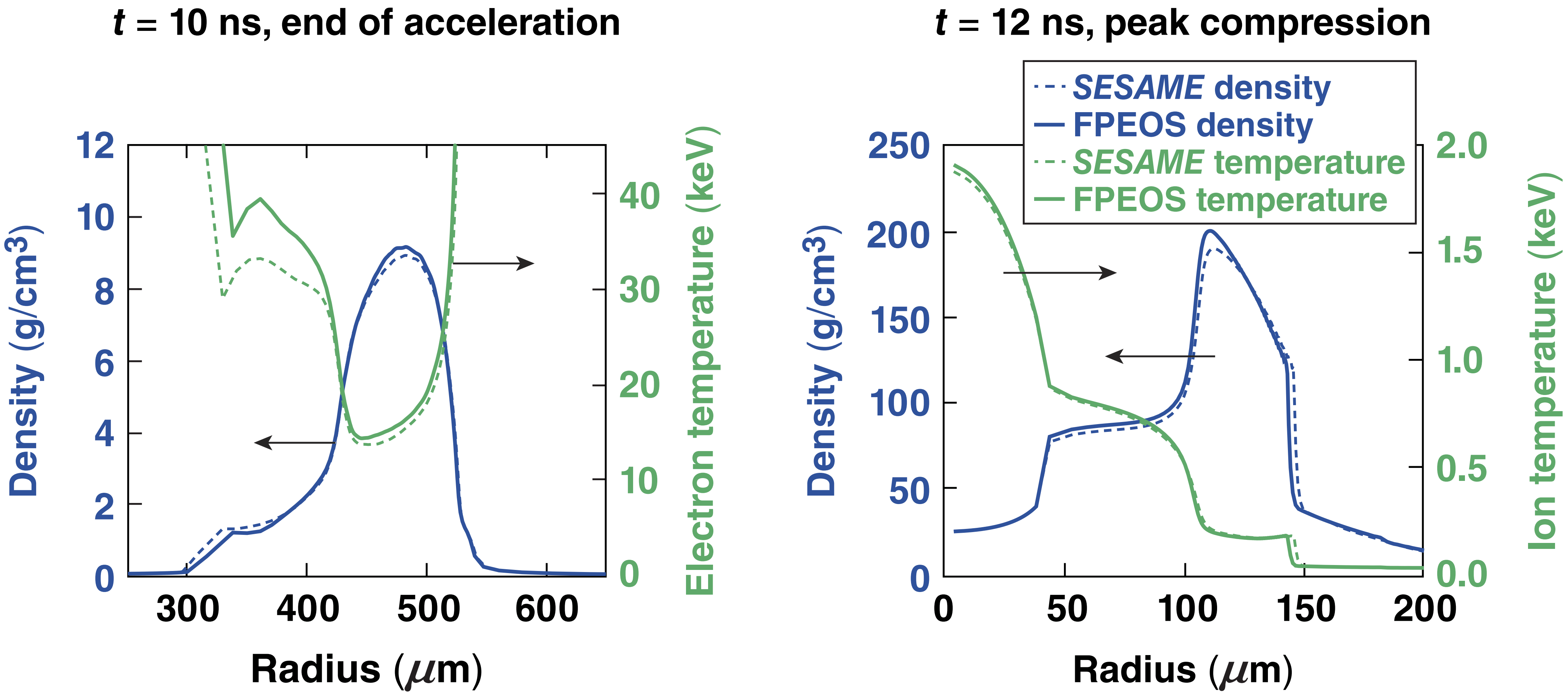
The FPEOS simulation predicted ~15% higher neutron yield than the *SESAME* simulation



This small difference between FPEOS and *SESAME* in hydro simulations is consistent with their good agreement with the Hugoniot.

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Summary/Conclusions

An accurate equation-of-state (EOS) table of beryllium has been built from first-principles calculations

- **Based on density-functional-theory (DFT) calculations, we have established a wide-range beryllium EOS table of density ρ = 0.001 to ρ = 500 g/cm^3 and temperature T = 2000 to 10^8 K**
- **The first-principles equation-of-state (FPEOS) table is in good agreement with the widely used *SESAME* EOS table (*SESAME* 2023), but shows a 10% difference in maximum compressibility from *Purgatorio***
- **By implementing the FPEOS table into our hydrocodes, we show that the FPEOS simulation predicts a higher neutron yield (~15%) compared to the simulation using the *SESAME* 2023 simulations**

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