Optimizing proton–boron-11 fuel for fast ignition inertial fusion applications

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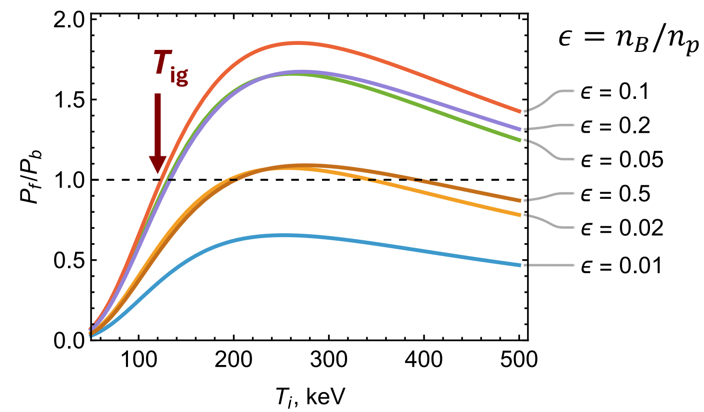
OUTLINE

- **Proton Boron compounds**
- **Implosion of spherical targets**
- **1D code verification for implosion**
- **Optimization methods**
- **Results**
- **Conclusions**

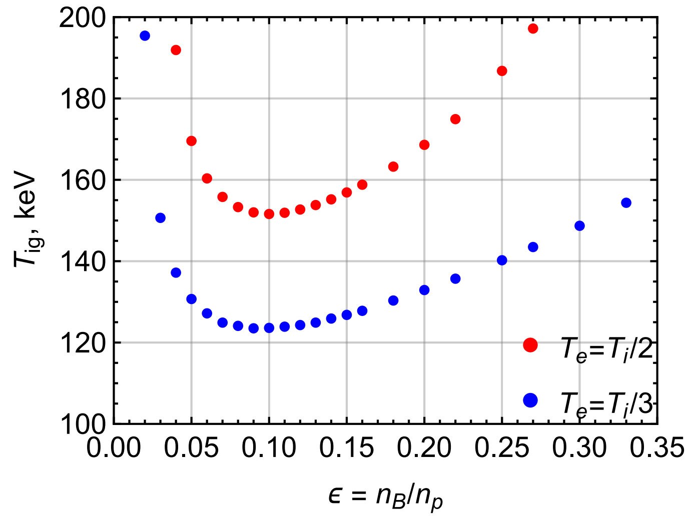
Formula	Crystal System	n_B/n_p	Z_{eff}	T_{ig}, keV
B_2H_8	monoclinic	0.25	3.22	140
B_2H_7		0.29	3.35	146
B_4H_{12}	monoclinic	0.33	3.50	155
$B_{16}H_{40}$	monoclinic	0.40	3.67	170
B_2H_5	trigonal	0.40	3.67	170
$B_{20}H_{44}$	monoclinic	0.45	3.78	185
B_2H_4	monoclinic	0.50	3.86	202
B_3H_6	cubic	0.50	3.86	202
B_4H_8	monoclinic	0.50	3.86	202

* $T_e = T_i/3$



Synthetised and tested

Formula	Crystal System	n_B/n_p	Z_{eff}	T_{ig}, keV
B_2H_6	monoclinic, hexagonal	0.33	3.50	155
$B_{10}H_{14}$	monoclinic	0.71	4.13	–
$B_{18}H_{22}$	monoclinic, orthorhombic	0.82	4.21	–

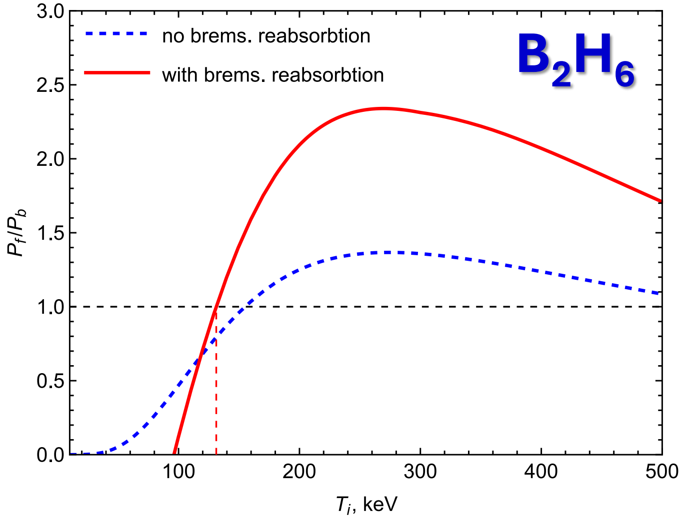


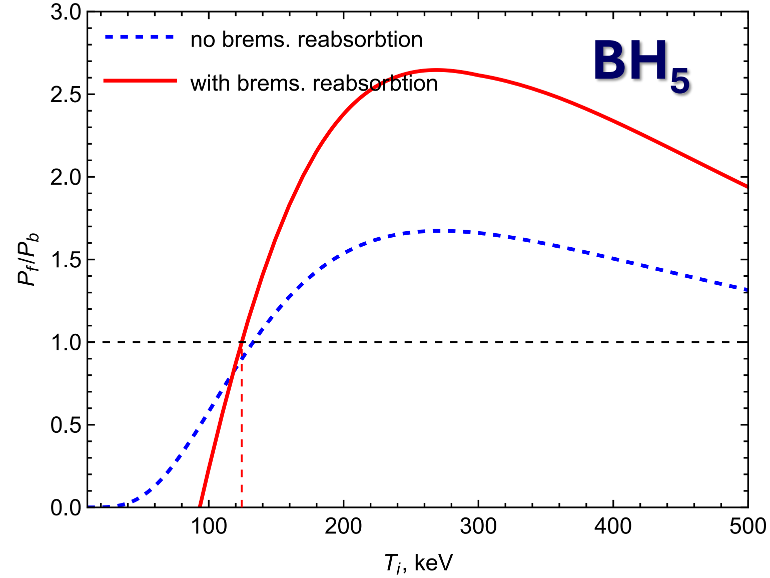
Study of possible target materials: Li-B-H systems*

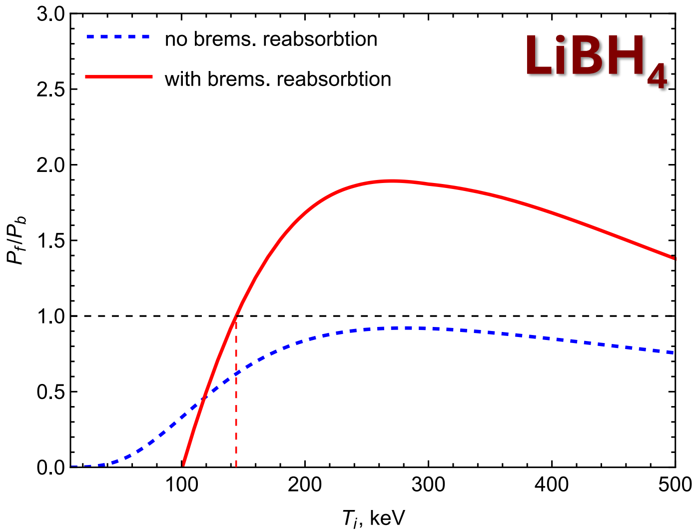
Formula	Crystal System	*n*(Li)/*n*(B)	*n*(B)/*n*(H)	Zeff	Tig, keV
$Li_2B_6H_{24}$	trigonal	0.33	0.25	3.20	162
LiB_2H_8	orthorhombic	0.50	0.25	3.19	177
$Li_2B_4H_{16}$	monoclinic, orthorhombic	0.50	0.25	3.19	177
LiB_4H_{12}	cubic	0.25	0.33	3.46	180
$LiBH_6$	monoclinic	1.00	0.17	2.86	186
$Li_2B_2H_{10}$	orthorhombic	1.00	0.20	3.00	212
LiB_3H_8	orthorhombic	0.33	0.38	3.54	217
$Li_2B_6H_{16}$	orthorhombic	0.33	0.38	3.54	217
LiB_2H_6	triclinic	0.50	0.33	3.42	232
$Li_2B_4H_{12}$	orthorhombic	0.50	0.33	3.42	232
LiB_2H_4	monoclinic	0.50	0.50	3.71	-
$Li_2B_2H_8$	monoclinic, triclinic, orthorhombic, hexagonal	1.00	0.25	3.17	-
$Li_4B_4H_{16}$	monoclinic, orthorhombic	1.00	0.25	3.17	-
$LiBH_4$	cubic	1.00	0.25	3.17	-

* **Data from NOMAD Lab and Materials Project which represent user-contributed raw simulation results obtained by DFT and quantum chemistry methods**

Ignition parameters considering bremsstrahlung reabsorption







Electron-to-ion temperature ratio:
$T_e = T_i/3$

Suprathermal effects:
20% for B-H compounds,
16% for Li-B-H compounds

The bremsstrahlung reabsorption ratio is estimated using 1D HELIOS hydro code and PROPACEOS opacity tables

Target designs

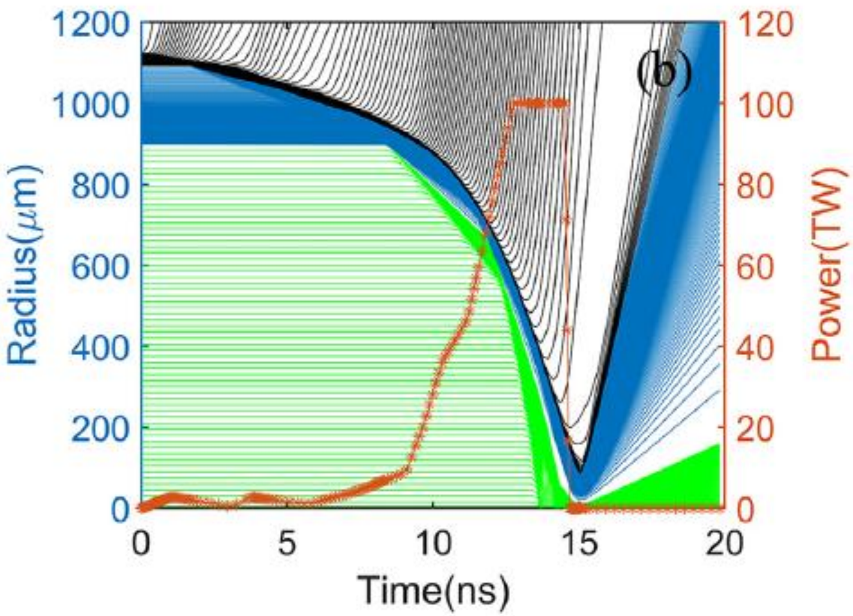
Materials	Melting temperature	Ignition energy	Neutron flux	Fuel gain isochoric, α = 1	Mass density, g/cc
$LiBH_4$	550 K	> 1 GJ	Very low	< 5	> 4000
B_2H_6	108.3 K	> 1 GJ	Very low	< 5	> 4000
BH_5	?	300 – 500 MJ	Very low	< 10	4000
$B_2(DT)_3$ + pB shell	108.3 K	30 – 150 kJ	Moderate	500 – 600	800 – 1500
DT gas + $B_2(DT)_3$ + pB shell	108.3 K	10 – 50 kJ	Moderate	500 – 650	700 – 1500
Solid DT + pB shell	19.8 K	0.5 – 10 kJ	Moderate	900 – 1500	500 – 1500
$B_2(DT)_3$	108.3 K	30 – 150 kJ	High	1200 – 1300	800 – 1500
DT gas + $B_2(DT)_3$	108.3 K	10 – 50 kJ	High	1300 – 1400	700 – 1500
DT gas + Solid DT	19.8 K	0.5 – 10 kJ	High	4700 – 7100	300 – 800

Towards Simulation of a Spherical Implosion

Main Considerations

Laser profile

- Pulse duration
- Beam parameters: (wavelength, focus position)
- Laser beam temporal profile



Target structure

- Geometry
- Regions (numbers and type)
- Mass density
- Temperature

Particle beam

- Type
- Power
- Time

HELIOS 1D code

- 1-D hydrodynamic code for planar, cylindrical, and spherical geometries
- Different temperatures of electrons and ions with ion-electron energy transfer
- Plasma thermal conduction (electrons)
- DT and $p^{11}B$ fusion

Helios

PRISM Computational Sciences, Inc.

Geometry: **spherical**

EOS & Opacity: **PROPACEOS**

Thermal conductivity: **Spitzer**

Hydro: $T_i \neq T_e$

Fusion: **off** in most cases

Codes compared

MULTI-IFE

Hydra

ILESTA-1D

Optimization methods

What is a good optimizer?

What is our choice?

efficient implosion → Designing an optimal laser profile and target structure

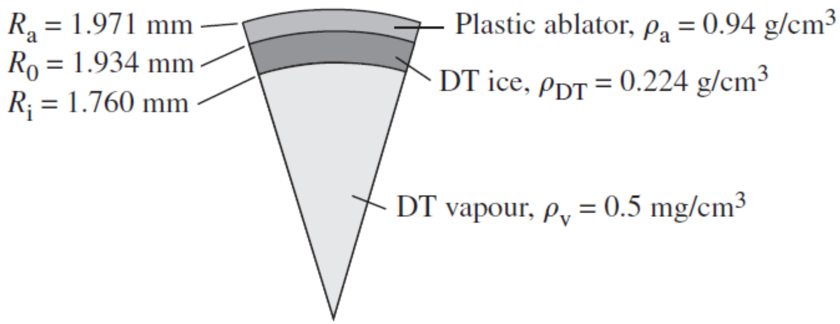
Different optimization methods

Theory / manual / algorithms

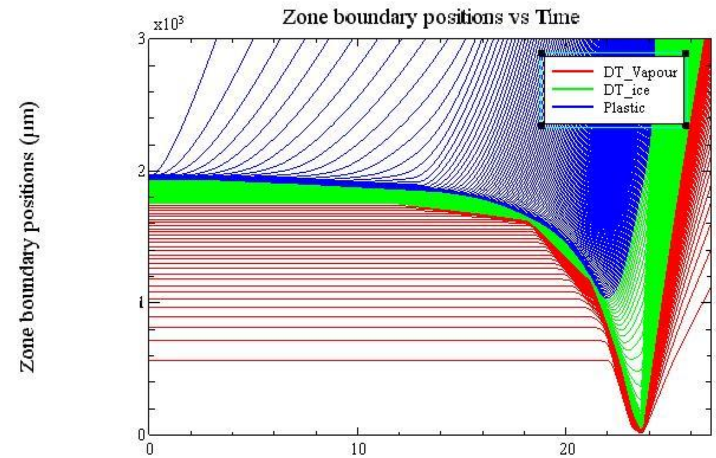
provide the ability significantly cut down on computational time and costs associated with the search for optimal target designs

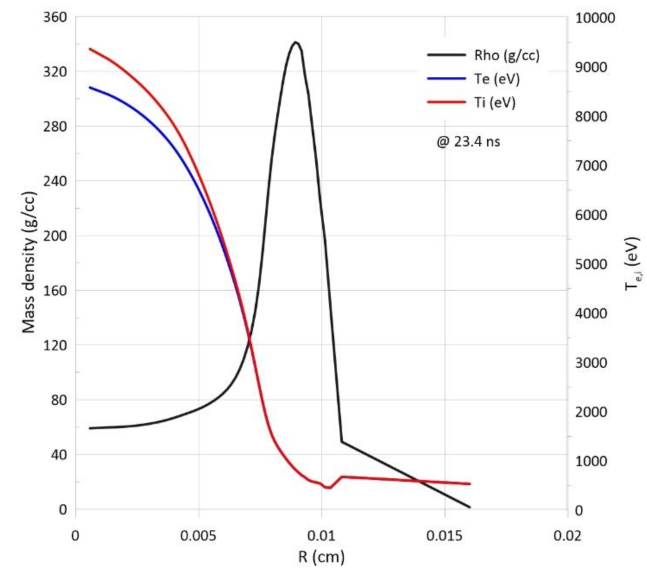
Targets simulated (Verifications)

DT fuel



regions	3		
	DT-gas	DT-ice	CH
R_{init} (cm)	0.176	0.1934	0.1971
T_{init} (eV)	0.025		
$\rho\ (g/cc)$	5×10^{-4}	0.224	0.94
Mass (mg)	0.0114	1.672	1.667





Atzeni, Stefano, and Jürgen Meyer-ter-Vehn. *The Physics of Inertial Fusion: BeamPlasma Interaction, Hydrodynamics, Hot Dense Matter*. No. 125. Oxford University Press, 2004, Ch. 3

Results up to now

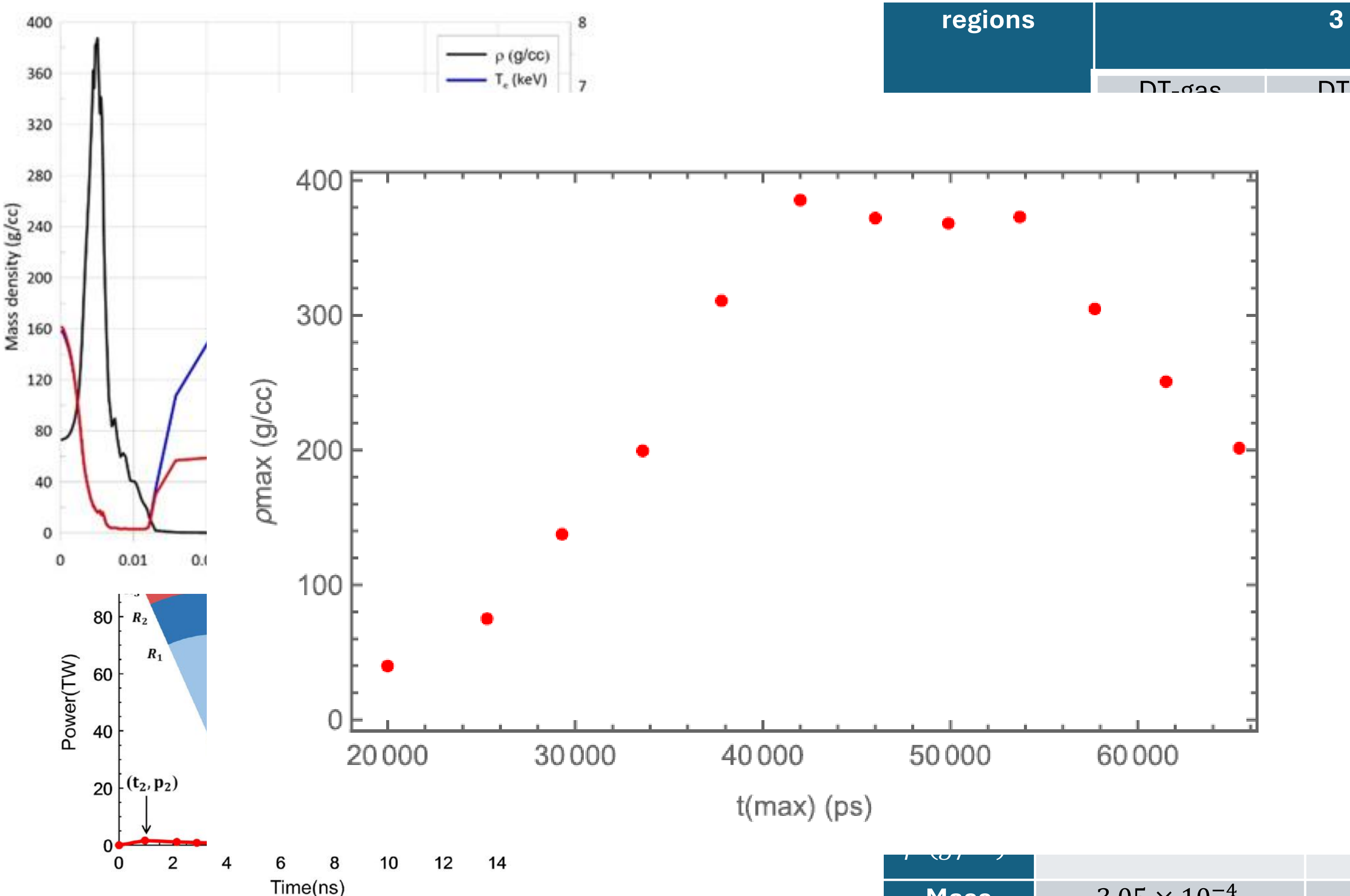


FIG. 2. Schematic of the laser pulse shape and the target structure to be optimized for establishing the implosion database.

regions	3		
	DT-gas	DT-ice	CH
		997	0.1027
		5	
			1.1
			0.425

			CH
			0.1123
		0.25	1.1
Mass (mg)	3.05×10^{-4}	0.604	0.509

Methods

Global optimizers → Bayesian Optimization

- Determine the optimal parameters
- The precise laser control is required for the implosion
- Effective global optimization
- Algorithm that can quickly and efficiently find the relatively optimal input parameters

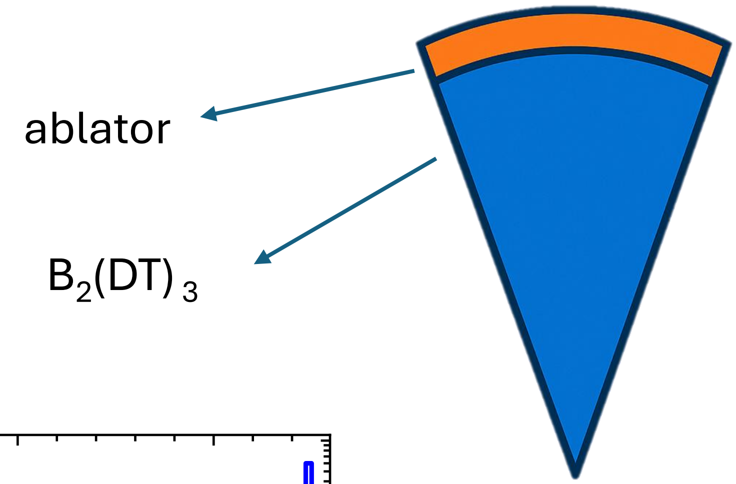
Challenges:

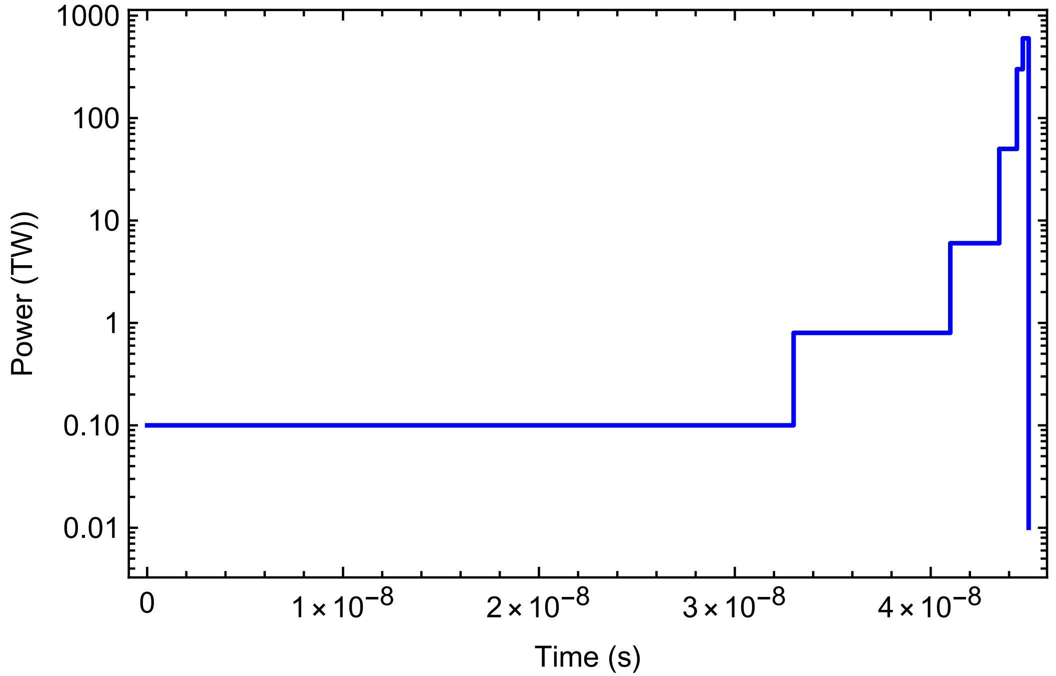
How to reduce the randomness in the optimization process and enhance the optimization efficiency

to compress the fuel to high enough density

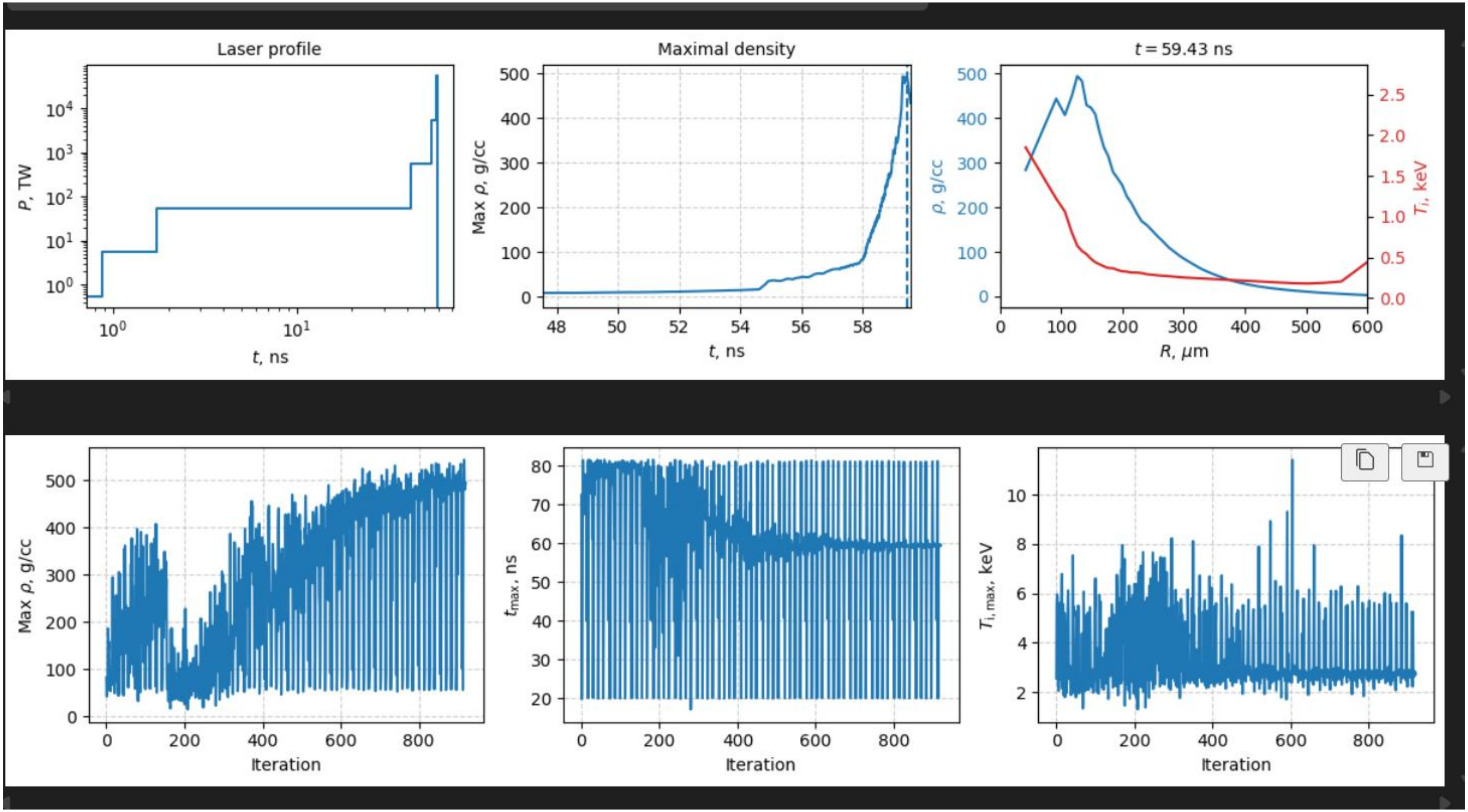
Our target structure

Fuel	$B_2(DT)_3$
Mass	Up to 50 mg
Laser profile	Simple step-like





Results up to now



Results up to now

Post processing

To be done:

- Troubleshooting the current algorithm
- Adding other free parameters
- Combine implosion parameters and burn propagation for real imploded targets for our target design
- Hybrid mode to better optimize the target structure

CONCLUSIONS

- **Optimization of implosion for the laser energy for large advanced fuels was presented.**
- **BO method is an efficient method, but other methods can also be investigated.**
- **Combination of methods could make improvement in the results.**
- **The optimization is performed under some ideal assumptions, and verifications. Using an actual model is also required.**

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