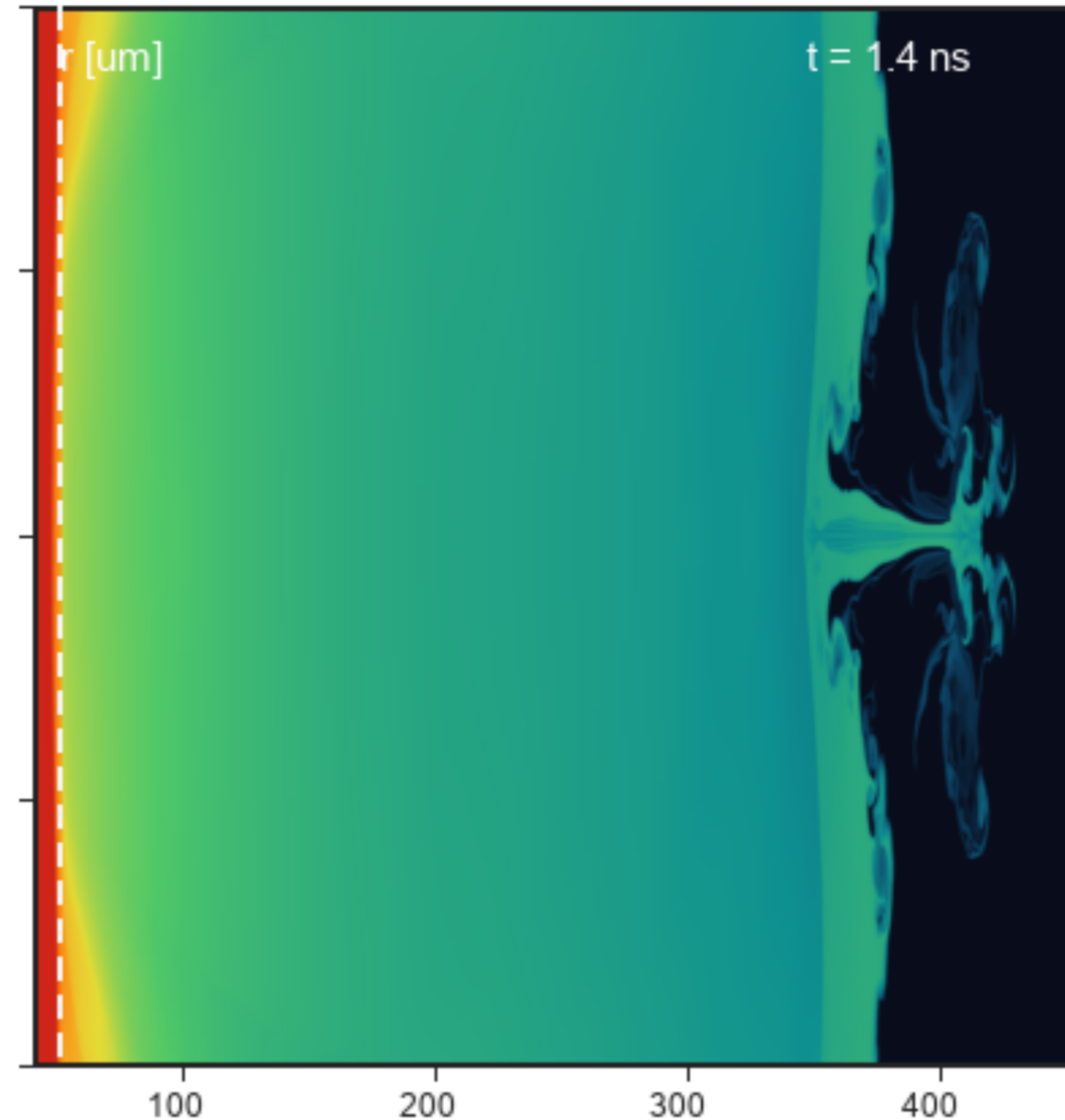


Modeling target– substrate distance in PLD

A validation-first path toward YBCO plume
transport in oxygen

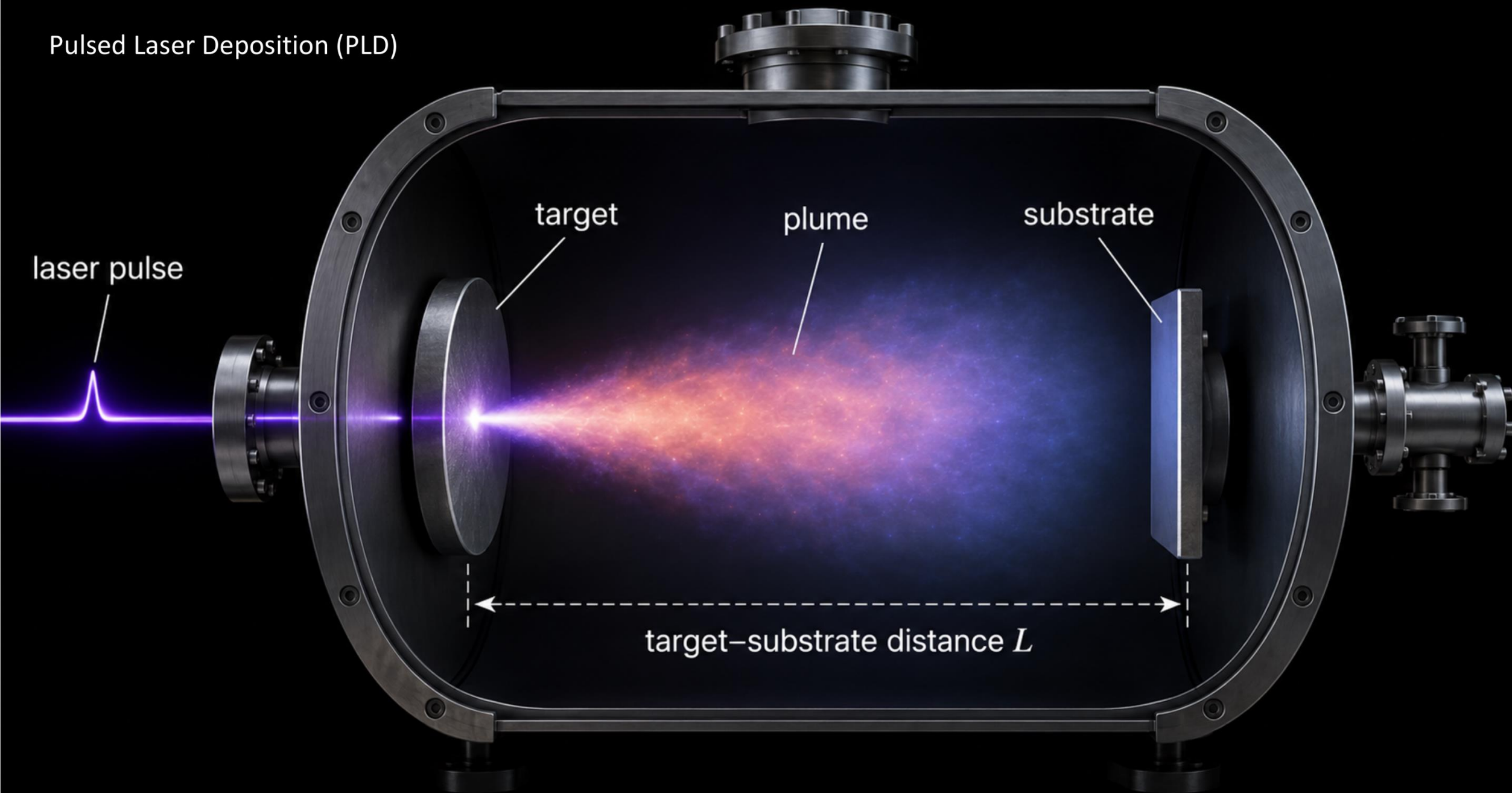
Shirsha Mukherjee

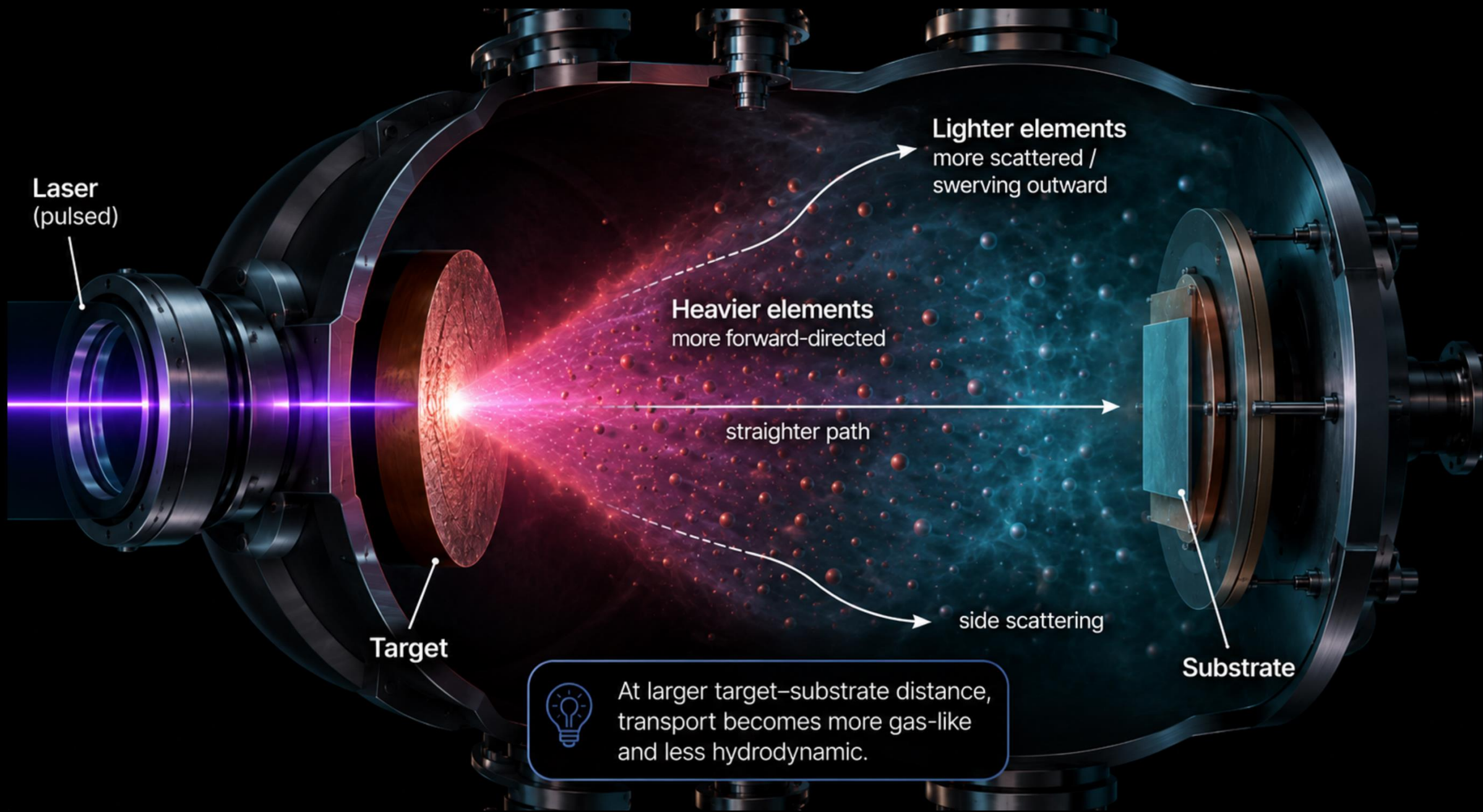
OU Research Experience for Undergraduates



What is PLD?

Pulsed Laser Deposition (PLD)





Distance changes what the substrate receives

CLOSER

Shorter path

Higher arrival energy
Fewer gas-phase collisions
Possible sputtering

CANDIDATE WINDOW

Useful arrival conditions

Enough flux to grow
Manageable impact energy
Desired oxygen interaction

FARTHER

Longer path

More slowing and spreading
More collisions and reactions
Possible change in thin film composition

Distance is simple to set, but hard to predict

Changing d changes:

This is why a “best distance” depends on a recipe, rather than just the material name

Plume density at substrate

Particle kinetic energy

Collisions with oxygen background gas

Radial spreading and uniformity

Arrival time and cooling



What distance is “just right” for YBCO deposition

1 Build

A physics-based plume transport model

2 Validate

The workflow against a published case

3 Map

Fluence, O₂ pressure, etc to optimum target-substrate distance

Goal: move from trial-and-error distance selection toward a physics-informed process window.

What do we want the model to do



Film measurements then test whether those arrival conditions actually improve structure and superconducting performance.

What are we using for our model?

What are we using for our model?

FLASH

What is FLASH?

The simulation engine we are validating before using it for YBCO PLD distance predictions

FLASH

A research simulation code for many different physics applications

- Solves the physics**
hydrodynamics, heat flow, plasma temperatures
- Adapts the grid**
adds resolution where the plume changes fastest
- Outputs predictions**
density, temperature, ionization, plume shape vs time

FLASH is a serious way to simulate PLD plume physics, and thus simulate optimal target-substrate distances

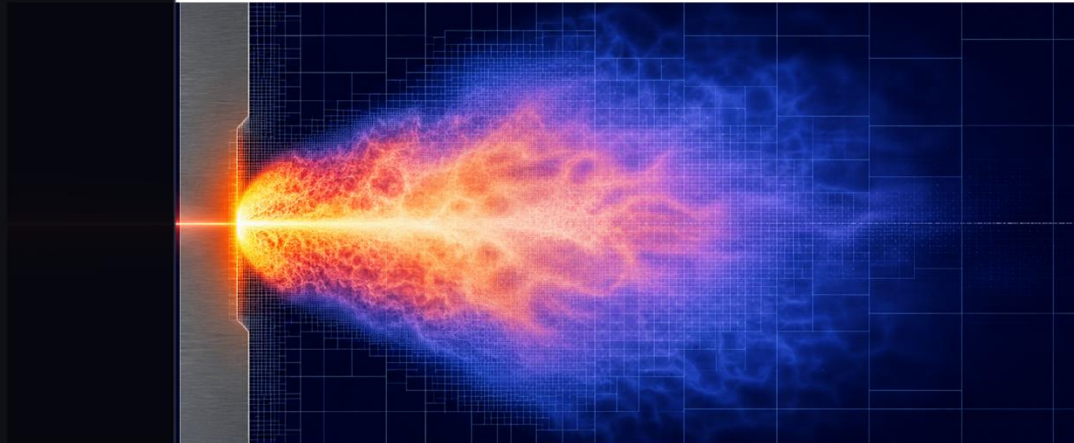
Validate on aluminum → adapt toward YBCO + oxygen → predict useful target-substrate distance

Simple idea: use FLASH to simulate how the plume travels, then connect plume behavior to the distance that gives the substrate the “right” material delivery.

Using FLASH for plume simulations

FLASH gives a physics-based way to calculate:

- ✓ laser heating and ablation
- ✓ plume expansion through gas
- ✓ shocks and density gradients
- ✓ adaptive mesh refinement
- ✓ electron/ion/radiation temperatures



This is the computational core I am building toward.

Workflow

STEP 1



Reproduce

Run a published aluminum laser-plasma case with FLASH for known geometry, pulse, and output times.

STEP 2



Compare

Check whether our results are the same

STEP 3



Adapt

Only then change the material and background gas for a staged YBCO-in-oxygen model.

What I have working now

FLASH

1.4 ns

build + run workflow full benchmark duration reached

15.3 mJ

AMR

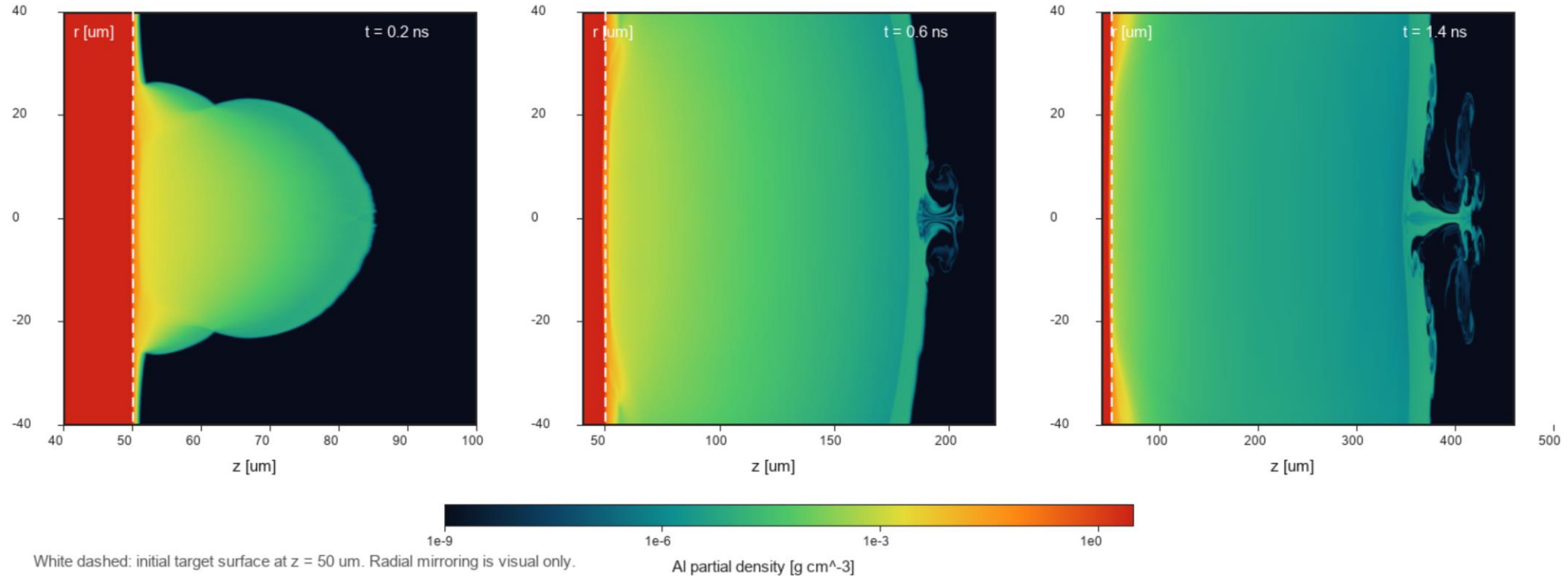
laser energy reproduced mesh follows plume structure

Why this matters: before using FLASH to predict YBCO PLD distance, I first needed to prove that I can run and analyze a known laser-ablation case.

The benchmark matched the expected plume scale

Aluminum plume shape from the 2D cylindrical FLASH output

Al partial mass density (dens x targ), mirrored about the $r = 0$ symmetry axis



The plume expands from roughly 90 → 200 → 400 μm over 0.2 → 0.6 → 1.4 ns.

Validation supports the method—not the final YBCO answer

WHAT IT SUPPORTS

The workflow is credible

- Laser energy enters the target
- The plume expands in time
- The output can be analyzed consistently
- The axial scale agrees approximately

WHAT IT DOES NOT YET SHOW

YBCO still needs its own physics

- Reliable YBCO material data
- Oxygen chemistry and reactions
- Species-dependent transport
- The distance that produces the best film

The benchmark answers “Can the workflow reproduce plume expansion?” The YBCO study asks “What arrives at the substrate?”

Target-substrate distance is a very significant, and hard to predict parameter of quality thin film production

A validated model can narrow the search by connecting fluence, O_2 pressure, and distance to what reaches the substrate.
