Bayesian Optimization Scheme for the Design of a Nanofibrous High Power Target

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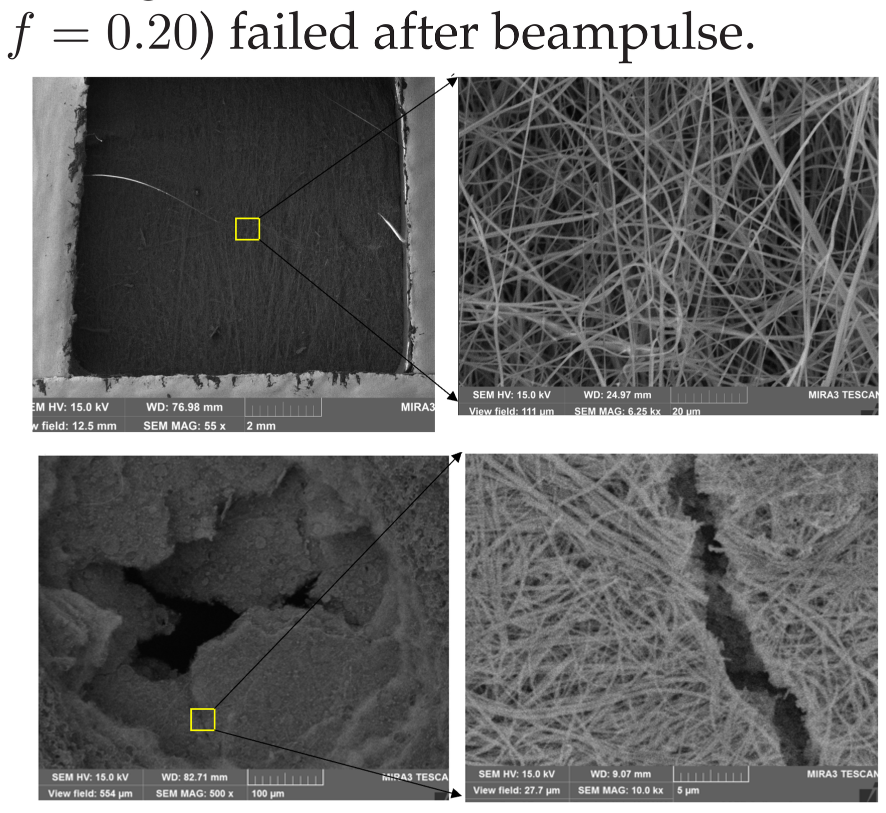
Background

Neutrinos are one of the biggest research areas to look for Beyond the Standard Model physics, and studying rare processes requires high intensity neutrino beams. For next generation facilities, robust targets need to be designed which can sustain the increased radiation damage and thermal shock from higher beam intensities (up to 4+ MW)
Record: 959 **kW (NuMI, May 2023)**
LBNF w/ PIP-II: 1.2 **MW**
LBNF w/ PIP-III: 2.4 **MW**

Nanofiber Targets

- High Power Targetry R&D Group at Fermilab studying nanofibrous target material—electrospun mats of Yttria-Stabilized Zirconia nanofibers [1,2].
- Several potential advantages:
  1. Empty space dissipates thermal stress waves
  2. Porosity allows cooling with gas flow
  3. Intrinsic radiation hardening
- Thermal shock test with single beam pulse at HiRadMat revealed survival depends on construction parameters.
- Top row: less dense nanofiber mat (Solid Volume Fraction (SVF) $f = 0.05$) appears undamaged. Bottom row: denser mat (SVF $f = 0.20$) failed after beampulse.

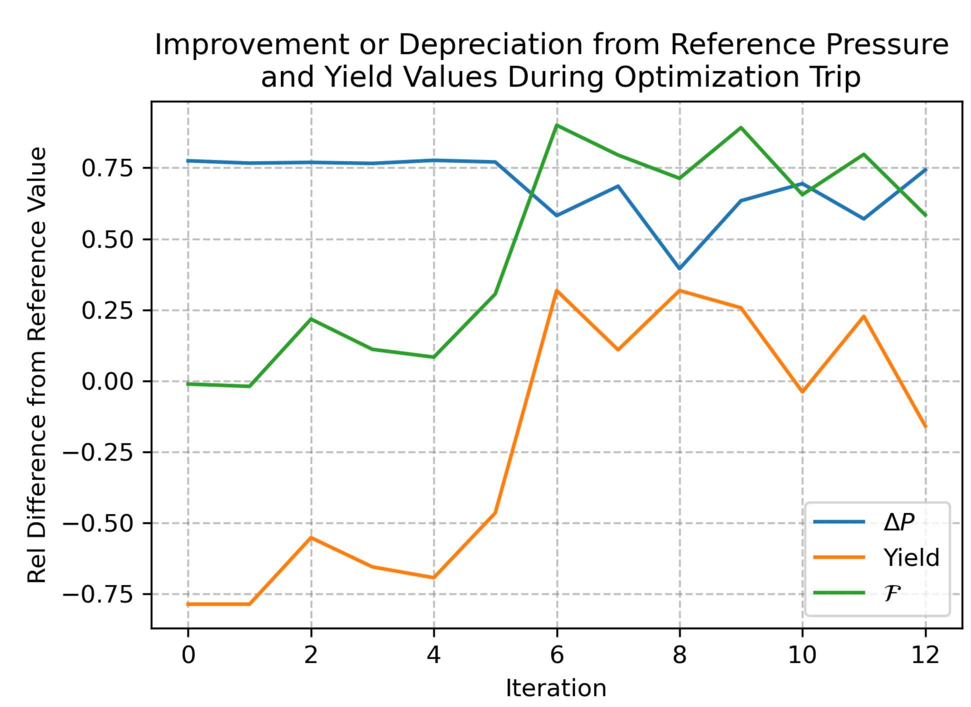


Objective of this work: use Bayesian Optimization to study trade-off between secondary particle production yield and target lifetime.

Bayesian Optimization

- Bayesian optimization is a strategy for global optimization
- Particularly useful if objective function $\mathcal{F}$ is expensive to compute or lacks a simple form or derivative information (black box)
- Works by treating $\mathcal{F}$ as random function with statistical model of your choosing. Knowledge of $\mathcal{F}$ at a finite number of points + Bayes' theorem $\longrightarrow$ posterior distribution
- Use posterior distribution to compute acquisition function—optimizing acq f'n tells you where to try next in parameter space
- **Predicting damage and yield to a nanofiber target is VERY computationally expensive. Advantage of BO is doing expensive calculation only at carefully chosen points**

Progress On Objectives



Progress on attaining our "objectives" of low pressure rise and high yield at each iteration of the loop.

Optimizer

- Used BoTorch Python library [10]
- Gaussian process as prior distribution for $\mathcal{F}$
- Training of hyperparameters by minimizing negative marginal log likelihood
- Expected Improvement as acquisition function, optimized using Monte-Carlo method
- Ran for 13 iterations, demonstrated convergence behavior to $f = 0.35$ and $R = 2500$nm, the maximum allowed values

Model

- Gas phase thermal conductivity [3] incorporates size effects and non-equilibrium
- Porous zone effective thermal conductivity [4], nonlinear combination of solid and gas
- Permeability to fluid flow (in Darcy's Law), α, given below [5]

$$\alpha = \frac{\epsilon\, R^2}{8\,(\ln\epsilon)^2}\,\frac{(\epsilon-\epsilon_p)^{x+2}}{(1-\epsilon_p)^x\,\left[(x+1)\,\epsilon-\epsilon_p\right]^2}$$

- Where $\epsilon = 1 - f$, R is avg fiber radius, $\epsilon_p = 0.11$, x depends on direction of fluid flow (for $\perp$, $x = 0.785$, for $\parallel$, $x = 0.521$)

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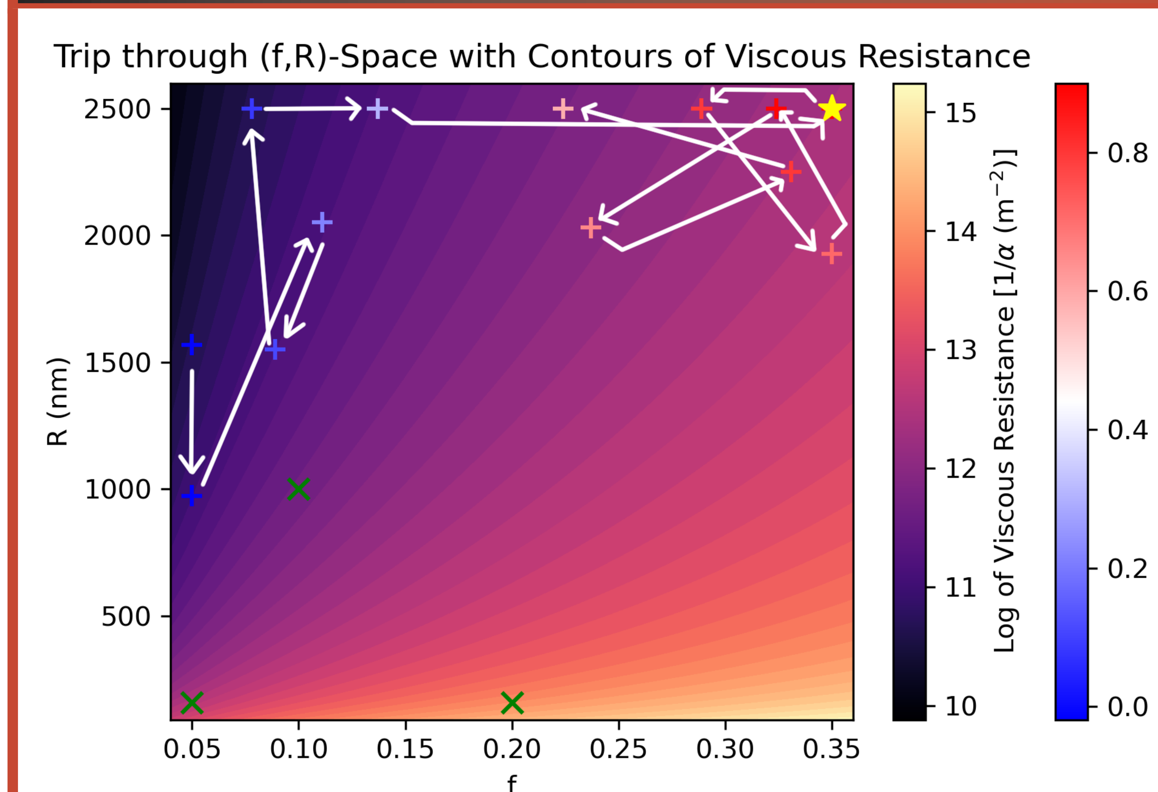
Objective Function

- Choose wisely: only connection between math and the physical problem
- Input space: SVF, f, and average fiber radius, R with bounds $f \in [0.05,\ 0.35]$ and $R \in [100\text{nm},\ 2.5\mu\text{m}]$
- Failure of HiRadMat high density target believed to be pressurization of air inside target $\implies$ small f improves survival
- Low f lowers secondary particle yield, so balance max pressure rise ΔP and yield $\mathcal{Y}$
- Thus, chose $\mathcal{F}(f, R)$ to be:

$$\mathcal{F}(f,R) := \left(\frac{\mathcal{Y}(f)-\mathcal{Y}_{\text{ref}}}{\mathcal{Y}_{\text{ref}}}\right) + \left(-\frac{\Delta P(f,R)-P_{\text{ref}}}{P_{\text{ref}}}\right)$$

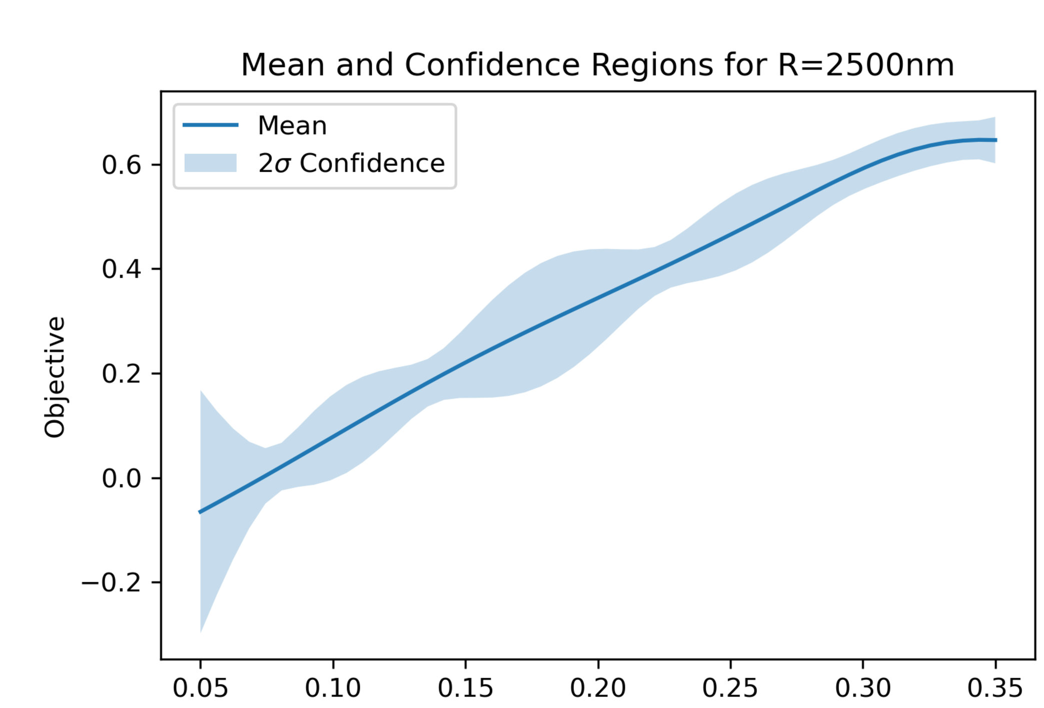
- $\mathcal{Y}_{\text{ref}} = 2.89 \times 10^{-3}$ (SH PPP)—yield of graphite target, $P_{\text{ref}} = 100\text{kPa}$

Parameter Space Trajectory



Contours of viscous resistance ($1/\alpha$, see "Model") overlaid with trip of Bayesian Optimizer through SVF (f) and fiber radius (R) parameter space. Green x's are training points, +'s are tested points (colored gradient from blue to red based on value of $\mathcal{F}$) and the gold star is the best point so far.

Mean and Confidences



Plot of final mean value and 2σ confidence intervals of $\mathcal{F}$ as function of SVF f for fixed $R = 2500$nm (optimum radius).

Conclusions

- Optimizer identified increasing R as improving α without changing f and the yield
- Neglected way to penalize R increasing, exiting realm of applicability of model and thermal stresses may become problem at large R
- Additional thermal or mechanical penalty terms may be needed.
- Pursuing multi-objective Bayes Optimization will allow study of Pareto fronts and understanding of trade-off better

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