Exploring multi-fidelity Bayesian optimization for inertial confinement fusion design

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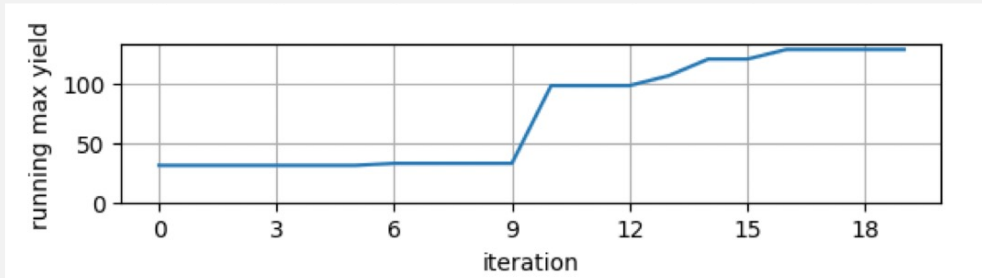
Multi-fidelity Bayesian optimization algorithm automatically searches the design parameter space for higher yield implosions

Traditional ICF design involves hand-tuning key physics levers in simulation to optimize yield. We employ an automated approach based on Bayesian optimization that can directly tune the experimental design parameters to improve the yield.

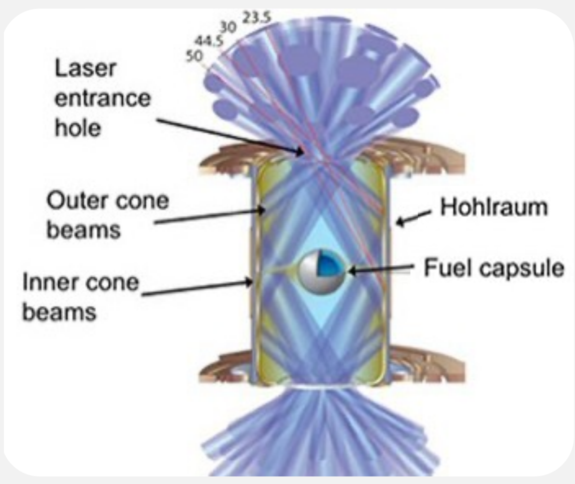
This algorithm leverages both high- and low-fidelity simulations to quickly and efficiently search the design space.



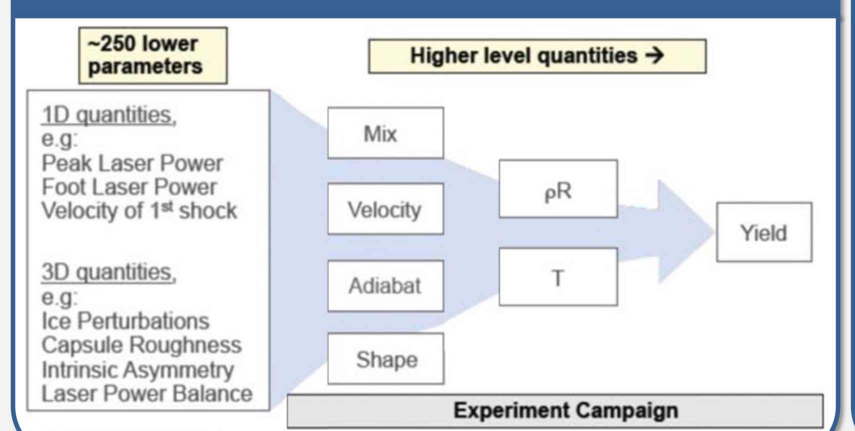
Optimizing an 8-parameter design for yield using our algorithm. Figure shows the highest yield found as the algorithm progresses.

Inertial confinement fusion (ICF) design relies on complex simulation codes with large design parameter spaces

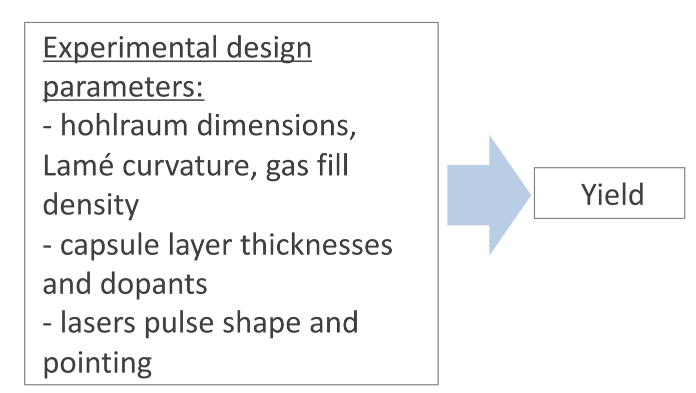
- ICF at NIF uses a gold hohlraum and 192 lasers to drive a capsule containing fusion fuel
- ICF experiments are developed by teams of design experts who use several high-fidelity multi-physics codes [1] to build their designs
- The design space spans over at least a few dozen independent parameters



Traditional design optimization workflow uses higher-level physics parameters [3]



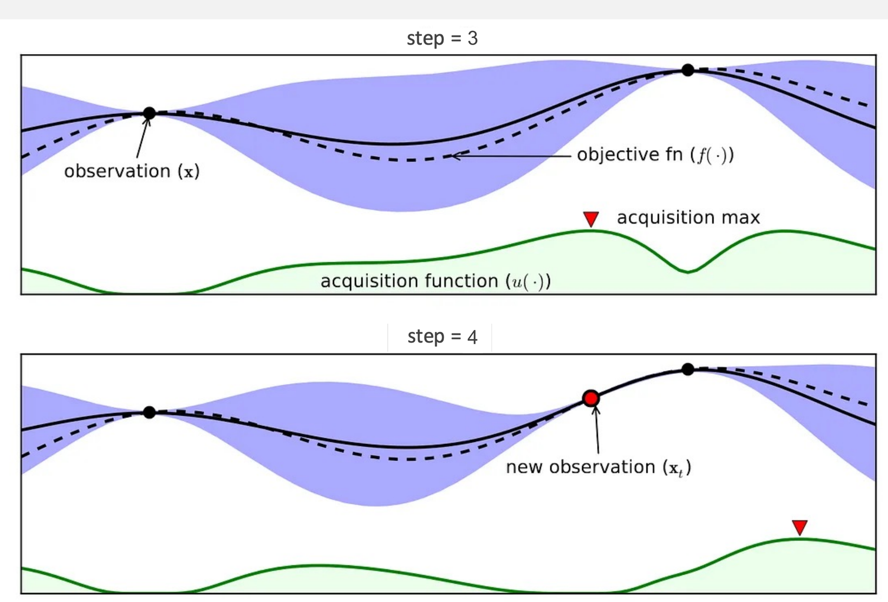
Our automated workflow directly optimizes the lower-level experimental design parameters



Bayesian optimization (Bayes opt) can be leveraged as a powerful tool for automating ICF design

Bayesian Optimization process:

1. Observe data points
2. Build a model to fit observed data and quantify uncertainty (**surrogate model**)
3. Determine the next candidate points to sample using the **acquisition function**
4. Sample the next point and add it to our set of data points
5. Repeat



[4]

Using a multi-fidelity approach avoids the need to run many expensive high-fidelity simulations

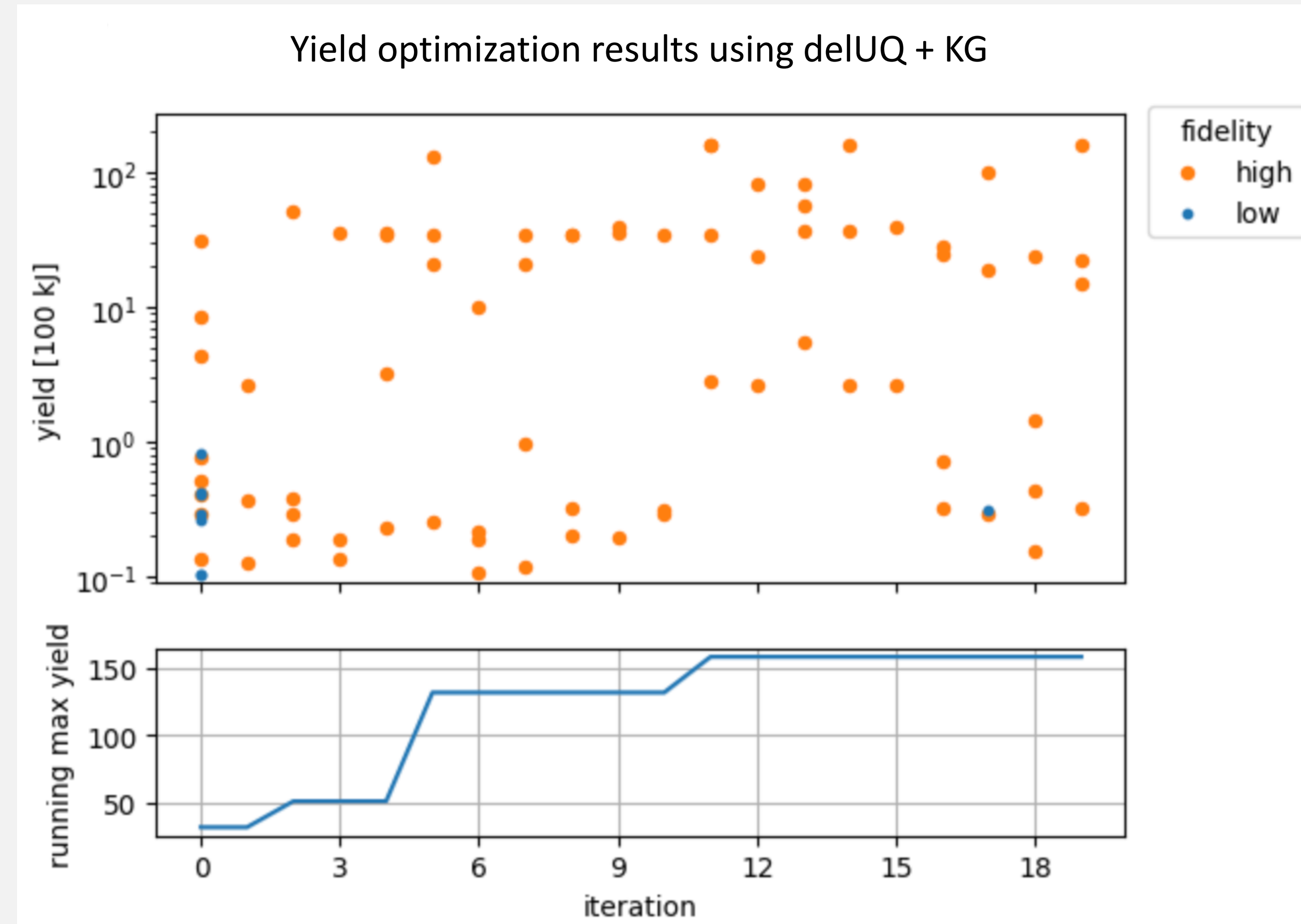
- Multi-fidelity Bayesian optimization uses cost-aware acquisition functions that automatically balances the cost of running more expensive, more informative simulations vs. less expensive, less informative ones
  —e.g. Knowledge Gradient (**KG**), Max-value entropy search (**MES**)
- Multi-fidelity surrogate models help pass information from the low fidelity simulations to the high-fidelity surrogate
  —e.g. Gaussian Process (**GP**), Neural Network with uncertainty (**delUQ**)
  —Allows Bayes opt to explore the search space more quickly and intelligently
- In our tests, high- and low- fidelity simulations are conducted with and without thermonuclear burn, respectively
  — In practice, the two (or more) fidelities will have more distinct run times to better exploit the faster lower fidelity simulations

To aid rapid debugging of our algorithm, we substitute the HYDRA simulator with an approximate neural network

Neural network approximator to HYDRA is constructed as follows:

1. Build a database of 1D HYDRA simulations in an 8-parameter design space
2. Train a neural network on high (burn on) and low (burn off) fidelity simulations to create a high-fidelity and a low-fidelity model
3. Substitute high- and low-fidelity HYDRA simulations in the algorithm with corresponding neural network

Since the neural network test function is an approximation to HYDRA, success on the test problem is a positive sign for future ICF design optimization



Results from algorithm optimizing yield in an 8-parameter design space. (top) Yield of each point chosen by the algorithm over 19 iterations. Algorithm preferentially chooses high-fidelity simulations, possibly due to low correlation between burn off and burn on yield. (bottom) Highest yield found by the algorithm so far. Consistent improvement in max yield found shows algorithm is performing as expected

References
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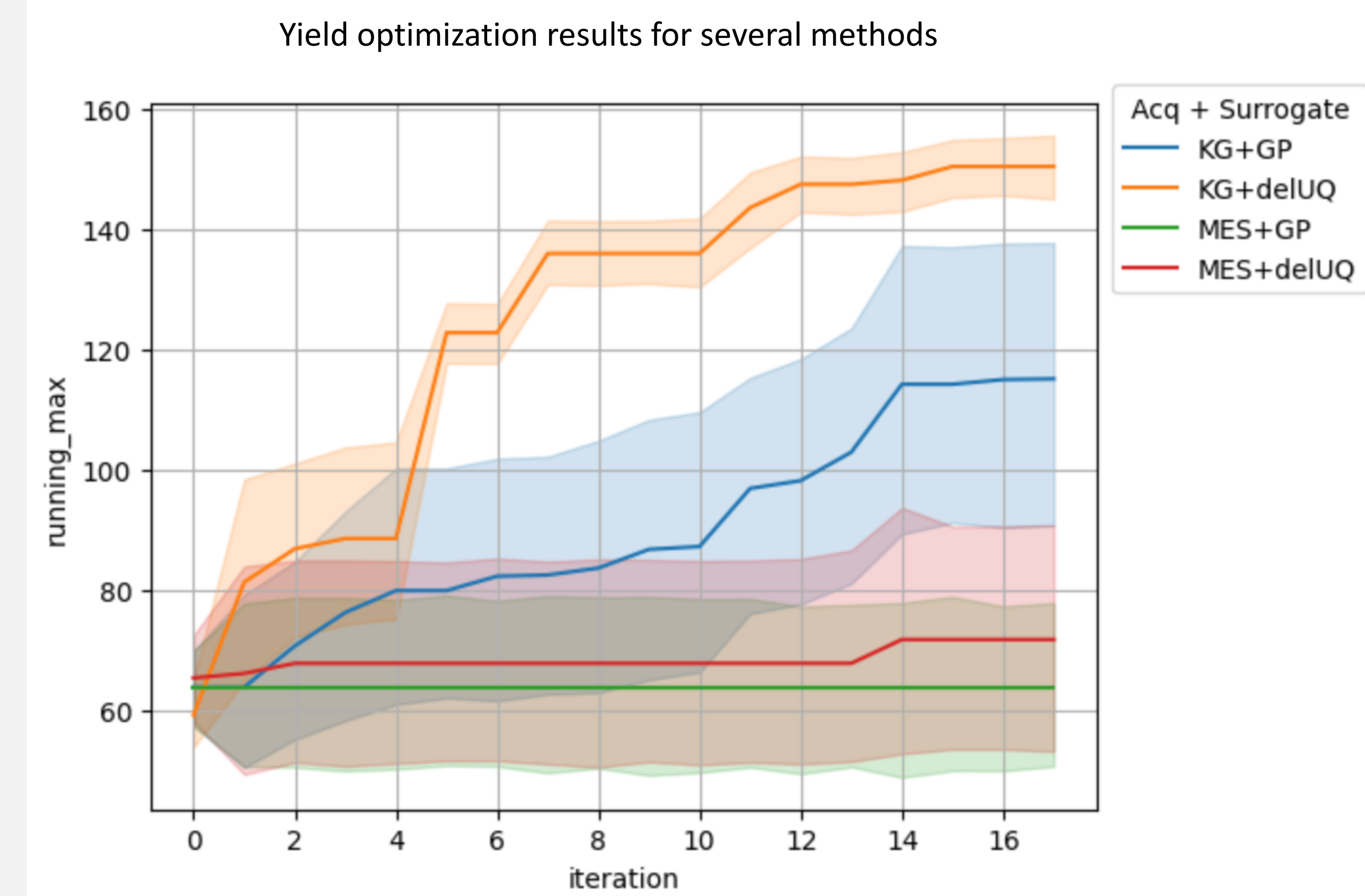
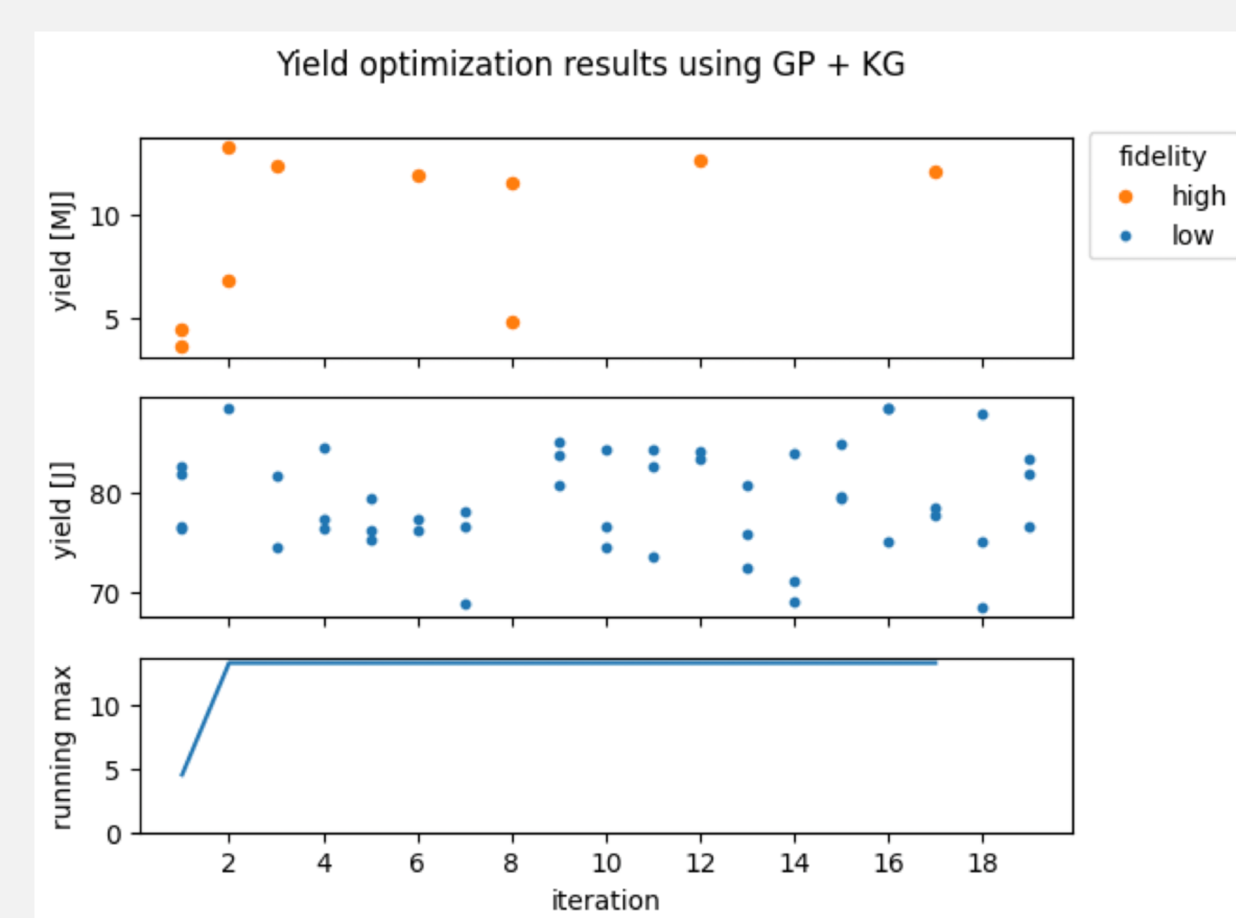
Optimization algorithm shows promise when applied to ICF test problem



- Knowledge gradient (KG) results in incremental improvement
- Max-value entropy search (MES) prioritizes low-fidelity exploration, and accumulates information before making an informed decision
  —Benefits from a final recommendation step (in progress)
- Neural networks are able to handle large scaling and nonlinearity required in high dimensional problems
  —delUQ in above figure outperforms GP surrogate model

We are beginning to evaluate performance of the algorithm with HYDRA fully integrated in the optimization loop



- 5-parameter scan using HYDRA [1] chooses both high- and low-fidelity points as it progresses
- Next steps include scaling to larger number of candidate points and moving to 2D simulations
- Eventually, we hope to modify the cost function and optimization algorithm to search more specific design spaces (e.g. designs robust to surface roughness of capsule)

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